

AERH2S

A Model for Calculating Emergency Response and Planning Zones

**Volume 1: Technical Reference Document,
Version 2.07**

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AERH2S: A Model for Calculating Emergency Response and Planning Zones, Volume 1: Technical Reference Document, Version 2.07

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NOMENCLATURE

Γ	Average vertical temperature gradient in the atmosphere, K/m
ρ_{equiv}	equivalent density of the release after it slows down and the liquids evaporate
\dot{m}_{ei}	initial mass flux at pipe exit for flow in one direction, kg/s
ρ_L	license condition density, kg/m ³
\dot{m}_E	modelled steady mass flux at exit, kg/s
TSD_{∞}	the effective release duration, equal to t_{eff} , s
\dot{m}_e	transient mass flux at pipe exit for flow in one direction, $\dot{m}_e(t)$, kg/s
γ_{gs}	gas gravity (air=1) that would result from separator conditions of 100 psig
γ_{gp}	gas gravity obtained at separator conditions of p and T
$^{\circ}API$	degrees American Petroleum Institute gravity, a scale measuring the density of petroleum liquids relative to water
$^{\circ}C$	degrees Celsius
α	initial time constant for double exponential pipeline blowdown model, s
A_E	area of exit
A_e/A_p	ratio of effective hole area to pipe area for flow from one direction, one half of flow from both directions. Ratio of area hole to area inside pipeline
AOF	Refers to a gas well, absolute open flow. Specifically, AOF is the flow at surface through the orifice to atmosphere, Rm ³ (at T_{REF} & P_{REF})
A_p	inside area of pipe
AS	source area, m ²
A_{Total}	total area of exit. For a guillotine rupture $A_{Total}/A_p=2$
β	time constant for double exponential pipeline blowdown model, s
B_A	a constant, 1/m
β_e	effective entrainment constant
B_o	oil formation volume factor for saturated oil
C_D	drag coefficient (0 to 1)
c_{Ea}	average speed of sound at exit, m/s, at P_{Ei} and T_{Ei}
c_{Ei}	initial speed of sound at exit, m/s, at P_{Ei} and T_{Ei}

<i>cmdaa</i>	dry mass fraction water
<i>CMEDO</i>	R-plane initial liquid mass fraction
<i>cmwa</i>	mass fraction water
<i>c_o</i>	Initial speed of sound at P_o and T_o , m/s
<i>cpa</i>	specific heat of dry air, J/(kg.K) at T_{REF} .
<i>cpaa</i>	specific heat of moist air, J/(kg.K)
<i>C_{Pi}</i>	specific heat of ideal gas component i, J/(kg.K)
<i>CPI</i>	specific heat of ideal gas source mixture, J/(kg.K)
<i>CPS</i>	vapour heat capacity at constant pressure, J/(kg.K)
<i>CPS</i>	Vapour specific heat capacity, J/(kg.K)
<i>CPSL</i>	Liquid heat capacity, J/(kg.K)
<i>CPSL</i>	Liquid specific heat capacity, J/(kg.K)
<i>cpwl</i>	Specific heat water liquid, J/(kg.K) at T_{REF}
<i>cpwv</i>	Specific heat water vapour, J/(kg.K) at T_{REF}
<i>D</i>	Pipeline outside diameter, mm
<i>DHE_C</i>	heat of vaporization, J/kg
<i>dhw</i>	Latent heat water, J/kg at T_{REF}
<i>d_i</i>	dry reference analysis gas molar fraction of a component
<i>D_o</i>	Pipeline outside diameter, mm
<i>EH2S%</i>	Expected maximum H ₂ S concentration, % (molar, dry gas phase), (at T_{REF} & P_{REF})
emergency	As defined in the Oil and Gas Conservation Rules, Pipeline Rules , and Geothermal Resource Development Rules .
EPZ	Emergency planning zone. An EPZ is a geographic area around wells, pipelines, or facilities where the presence of hazardous substances requires specific emergency preparedness by the duty holder. An EPZ is a hazard distance to a specific endpoint. A release scenario may result in many calculated hazard distances. The EPZ is selected from that set, such as the average or maximum distance for a specific regulatory purpose.
ERP	Emergency response plan. A comprehensive plan to protect the public that includes criteria for assessing an incident (emergency) and procedures for mobilizing response personnel and agencies and establishing communication and coordination among the parties.
ESD	Emergency Shutdown [valve]

f	Moody friction factor for turbulent flow, which is 4 times the Fanning friction factor
F_B	buoyancy flux, m^4/s^3
F_M	Momentum flux, m^4/s^2
F_R	Froude number
g	gravity constant, m/s^2
GF	Gas fraction factor
GLR	Expected maximum Gas to Liquid Ratio, expressed as standard m^3 Gas to stock tank m^3 Liquid
GVF	Gas volume fraction relative to reference conditions
H_2S	Hydrogen Sulphide. A naturally occurring gas found in geological formations or formed by the natural decomposition of organic matter in the absence of oxygen. It is colourless, has a molecular weight heavier than air and is highly toxic. In small concentrations, it smells like rotten eggs and causes eye and throat irritation.
H_2S_{RR}	Hydrogen sulphide release rate, Rm^3/s (at T_{REF} & P_{REF})
h_{Ea}	average enthalpy at exit (J/kg)
h_{Ei}	enthalpy at exit (J/kg)
hfg	Liquid heat of vaporization, J/kg
h_o	initial enthalpy (J/kg)
hpr	plume rise, m
$hprf$	final plume rise, m
h_Q	enthalpy at the Q-plane, J/kg
h_R	enthalpy at the R-plane, J/kg
HS	Source release height above ground, m
$IDSPL$	spill source type, 1 through 6
$iHOPT$	plume rise calculation option, 0=SLAB, 1=ISC, 2=BRIGGS
IIZ	Initial isolation zone. The area in close proximity to a continuous hazardous release where indoor sheltering may provide only temporary protection due to the proximity of the release. An IIZ is a hazard distance to a specific endpoint. A release scenario may result in many calculated hazard distances. The IIZ is selected from that set, such as the average or maximum distance for a specific regulatory purpose.
K	degrees Kelvin

k_a	average specific heat at exit, C_p/C_v
k_t	Ratio of specific heats for an ideal gas source mixture at reference conditions
k_i	ratio of specific heats for real gas
$K_{inertial}$	inertial delay factor
L_{eff}	effective length of a pipeline segment, m
L_{ESD}	length of pipe from release location to the ESD, m
L_{extra}	extra length of pipeline beyond the ESD as a result of mass flow until the valve closes, m
$LH2S\%$	Licensed maximum H ₂ S concentration, % (molar, dry gas phase), (at T_{REF} & P_{REF})
L_p	lift-off parameter
$M_{escaped}$	the mass that escapes from the release up to the time the ESD valve closes, kg
m_i	Calculated dry combined gas molar fraction with respect to input specified H ₂ S component, m_{H2S} .
M_S	R-plane velocity ratio to density ratio
$M_{unignited}$	mass released until the time of ignition, kg
MW	molecular weight, kg/kmol
$NAD83$	North American Datum, 1983
$NCALC$	numerical sub-step parameter for SLAB
N_{poll}	PROC number of cycles until final decision
$P(x,t)$	pressure at a location x [m] at time t [s]
P_A	local elevation ambient pressure, kPa
PAZ	Protective action zone. An area downwind of a hazardous release where outdoor pollutant concentrations may result in life-threatening or serious irreversible health effects on people. A PAZ is a hazard distance to a specific endpoint. A release scenario may result in many calculated hazard distances. The PAZ is selected from that set, such as the average or maximum distance for a specific regulatory purpose.
P_{Ea}	average pressure at exit, kPa (abs)
P_{Ei}	initial pressure at exit, kPa (abs)
P_{Eig}	ideal gas pressure at exit assuming gas is choked, kPa (abs)
P_{ESD}	ESD valve low pressure (LP) trigger, kPa (gauge)
P_{ESDg}	Low pressure activation pressure setting for ESD, kPa (gauge)

P_i	Expected maximum Operating Pressure, kPa (gauge)
P_L	Licensed Maximum Operating pressure, kPa (gauge)
P_o	initial pressure of gas in pipeline, kPa (abs)
P_{REF}	reference pressure, 101.325 kPa
$PROC$	ESD valve pressure rate of change trigger (dPESD/dt), kPa/s
Q_{LIQUID}	is the liquid flow rate in a liquid pipeline, m ³ /d of oil and water at T_{REF} and P_{REF}
QS	mass source rate, kg/s
QSi	initial release rate for transients, kg/s
$QTIS$	Instantaneous source release mass (not used in AERH2S), kg
RH	Relative humidity, %
ρ_{hoa}	density of moist air , kg/m ³
$RHOLV$	density under license condition, kg/m ³
$RHOSL$	Liquid density of source material, kg/m ³
$RHOSL$	Liquid density, kg/m ³
ρ_{howl}	density water liquid state, kg/m ³ (at T_{REF} & P_{REF})
R_i^*	local cloud Richardson number
R_{iCRIT}	critical cloud Richardson number
Rm^3	cubic meter at reference temperature T_{ref} and reference pressure P_{ref}
$rpwa$	water relative partial pressure
R_s	dissolved gas to fluid ratio
R_s	gas constant for source mixture, J/(kg.K)
R_U	Universal gas constant, J/(kmol.K)
S	Pipeline segment length between two logical nodes or changes in physical properties, m
$SCSSSV$	Surface control sub-surface safety valve. Is well safety device installed for production near the surface grade to prevent a release in the event of containment failure above the valve.
S_{ESD}	Equivalent segment length between ESDs, m. This is the length, S, of a pipeline segment plus any volume of gas or liquid that naturally flows into that segment expressed as a pipeline length with the same pipeline properties as pipeline, S.

sour gas	Natural gas, including solution gas, with H ₂ S. Depending on the particular mix of gases, gas properties, and ambient conditions, a sour gas release may ... <ul style="list-style-type: none"> • be heavier than air (dense), so it will tend to drop towards the ground with time, • be lighter than air (buoyant), so it will tend to rise with time, or • be about the same weight as air (neutrally buoyant), so it will tend to neither rise nor drop but will disperse with time.
sour pipeline	A pipeline to convey gas or liquid or both that contains sour gas.
sour well	An oil or gas well where formations bearing sour gas may be encountered during drilling or an oil or gas well capable of producing sour gas.
<i>spaw</i>	intercept, Antoine saturation pressure constant, moisture content of ambient air at standard atmospheric pressure
<i>spawpp</i>	intercept for the partial pressure corrected for ambient pressure
<i>SPB</i>	Antoine saturation pressure constant
<i>spbw</i>	slope, Antoine saturation pressure constant, moisture content of ambient air at standard atmospheric pressure, K
<i>SPC</i>	Antoine saturation pressure constant
<i>spcw</i>	correction factor, Antoine saturation pressure constant, moisture content of ambient air at standard atmospheric pressure, K
<i>spv</i>	specific volume, Rm ³ /kmol
<i>STAB</i>	Pasquill-Gifford stability class, A through F, or often for models the range 1 through 6 is used, respectively.
<i>t</i>	Pipeline wall thickness, mm
<i>T_A</i>	local ambient temperature at surface, K
<i>TACH</i>	local building air changes per hour, 1/h
<i>t_{arrival}</i>	time for pressure deviation to reach the ESD from the release location, s
<i>TAV</i>	Concentration averaging time, s
<i>T_{B,site}</i>	boiling point of water at site elevation
<i>TBP</i>	Boiling point temperature, K
<i>TBP</i>	Boiling point temperature, K
<i>t_{close}</i>	ESD valve closure time once triggered, s
<i>t_{close}</i>	time from initiation of ESD activation to valve is closed condition, s
<i>TCPL</i>	Toxic load endpoint for planning steady ppm for 3 minutes, ppm
<i>TCRE</i>	Toxic load endpoint for response, steady ppm for 3 minutes, ppm

T_{DEW}	Dew point temperature, K
T_{Ea}	average temperature at exit, K
T_{Ei}	initial temperature at exit, K
T_{Eig}	ideal gas temperature at exit assuming gas is choked, K
T_F	isenthalpic flash stagnation temperature, K
T_F	Isenthalpic flash temperature to P_A
$TH2S$	Percent H ₂ S in source mixture, mole percent
T_l	Expected minimum gas temperature, °C
$TIGN$	time to ignition or mitigation, s
$t_{ignition}$	Time from initial release until ignition or stop flow, minutes
TKL	toxic load factor to account for fluctuations
T_L	Level designation temperature, K.
t_{manual}	Time from initial release until ESDs manually or remotely closed, minutes
$TMAXEX$	maximum exposure time, s
TN	concentration exponent for toxic load
T_o	initial temperature of gas in pipeline, K
T_{OSS}	effective source temperature accounting for the kinetic energy of the high-speed jet and the evaporation of the liquid droplets, K
t_{poll}	ESD valve pressure rate of change PROC sampling time, s
t_{PROC}	Time from the release start to when the rate of change of pressure at the ESD location has reached $PROC_{trigger}$
T_R	R-Plane temperature, K
T_{REF}	reference temperature, 15°C
TS	source temperature, K
TSD	Source duration, s
TSD	Time from initial release until ignition or stop of flow, minutes
$TSD_{ignition}$	the release duration until ignition occurs, s
t_{set}	time from the release start to when the pressure at the ESD has reached $P(ESD)/P_o \leq P_{ESD}/P_o$
t_{shut}	time from release to ESD is shut, s
u^*	friction velocity, u-star, m/s

U_C	is the average velocity of the plume over the height of the plume, m/s
U_{ref}	Ambient wind speed at measurement height, m/s
U_{ref}	ambient windspeed at measurement height, m/s
V_D	velocity at the D-plane (drag), m/s
V_{ESD}	Equivalent cumulative pipeline volume between ESDs, m ³ .
V_{free}	Volume of gas in free state, m ³
V_P	pipeline segment volume, m ³
V_Q	velocity of release jet at the Q-plane, m/s
V_R	R-plane velocity, m/s
V_{sol}	Volume of gas entrained in solution, m ³
w_{H2S}	H ₂ S mole fraction
$w_{H2S,L}$	maximum licensed H ₂ S mole fraction
w_i	Calculated wet combined gas molar fraction with respect to input specified H ₂ O component, w_{H2O} .
w_{ma}	molar mass dry air, kg/kmol
w_{mae}	molar mass of moist air, kg/kmol
WMS	molar mass of source material, kg/mole
WMS	source molecular weight, kg/kmol
w_{mw}	molar mass water, kg/kmol
X_{Ea}	average liquid mass fraction at exit, at P_{Ei} and T_{Ei}
X_{Ei}	initial liquid mass fraction at exit, at P_{Ei} and T_{Ei}
X_F	Isenthalpic flash liquid mass fraction, at P_A and T_A
X_F	stagnation liquid mass fraction
$XFFM$	maximum downwind distance to be modelled, m
X_o	Initial liquid mass fraction at P_o and T_o
X_R	R-plane liquid mass fraction
$xxALPHA$	time factor
$xxBETA$	final time constant, s
Z_C	height above ground of the centreline of the plume
Z_L	license condition compressibility

Z_o	initial condition compressibility
Z_o	Meteorological surface roughness, m
ZP	height above ground level of concentration calculation, m
Z_{ref}	Ambient wind speed measurement height, m
ρ_{Ea}	average density at exit, kg/m ³ , at P_{Ei} and T_{Ei}
ρ_{Ei}	initial density at exit, kg/m ³ , at P_{Ei} and T_{Ei}
ρ_F	Isenthalpic flash density, kg/m ³ , at P_A and T_A
ρ_o	Initial density at P_o and T_o , kg/m ³
ρ_R	R-plane density, kg/m ³
h	vertical depth of plume in SLAB model, m
B	horizontal width of plume in SLAB model, m
V_e	vertical entrainment velocity in SLAB model, m/s
W_e	horizontal entrainment velocity in SLAB model, m/s
t_{cld}	cloud duration at the location of a receptor, s
t_{peak}	time of the peak concentration as it passes over a receptor, s
\bar{C}	concentration at a receptor, the bar means average concentration, ppm
\bar{C}_i	indoor concentration at a receptor, the bar means average concentration, ppm
\bar{C}_o	outdoor concentration at a receptor, the bar means average concentration, ppm
i	concentration intensity defined as standard deviation of instantaneous concentration divided by average concentration, c'/\bar{c}
i_{ref}	concentration intensity at some reference time
i_p	conditional concentration intensity defined as standard deviation of instantaneous conditional concentration divided by conditional average concentration, c'_p/\bar{c}_p , where the conditional concentration has zero periods of concentration removed
γ	intermittency factor
LO	toxic load, ppm ⁿ .s
n	exponent in the toxic load model
τ_b	building time constant, 3600/ACH, 1/s
ACH4	measured building air changes per hour based upon 4 mPa pressure test

- ACH50 measured building air changes per hour based upon 50 mPa pressure test
- ACHn natural or local air changes per hour for site temperature, wind speed and pressure
- ε pipe absolute roughness, mm
- W released gas water content, mg/m³ at T_{REF} and P_{REF}

1 INTRODUCTION

In December 2010, the Energy Resources Conservation Board (ERCB) released *ERCBH2S: A Model for Calculating Emergency Response and Planning Zones for Sour Wells, Sour Pipelines, and Sour Production Facilities, Volume 1: Technical Reference Document, Version 1.20* (ERCBH2S). ERCBH2S addressed the *Provincial Advisory Committee on Public Safety and Sour Gas* recommendations for a review of the calculation method of emergency planning zones (EPZ) for sour operations. To address these recommendations the Alberta Energy Regulator (AER) revised *Directive 071: Emergency Preparedness and Response Requirements* (Directive 071) for sour wells, sour pipelines, and sour production facilities. At that time, a significant change was the requirement (as per Directive 056, Section 4.8.5.4 (69)) to use *ERCBH2S* instead of the previously adopted nomograph method of calculating an EPZ. In 2025, the AER updated and rebranded ERCBH2S to AERH2S. AERH2S is a complex tool that calculates site-specific EPZs using thermodynamics, fluid dynamics, atmospheric dispersion modelling, and toxicology. The development of AERH2S (and previously ERCBH2S) has been a considerable undertaking with input from experts in a wide range of backgrounds, disciplines and expertise, and industry and public stakeholders. Documents pertaining to AERH2S are:

Directive 071, Emergency Preparedness and Response Requirements	This directive provides the requirements for the industrial operator. It covers not only sour operations but any activity where a hazard exists with the potential to cause a risk to the public.
Volume 1 Technical Reference Document Version 2.07	Written for the technical specialist to document the complex science within AERH2S. It provides the equations required to calculate the EPZ and the basis for selecting the components used to make the calculations within AERH2S.
Volume 2 Emergency Response Planning Endpoints	Written for the technical specialist with a particular interest in toxicology. It presents the data available to choose an EPZ endpoint, toxicological calculations, uncertainty factors and the EPZ endpoint values.
Volume 3 User Guide Version 2.07	Written for the AERH2S user, it provides a description on how to install and operate the computer software application with tutorial notes.

This document, Volume 1, provides a technical description of the formulations and assumptions used in the computer model AERH2S. Following this brief introduction, the AERH2S user inputs required to determine the hazard distances for sour gas well blowouts, sour gas pipeline ruptures or releases from sour liquid wells or pipelines are discussed. For many entries, AERH2S uses defaulted values which are used when the inputs to the model left blank or are out of range. The default values are highlighted in the tables in the following sections.

This technical reference includes the following descriptions of formulations used in the model:

- The constants and physical properties of the release and atmosphere are presented. Because of the high pressures, the thermodynamic calculations must employ real fluid properties to account for compressibility. The AERFLASH computer program was developed to determine the real fluid properties of the sour gas release.
- The release rate and duration of uncontrolled sour gas releases are then discussed. Releases from gas pipelines, wells and liquid pipelines and liquid wells are modelled as continuous steady releases, but the transient nature of blowdowns from gas pipelines is accounted for in the dispersion modelling. The extra mass that flows by the valves that isolate a pipeline segment is accounted for. The initial behavior of the release in the atmosphere is simulated to determine inputs to the dispersion model. A new method is used to determine if the release is dense and remains ground based or if it is buoyant and may rise above the ground.
- Hydrogen sulphide (H₂S) dispersion modelling to predict the downwind concentrations for the specified steady release rate and duration is then discussed. The AERSLAB computer program was developed by modifying the SLAB dense gas dispersion model that is publicly available from the United States Environmental Protection Agency. The approach used to transform the steady release rate predictions to transient release rate predictions for gas pipelines is described. The concentration predictions output from AERSLAB are then used to determine the toxic load equivalent outdoor exposure H₂S concentration accounting for concentration fluctuations. The indoor concentrations are also calculated from the outdoor predictions and used to determine the toxic load equivalent indoor exposure H₂S concentration. The output of AERH2S is the distance from the well or pipeline to the response and planning endpoints toxic load exposure.
- A description of the worst expected hazard distances calculated by AERH2S Version 2.07 to define the response and planning zones is then provided. The worst source under the worst-case dispersion resulting in the maximum distance is now used for planning. This is followed by a sensitivity analysis to input variables.

The report concludes with references and appendices.

- Appendix 1 describes the AERFLASH program (Clearstone report) to determine real fluid properties.
- Appendix 2 is a report (Wilson report) by Dr. D.J. Wilson of the University of Alberta deriving several of the approaches used in the AERH2S.
- Appendix 3 summarizes the selection of the drag coefficient for uncontrolled releases.

2 USER INPUTS

User inputs to calculate the hazard zones include administrative information to identify the facility, calculation controls, the sour gas facility details and the sour gas composition. All inputs are entered on the INPUTS page of the AERH2S Version 2.07 Microsoft Excel workbook. Upon completing these required inputs, the AERH2S programs are run. The following convention is used to identify inputs to the model in this report:

- User inputs are in **regular font in bold boxes**,
- Source mitigation inputs for the release are in **bold font in bold boxes**. The user can input alternate values to replace the default AER input to mitigate the release and the hazard zones.
- Default inputs that are set by the AER and cannot be changed by the user are in **bold font in shaded boxes**,
- Calculated values or constants are in **regular font in regular boxes** and cannot be changed by the user.

Variable names are in *italics* and the units are specified. Some user inputs that are not required for calculations but are required for AER submissions. The BATCH page allows for inputting many different facilities included in an Emergency Response Plan and is discussed in the User Guide. Only one type of sour gas or liquid operation can be calculated at a time.

2.1 Administrative

The following inputs are required to identify the applicant and source:

BA Code	Not required for calculation
Licensee/Applicant Name	Not required for calculation
Engineer Responsible for Providing Inputs - Name	Not required for calculation
Engineer Responsible for Providing Inputs - Company	Not required for calculation
Engineer Responsible for Providing Inputs - eMail	Not required for calculation
Engineer Responsible for Providing Inputs – Professional License Number	Not required for calculation
Name of Well or Pipeline License Number	Label 1 Not required for calculation
Well License Number or Well Application Number	Not required for calculation

Legal Surface Location of Well or Pipeline Line Number	Label 2 (LSD-SEC-TWP-RGE W?M) <i>Not required for calculation</i>
Pipeline Segment From Location	(LSD-SEC-TWP-RGE W?M) Not required for calculation
Pipeline Segment To Location	(LSD-SEC-TWP-RGE W?M) Not required for calculation
Surface Elevation, Z_{ASL}	m, (Average Sea Level)

Label 1 (name), Label 2 (location) and Label 3 (scenario) are concatenated to form a label that appears on the printouts.

The average EPZ elevation is used to calculate the local atmospheric pressure. It can be based on the wellhead surface elevation as specified in the well license or on a representative average elevation for the surrounding area within the EPZ.

Surface locations in Longitude/Latitude NAD83 (North American Datum of 1983, minimum 4 decimals) are now a required entry to allow for links to graphics packages for plotting the EPZs for an Emergency Response Plan (ERP). The surface locations are required for pipeline segment line numbers which are sub-segmented with an Emergency Shut Down (ESD). If the pipeline segment is not sub-segmented, then the ESDs would be located as the gas gathering network analysis at known end nodes for a line number. However, if an ESD is located at location along a line number, then location of the ESD is a required input.

2.2 Calculation Controls

Calculation controls include:

Scenario Name	Label 3 a unique description of the scenario being modelled
Operations Type	1-Gas Well 2-Gas Pipeline (H ₂ S > 10 mol/kmol) 3- Gas Pipeline (H ₂ S ≤ 10 mol/kmol) 4-Oil/Liquid/Other Well (GLR > 1000) 5-Oil/Liquid/Other Well (GLR ≤ 1000) 6-Oil Effluent Pipeline (GLR > 1000) 7-Oil Effluent Pipeline (GLR ≤ 1000) 8-Acid Gas Pipeline 9-Crude Oil Pipeline (GLR ≤ 1000) 10-LVP Products Pipeline (GLR ≤ 1000) 11-Salt Water Pipeline (GLR ≤ 1000) 12-Brine Hosted Minerals (GLR ≤ 1000)
Analysis Type	1-No Mitigation, or 2-With Mitigation

The analysis scenario name allows each calculation to be uniquely identified. Label 1 (name), Label 2 (location) and Label 3 (scenario) are concatenated to form a label that appears on the printouts.

By selecting a type of sour operations one of three types of models are run, depending on the Gas to Liquid Ratio (*GLR*):

- 1) GAS PIPELINE (includes oil effluent pipelines with Gas to Liquid Ratio > 1000) using a transient jet source model,
- 2) GAS WELL (includes oil/liquid/ other wells with Gas to Liquid Ratio > 1000) using a steady jet source model, or
- 3) LIQUID PIPELINE or LIQUID WELL (includes oil effluent pipeline, oil well, other pipelines and other wells) with Gas to Liquid Ratio ≤ 1000 using a steady pool source model.

Input cells are opened or closed, and defaults are set depending on the selection. Similarly, the analysis type selection opens cells for input and provides the default values, checks to see if the value is within limits and displays the value to be used in the calculation. Warnings are provided if the value entered is out of bounds, but the model will calculate the EPZ.

2.3 Gas Pipeline

A gas pipeline (includes oil effluent pipeline with Gas to Liquid Ratio > 1000) transient jet release is defined by:

Pipeline Segment From Location Coordinates Longitude/Latitude NAD83	X (east-west) and Y (north-south)
Pipeline Segment To Location Coordinates Longitude/Latitude NAD83	X (east-west) and Y (north-south)
Licensed Maximum Operating pressure (P_L)	kPa (gauge)
Expected Maximum Operating Pressure (P_i)	kPa (gauge)
Pipeline outside diameter (D)	mm
Pipeline wall thickness (t)	mm
Pipe Absolute Roughness Dropdown Box selection (Steel:0.05; Plastic/Liner:0.01; Fibreglass:0.005)	mm
Segment length (S)	m
Equivalent Segment Length between ESDs (enter Length or Volume below), (S_{ESD})	m

Equivalent Cumulative Pipeline Volume between ESDs (enter Volume or Length above), (V_{ESD})	m^3
Expected Maximum Gas to Liquid Ratio, (GLR) (if oil effluent pipeline with $GLR > 1000$)	standard m^3 Gas to stock tank m^3 Liquid
Licensed Maximum H ₂ S Concentration ($LH_2S\%$)	% (molar, dry gas phase), (at T_{REF} & P_{REF})
Expected Maximum H ₂ S Concentration ($EH_2S\%$)	% (molar, dry gas phase), (at T_{REF} & P_{REF})
Expected Minimum Gas Temperature (T_i)	°C
ESD Valve Closure Time once Triggered (t_{close})	s
ESD Valve Low Pressure (LP) Trigger (P_{ESD})	kPa (gauge)
ESD Valve Pressure Rate of Change (PROC) Trigger (dP_{ESD}/dt)	kPa/s
ESD Valve Pressure Rate of Change PROC sampling time (t_{poll})	s
PROC Number of Cycles until Final Decision (N_{poll})	--
Time from initial release until ESDs manually or remotely closed (t_{manual})	minutes
Time from initial release until ignition or stop flow ($t_{ignition}$)	minutes

The segment length is the distance between nodes such as ESD valves, check valves, manual valves or junctions. The BATCH page GAS GATHERING SYTEM - PIPELINE NETWORKING section can be used to determine the equivalent segment length between ESDs, as described in Section 5.1.12. The user enters either the equivalent segment length between ESDs or the equivalent cumulative pipeline volume (S_{ESD} or V_{ESD}), the other value not entered is calculated from the value entered and the pipeline outside diameter D and wall thickness t .

The pipe absolute roughness is a new input using a dropdown box. It is used to adjust the friction factor for steel (0.05 mm), plastic liners (0.01 mm), and fiberglass (0.005 mm). Smoother pipe surfaces blowdown quicker.

The expected conditions during the operation of the pipeline are used for the hazard zone calculations. This includes the expected maximum operating pressure and the expected maximum H₂S concentration. The licensed conditions for the pipeline are input for the setback volume calculations. The input H₂S concentrations may differ from the representative analysis provided as the program will normalize the representative analysis to the input H₂S. The source mitigation inputs define the ESD valve time delays and trigger settings and are discussed in Section 5.1.4.

The source mitigation input is the time before ignition and is discussed in Section 5.1.4. Default mitigation settings result in a larger EPZ. Section 13 of the *Pipeline Rules* requires an Engineering

Assessment for ESD valve settings. The default ESD settings in AERH2S are worst case settings and represent settings where the valve does not respond to close automatically. Default ESD valve settings should not be used as actual operating settings unless those settings are not used in the operation or when those settings can be justified.

2.4 Gas Well

A gas well (includes oil well and other well with Gas to Liquid Ratio>1000) steady jet release is described by:

Phase of well operations?	2-Drilling, or 3-Completion/Service/Workover, or 4-Producing/Injection/Suspended
Is well classified as critical?	1-Critical, or 2-Non-Critical <i>Not required for calculation</i>
Unique well identifier	As issued by AER <i>Not required for calculation</i>
Well Centre Surface Coordinates -- Longitude/Latitude NAD83	X (east-west) and Y (north-south)
Casing or tubing inside diameter at exit (<i>D</i>)	mm
Wet Gas Release Rate (Absolute Open Flow), (Cumulative if Multi-zone)	10 ³ Rm ³ /d, (at <i>T_{REF}</i> & <i>P_{REF}</i>)
Licensed Maximum H ₂ S concentration (<i>LH₂S</i> % of mixture) (not molar fraction, but molar fraction times 100)	% (molar, dry gas phase), (at <i>T_{REF}</i> & <i>P_{REF}</i>)
Expected Maximum H ₂ S concentration (<i>EH₂S</i> % of mixture) (not molar fraction, but molar fraction times 100)	% (molar, dry gas phase), (at <i>T_{REF}</i> & <i>P_{REF}</i>)
H ₂ S Release Rate (Obsolete Entry) (<i>H₂S_{RR}</i>) (Directive 056 requires assessment done by APEGA member)	Rm ³ /s (at <i>T_{REF}</i> & <i>P_{REF}</i>)
Is Surface-Controlled Sub Surface Safety Valve Installed? (Producing Well Only)	1-SCSSSV, or 2-No SCSSSV
Time from initial release until ignition or stop flow (<i>TSD</i>)	minutes

The input H₂S concentrations (percent) may not be equivalent to the representative gas analysis provided (molar fraction) as the program will normalize the representative analysis to the input H₂S. Note that the H₂S release rate entry is now an obsolete entry and is no longer required to be entered because it is calculated from the input expected maximum H₂S concentration and the input wet gas release rate. It is still provided to allow data from ERCBH2S to be input into AERH2S. The calculated H₂S release rate

must match the values determined in the H₂S release rate assessment. For releases from multiple zones such as during drilling through open zones or commingled production, the cumulative gas release rate and the flow weighted average H₂S concentration must be input. The MULTiZONE page determines the required inputs. The wet gas release rate input depends on the well bore diameter so caution should be used when the values are adjusted independently of each other.

Directive 056: Energy Development Applications and Schedules (Directive 056) Section 4.8.5.4 (69) requires the H₂S release rate assessment to be done by a member of the Association of Professional Engineers and Geoscientists of Alberta (APEGA). If an annulus flow is being modelled, such as a release flowing between the tubing and casing, the equivalent diameter of the flow area is input. The source mitigation input is the time before ignition and is discussed in Section 5.2.2.

2.5 Liquid Pipeline or Liquid Well

Liquid pipeline or liquid well (as oil effluent, crude oil, low vapour pressure (LVP) products, or salt water) with a Gas to Liquid Ratio ≤ 1000 are modelled as steady releases from a liquid pool defined by following inputs:

Phase of well operations? (if well)	2-Drilling, or 3-Completion/Service/Workover, or 4-Producing/Injection/Suspended
Is well classified as critical? (if well)	1-Critical, or 2-Non-Critical <i>Not required for calculation</i>
Unique well identifier (if well)	As issued by AER <i>Not required for calculation</i>
Well Centre Surface Location Coordinates or Pipeline Segment From Location Coordinates Longitude/Latitude NAD83	X (east-west) and Y (north-south) <i>Not required for calculation</i>
Pipeline Segment To Location Coordinates (if pipeline) Longitude/Latitude NAD83	X (east-west) and Y (north-south) <i>Not required for calculation</i>
Licensed Maximum Operating Pressure	kPa (gauge)
Expected Maximum Operating Pressure	kPa (gauge)
Oil Gravity	°API
Produced Water/Brine Water Salt Content (salinity)	% salt of liquid as mass fraction
Pipe outside diameter (<i>D</i>)	mm
Pipe wall thickness (<i>t</i>)	mm

Segment length (S) (if Oil effluent pipeline)	m
Equivalent Segment Length between ESDs (enter Length or Volume below), (S_{ESD}) (if Oil effluent pipeline)	m
Licensed Maximum H ₂ S Concentration (LH ₂ S%) (not molar fraction, but molar fraction times 100)	% (molar, dry gas phase), (at T_{REF} & P_{REF})
Expected Maximum H ₂ S Concentration (EH ₂ S%) (not molar fraction, but molar fraction times 100)	% (molar, dry gas phase), (at T_{REF} & P_{REF})
Well Maximum H ₂ S Release Rate (Obsolete Entry) (H_2S_{RR})	Rm ³ /s (at T_{REF} & P_{REF})
Expected Maximum Liquid Flow Rate of Well or Pipeline Fluid (Q_{LIQUID})	Rm ³ /d (at T_{REF} & P_{REF})
Expected Maximum Gas to Liquid Ratio of Well or Pipeline Fluid (GLR)	standard m ³ Gas to stock tank m ³ Liquid
Expected Minimum Liquid Temperature (T_L)	°C
Is Surface-Controlled Sub Surface Safety Valve Installed? (Producing Well Only)	1-SCSSSV, or 2-No SCSSSV
Time from initial release until stop flow or ignition (TSD)	minutes

The expected maximum pressure and H₂S concentration for pipelines and wells are input for the emergency planning zone determination. The expected maximum daily production rate of liquid (oil and/or water) from the well or through the pipeline, Q_{LIQUID} along with the gas to liquid ratio, GLR determine the rate of gas coming out of solution when the fluid is released at reference conditions. The H₂S concentration is the expected maximum at stock tank conditions (percent) and may not be equivalent to the representative gas analysis for the solution gas (molar fraction). The H₂S release rate from wells and pipelines is calculated from these three entries.

The licensed pressure and H₂S concentration for oil effluent pipelines and wells are input for the setback determination. The oil gravity or produced water/brine water salt content allow the bubble point of the gas coming out of solution to be determined. This allows for a better estimate of the amount of H₂S in the pipeline segment to determine the setback level.

For pipelines, the segment length is the distance between nodes such as ESD valves, check valves, manual valves or junctions. The BATCH page LIQUID GATHERING SYSTEM - PIPELINE NETWORKING columns can be used to determine the equivalent segment length between ESDs, as described in Section 5.3.5. The user enters the equivalent segment length between ESDs (S_{ESD}).

The source mitigation input is the time before the well or pipeline is shut-in and is discussed in Section 5.3.3.

2.6 Sour Gas Composition

The user is required to input a representative dry sour gas molar (d_i) compositional analysis. This composition is adjusted to the expected or modelled ($EH_2S\%$ or $LH_2S\%$) H_2S mole fraction m_{H_2S} . Then the composition is adjusted to wet conditions (w_i) as follows:

Table 2-1: Gas Composition Normalization Equations for Dry and Wet Compositions

Component mole fractions	User Inputs d_i Dry Reference Analysis	User Input $H_2S\%$ Calculated Composition Dry at Specified H_2S $m_i =$	Calculated Composition Wet at Specified H_2S $w_i =$
H_2	d_{H_2}	$d_{H_2} \cdot (1 - m_{H_2S}) / (1 - d_{H_2S})$	$m_{H_2} \cdot (1 - w_{H_2O})$
He	d_{He}	$d_{He} \cdot (1 - m_{H_2S}) / (1 - d_{H_2S})$	$m_{He} \cdot (1 - w_{H_2O})$
N_2	d_{N_2}	$d_{N_2} \cdot (1 - m_{H_2S}) / (1 - d_{H_2S})$	$m_{N_2} \cdot (1 - w_{H_2O})$
CO_2	d_{CO_2}	$d_{CO_2} \cdot (1 - m_{H_2S}) / (1 - d_{H_2S})$	$m_{CO_2} \cdot (1 - w_{H_2O})$
H_2S	d_{H_2S}	$m_{H_2S} = H_2S\% / 100$	$m_{H_2S} \cdot (1 - w_{H_2O})$
CH_4	d_{CH_4}	$d_{CH_4} \cdot (1 - m_{H_2S}) / (1 - d_{H_2S})$	$m_{CH_4} \cdot (1 - w_{H_2O})$
C_2H_6	$d_{C_2H_6}$	$d_{C_2H_6} \cdot (1 - m_{H_2S}) / (1 - d_{H_2S})$	$m_{C_2H_6} \cdot (1 - w_{H_2O})$
C_3H_8	$d_{C_3H_8}$	$d_{C_3H_8} \cdot (1 - m_{H_2S}) / (1 - d_{H_2S})$	$m_{C_3H_8} \cdot (1 - w_{H_2O})$
i-C ₄ H ₁₀	$d_{iC_4H_{10}}$	$d_{iC_4H_{10}} \cdot (1 - m_{H_2S}) / (1 - d_{H_2S})$	$m_{iC_4H_{10}} \cdot (1 - w_{H_2O})$
n-C ₄ H ₁₀	$d_{nC_4H_{10}}$	$d_{nC_4H_{10}} \cdot (1 - m_{H_2S}) / (1 - d_{H_2S})$	$m_{nC_4H_{10}} \cdot (1 - w_{H_2O})$
i-C ₅ H ₁₂	$d_{iC_5H_{12}}$	$d_{iC_5H_{12}} \cdot (1 - m_{H_2S}) / (1 - d_{H_2S})$	$m_{iC_5H_{12}} \cdot (1 - w_{H_2O})$
n-C ₅ H ₁₂	$d_{nC_5H_{12}}$	$d_{nC_5H_{12}} \cdot (1 - m_{H_2S}) / (1 - d_{H_2S})$	$m_{nC_5H_{12}} \cdot (1 - w_{H_2O})$
n-C ₆ H ₁₄	$d_{nC_6H_{14}}$	$d_{nC_6H_{14}} \cdot (1 - m_{H_2S}) / (1 - d_{H_2S})$	$m_{nC_6H_{14}} \cdot (1 - w_{H_2O})$
n-C ₇ H ₁₆₊	$d_{nC_7H_{16+}}$	$d_{nC_7H_{16+}} \cdot (1 - m_{H_2S}) / (1 - d_{H_2S})$	$m_{nC_7H_{16+}} \cdot (1 - w_{H_2O})$
H_2O	<i>w</i>	0.0	w_{H_2O}
Total	1.0000	1.0000	1.0000

The analysis should be representative of the vapours that would exist at stock tank conditions of 15°C and 101.325 kPa (i.e. at T_{REF} & P_{REF}). The H₂S fraction of the representative analysis d_{H2S} does not have to equal the licensed $LH2S\%$ used for setback release calculations or the expected $EH2S\%$ that the ERP zones will be based on (d_{H2S} can be zero but a representative analysis should be entered). ***The dry compositional analysis input by the user must add up to one for the calculation to proceed.*** Warnings are provided if the input fraction of heavier hydrocarbons exist as liquids at reference conditions indicating reference conditions where not used.

For existing pipelines and wells, a gas analysis from the pipeline or well should be used. For proposed wells, the gas composition used to determine the release rate should be used. For proposed pipelines, the gas composition used to design the equipment should be used.

The AERH2S entries for the dry mixture gas phase composition are:

- gas model: use recombined vapour and liquid analysis
- liquid model: use vapour from separator or stock tank, at T_{REF} & P_{REF}

AERH2S uses the combined composition of the released material; that is, the combined vapour and liquid molar fractions. In the past, many users used the gas analysis without regard for whether it was a combined analysis or what pressure and temperature it was taken under. However, in a real gas the H₂S fraction in the gas phase may change with pressure and temperature as the mass fraction of vapours and liquids change. From a dispersion perspective, AERH2S requires the fraction of H₂S at atmospheric conditions. For this reason, the analysis should be representative of the vapours that would exist at stock tank conditions of 15°C and 101.325 kPa (i.e. at T_{REF} & P_{REF}).

The water content, W , is discussed in Section 3.2.

2.7 Advanced User Selected Case

A regulatory screening meteorology matrix consisting of 54 combinations of stability class and wind speed is used to determine the hazard zones, as discussed in Section 7.5. For gas pipelines, 11 different hole size fractions from 0.01 (a leak) to 2 (a guillotine rupture) are used to determine the ERP Zones, as discussed in Section 5.1.2. Advanced users can select the following inputs to review case specific results and intermediate calculation results:

Ambient Wind Speed at measurement height (U_{ref})	m/s
Stability Class	Stability Class (A=1, B=2, C=3, D=4, E=5, F=6, none=7=default)
Gas Pipeline Release Hole Size Fraction (A_e/A_p)	fraction

These cells must be blank for the AER regulatory submission.

3 PHYSICAL PROPERTIES

The CONSTANTS page of AERH2S provides the following values of constants and properties of sour gas, air and water used in the calculations. They are in regular font in regular boxes as the user cannot change them. The Gas Processors Suppliers Association (GPSA) is the source for most of the data.

Default inputs that are set by the AER and cannot be changed by the user are in

bold font in shaded boxes.

3.1 Constants

The constants (from Fig. 23-2 of the GPSA 2016) are:

Table 3-1: Physical Constants

Reference temperature, T_{REF}	288.15	K
Reference pressure, P_{REF}	101.325	kPa
Universal gas constant, R_U	8314.46261815324	J/(kmol·K)
Molar Volume, V/N at T_{REF} & P_{REF}	23.64483	Rm ³ /kmol
Gravity constant, g	9.80665	m/s ²

3.2 Sour Gas

The molar mass, specific heat and boiling point and lower flammability limit (LFL) (from Fig. 23-2 of the GPSA (2016)) properties of pure components are:

Table 3-2: Chemo-Physical Constants

Component	Sour Gas Composition Wet, at Expected or Licensed H ₂ S (Mole Fraction) w_i	Molar Mass (kg/kmol) MW_i	Mass Specific Heat at Constant Pressure (kJ/(kg·K) at T_{REF} and P_{REF}) C_{Pi}	Boiling Point (K)	Lower Flammability Limit (%)
H ₂	W_{H_2}	2.0159	14.2647	20.39	4
He	W_{He}	4.0026	5.1932	4.23	na
N ₂	W_{N_2}	28.0134	1.0395	77.36	na

CO ₂	W_{CO_2}	44.0096	0.8334	194.75	na
H ₂ S	W_{H_2S}	34.0809	0.9976	212.86	4.3
CH ₄	W_{CH_4}	16.0425	2.2036	111.67	5
C ₂ H ₆	$W_{C_2H_6}$	30.0690	1.7054	184.55	2.9
C ₃ H ₈	$W_{C_3H_8}$	44.0956	1.6291	231.08	2
i-C ₄ H ₁₀	$W_{iC_4H_{10}}$	58.1222	1.6162	261.53	1.8
n-C ₄ H ₁₀	$W_{nC_4H_{10}}$	58.1222	1.6511	272.64	1.5
i-C ₅ H ₁₂	$W_{iC_5H_{12}}$	72.1488	1.6003	300.99	1.3
n-C ₅ H ₁₂	$W_{nC_5H_{12}}$	72.1488	1.6216	309.25	1.4
n-C ₆ H ₁₄	$W_{nC_6H_{14}}$	86.1754	1.6125	341.88	1.1
n-C ₇ H ₁₆ ⁺	$W_{nC_7H_{16+}}$	100.2019	1.6057	371.56	1
H ₂ O	W_{H_2O}	18.0153	1.8620	373.12	na

The water content W_{H_2O} should be representative of the vapours that would exist at stock tank conditions of 15°C and 101.325 kPa (i.e. at T_{REF} & P_{REF}). Predicted hazard distances are not sensitive to the typical water contents encountered, (to be demonstrated in Section 10), therefore the AER default value entered on the CONSTANTS page is a dry gas with W set to zero.

Released Gas Water Content, (W_{H_2O}, Mole fraction)	Range 0 to 1 (at T_{REF} and P_{REF})	Default 0 (at T_{REF} and P_{REF})
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The following sour gas mixture properties are calculated from the input composition that has been adjusted to wet mole fractions at the specified H₂S concentration (w_i). Source mixture molar mass (kg/kmol) is calculated for the expected and licensed H₂S concentration mixtures:

$$WMS = \sum_{i=1}^n w_i \cdot MW_i \quad (3.1)$$

Gas constant for source mixture (J/(kg·K)) is calculated for the expected and licensed H₂S concentration mixtures:

$$R_S = \frac{R_U}{WMS} \quad (3.2)$$

Specific heat of ideal gas source mixture (J/(kg·K)) is calculated for the expected H₂S concentration mixture:

$$CPI = \sum_{i=1}^n \frac{w_i \cdot MW_i \cdot C_{Pi}}{WMS} \quad (3.3)$$

Ratio of specific heats for an ideal gas source mixture at reference conditions is calculated for the expected H₂S concentration mixture:

$$k_I = \frac{CPI}{CPI - R_s} \tag{3.4}$$

3.3 Air

The following air and water properties are from Fig. 23-2 of the GPSA (2016) except *dhw* which is from Fig. 24-30 of GPSA (2016), all at *T_{REF}* of 15 °C. They are used in AERSLAB for consistency and are slightly different than the values in SLAB:

Table 3-3: Properties of Air

Molar mass dry air (<i>wma</i>)	28.9655	kg/kmol
Specific heat dry air (<i>cpa</i>)	1004.2833	J/(kg·K) at <i>T_{REF}</i>
Molar mass water (<i>wmw</i>)	18.0153	kg/kmol
Density water liquid (<i>rho_{wl}</i>)	999.102	kg/m ³ at <i>T_{REF}</i> and <i>P_{REF}</i>
Specific heat water vapour (<i>cp_{wv}</i>)	1862.0	J/(kg·K) at <i>T_{REF}</i>
Specific heat water liquid (<i>cp_{wl}</i>)	4188.8	J/(kg·K) at <i>T_{REF}</i>
Latent heat water (<i>dhw</i>)	2465900	J/kg at <i>T_{REF}</i>

The local atmospheric pressure *P_A* (kPa) is calculated from the input site elevation using (AENV 1988):

$$P_A = P_{REF} \left(1 - \frac{\Gamma \cdot z_{ASL}}{T_{REF}} \right)^{\frac{wma \cdot g}{R_u \cdot \Gamma}} \tag{3.5}$$

The United States standard atmosphere at sea level is used with an average vertical temperature gradient in the atmosphere of:

Average vertical temperature gradient in the atmosphere (Γ)	0.0065	K/m
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The SLAB program allows for the moisture content of the ambient air at standard atmospheric pressure; thus, some code changes were required in AERSLAB to allow for the local atmospheric pressure. The following saturation pressure constants have been changed in the AERSLAB code.

The intercept for standard conditions is:

$$spaw=17.14 \tag{3.6}$$

The slope is:

$$spbw = 4285 \text{ K} \quad (3.7)$$

A temperature correction factor is included to give a 100 °C boiling point at the reference pressure:

$$spcw = -30.19 \text{ K} \quad (3.8)$$

Air moisture properties depend on the ambient air temperature T_A (K) and relative humidity RH (%) which are discussed in Section 7. The following parameters are calculated in AERH2S, just as they are calculated in SLAB, to determine the density of moist air at site conditions:

The intercept for the partial pressure:

$$SPA_{wPP} = SPA_w - \ln(P_A * 1000) + \ln(1000) \quad (3.9)$$

The water boiling point for site pressure (K):

$$T_{Bsite} = \frac{SPBw}{SPA_{wPP}} - SPCw \quad (3.10)$$

Water relative partial pressure:

$$rpwa = 0.01 \cdot RH \cdot \exp\left(spawPP - \frac{spbw}{T_A + spcw}\right) \quad (3.11)$$

Mass fraction water:

$$cmwa = \frac{wmw \cdot rpwa}{wma + (wmw - wma)rpwa} \quad (3.12)$$

Mass fraction dry air:

$$cmdaa = 1 - cmwa \quad (3.13)$$

Specific heat of moist air (J/(kg·K)):

$$cpaa = cmdaa \cdot cpa + cmwa \cdot cpwv \quad (3.14)$$

Molar mass of moist air (kg/kmol):

$$wmae = \frac{wma \cdot wmw}{wmw + (wma - wmw)cmwa} \quad (3.15)$$

Density of moist air (kg/m³) at site conditions:

$$rhoa = \frac{wmae \cdot P_A \cdot 1000}{R_U \cdot T_A} \quad (3.16)$$

4 AERFLASH - REAL FLUID PROPERTIES

Many hazard models use ideal gas properties to simplify the analysis. Ideal gas modelling does not allow for the change in specific heat with pressure and the potential for phase change due to the low temperatures at the exit. When the ideal gas assumption is used, the isenthalpic temperature of the release at atmospheric pressure is set at the initial temperature. Therefore, ideal gas modelling overestimates the temperature and ignores the potential aerosol liquid formation, thus underestimating the density of the release. Assuming ideal gas behaviour for sour gas releases introduces errors in the hazard distance calculations and is unacceptable. The AERFLASH program provides the real fluid properties of the release. Appendix 1 provides details of how the properties are calculated.

The inputs and outputs described below are in regular font in regular boxes as the user cannot change them.

4.1 Inputs

The AERFLASH page provides the input parameter variables to *AERFLASH*. The *AERFLASH* inputs table is shown below with the units for variable. The AERH2S page displays a warning if the entries are current or out of date.

AERFLASH Input	Variable/Units
Configuration	GAS PIPELINE, GAS WELL, or LIQUID PIPELINE/WELL
Operating Composition	Mole Fraction
hydrogen	$W_{H_2,E}$
helium	$W_{He,E}$
nitrogen	$W_{N_2,E}$
carbon dioxide	$W_{CO_2,E}$
hydrogen sulphide	$W_{H_2S,E}$
methane	$W_{CH_4,E}$
ethane	$W_{C_2H_6,E}$
propane	$W_{C_3H_8,E}$
isobutane	$W_{iC_4H_{10},E}$
n-butane	$W_{nC_4H_{10},E}$
isopentane	$W_{iC_5H_{12},E}$
n-pentane	$W_{nC_5H_{12},E}$
n-hexane	$W_{nC_6H_{14},E}$

AERFLASH Input	Variable/Units
n-heptane plus	$W_{nC7H16+,E}$
water	$W_{H2O,E}$
Total	1.00000
Operating Conditions	
Initial pressure	P_O , kPa (abs)
Initial temperature	T_O (K)
Mass flux at exit	\dot{m}_E / A_E (kg/(s·m ²))
Exit pressure	P_E (kPa abs)
Exit temperature	T_E (K)
Drag coefficient	C_d'
Atmospheric pressure	P_A (kPa abs)
Ambient temperature	T_A (K)
Licensed Composition	Mole Fraction
hydrogen	$W_{H2,L}$
helium	$W_{He,L}$
nitrogen	$W_{N2,L}$
carbon dioxide	$W_{CO2,L}$
hydrogen sulphide	$W_{HS2,L}$
methane	$W_{CH4,L}$
ethane	$W_{C2H6,L}$
propane	$W_{C3H8,L}$
isobutane	$W_{iC4H10,L}$
n-butane	$W_{nC4H10,L}$
isopentane	$W_{iC5H12,L}$
n-pentane	$W_{nC5H12,L}$
n-hexane	$W_{nC6H14,L}$
n-heptane plus	$W_{nC7H16+,L}$
water	$W_{H2O,L}$
Total	1.00000
Licensed Conditions	
Licensed pressure	P_L (kPa abs)
Level temperature	T_L (K)

The input data to AERFLASH are the configuration of the release (GAS PIPELINE, GAS WELL OR LIQUID PIPELINE/WELL) and the adjusted sour gas composition analysis (wet at specified H₂S, w_i). Liquid release calculations within AERFLASH are the same as for a gas well. The operating expected

condition inputs are discussed in Section 5 and are the: initial pressure, initial temperature, mass flux at the exit, an initial guess for exit pressure and exit temperature, drag coefficient, atmospheric pressure and ambient temperature.

4.2 Outputs

The AERFLASH OUTPUT page of AERH2S includes the pressure, temperature, density, speed of sound (or exit velocity if less than the speed of sound) and the liquid mass fraction at the initial conditions before the release and at the initial flow and average flow exit conditions. A specific heat ratio representative of the flow is provided (initial for well, average for pipeline). The temperature, density, and the liquid mass fraction at isenthalpic flash conditions and the R plane are then provided. These are followed by other properties at the R plane for input to the dispersion model. Some of these variables are not used in the calculations. The AERFLASH OUTPUT page (shown below) lists the output parameter variables, units and whether the inputs are current or out of date are provided in the following table.

AERFLASH Output	Units
P_o Initial pressure	kPa (abs)
T_o Initial temperature	K
ρ_o Initial density at P_o and T_o	kg/m ³
c_o Initial speed of sound at P_o and T_o	m/s
X_o Initial liquid mass fraction at P_o and T_o	
P_{Ei} Initial exit pressure	kPa (abs)
T_{Ei} Initial exit temperature	K
ρ_{Ei} Initial exit density at P_{Ei} and T_{Ei}	kg/m ³
c_{Ei} Initial exit speed of sound at P_{Ei} and T_{Ei}	m/s
X_{Ei} Initial exit liquid mass fraction at P_{Ei} and T_{Ei}	
P_{Ea} Average exit pressure	kPa (abs)
T_{Ea} Average exit temperature	K
ρ_{Ea} Average exit density at P_{Ea} and T_{Ea}	kg/m ³
c_{Ea} Average exit speed of sound at P_{Ea} and T_{Ea}	m/s
X_{Ea} Average exit liquid mass fraction at P_{Ea} and T_{Ea}	
k_a Average ratio of specific heats C_p/C_v	
T_F Isenthalpic flash temperature to P_A	K
ρ_F Isenthalpic flash density at P_A and T_F	kg/m ³
X_F Isenthalpic flash liquid mass fraction at P_A and T_F	
V_R R-plane velocity	m/s

AERFLASH Output	Units
T_R R-plane temperature	K
ρ_R R-plane density	kg/m ³
X_R R-plane liquid mass fraction	
T_{DEW} Dew point temperature	K
CPS Vapour specific heat capacity	J/(kg·K)
TBP Boiling point temperature	K
hfg Liquid heat of vapourization	J/kg
$CPSL$ Liquid specific heat capacity	J/(kg·K)
$RHOSL$ Liquid density	kg/m ³
SPB Saturation pressure constant	
SPC Saturation pressure constant	
ρ_o $RHOLV$, density under license condition	kg/m ³
Vapour Phase Mass Fraction after initial isenthalpic flash	

AERFLASH produces an errorlog.txt file if a problem is encountered while running. Like most thermodynamic flash models, AERFLASH is a two-phase program (vapour and liquid) but in some situations three phases may exist (vapour, and two immiscible liquids such as hydrocarbons and water or hydrogen sulphide). Occasionally, especially if the fraction of water or heavier hydrocarbons is high or the temperature is very low, the program cannot converge on a solution. To prevent this error, an initial isenthalpic flash from licensed conditions is done to the reference pressure and the vapour phase composition is used thereafter.

5 RELEASE DESCRIPTION

This section provides the equations used to describe the release for gas pipelines, gas wells, and liquid pipelines and liquid wells. The rate, duration, and initial and exit conditions are defined to model gas pipelines as transient jets, gas wells as steady jets, and liquid pipelines and liquid wells as steady pool releases. Recall that:

- **User inputs are in regular font in bold boxes**,
- **Default inputs are in bold font in shaded boxes**, and
- **Ranges of inputs are in bold font in bold boxes**

This section describes how the user inputs (Section 2) are used to define the release. Only source mitigation values input by the user and AER default values are discussed in this section. Default inputs are used for source mitigation if the user does not provide a value or if no source mitigation is selected. The range of acceptable source mitigation values is also provided.

5.1 Gas Pipeline

The GAS PIPELINE page performs the release calculations. For gas pipelines, the transient mass release rate is described by the double exponential blowdown model (see Appendix 2) which is based on an isothermal blowdown of a quasi-ideal gas. Initial conditions in the pipeline segment are defined by user inputs in Section 2.3. This allows an effective release duration and steady release rate to be calculated for hole sizes ranging from ruptures that shut down the pipeline to leaks which do not immediately impair the operation. Inputs to the dispersion model are based on real fluid properties at the effective duration and effective mass release rate.

5.1.1 *Initial and Exit Conditions*

Initial conditions for a pipeline release are the conditions in the segment before a rupture. For pipelines, the initial expected maximum operating pressure P_o and the minimum initial pipeline temperature T_l are specified by the user. Both the initial release rate when the rupture occurs (which is needed for the blowdown equation) and the effective release rate (which is input to AERSLAB), are defined from the user input.

The initial temperature input is:

Expected Minimum Gas Temperature T_o (°C)	Range 0 to 150	Default 5
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The model uses the stagnation temperature and since the velocity of flow in a pipeline is low, the kinetic energy can be ignored, and the stagnation temperature equals the static temperature. A stagnation temperature of 5 °C, a typical Alberta ground temperature at pipeline depths, is the default. This conservatively assumes the sour gas in the pipeline has cooled to the ground temperature before a rupture occurs. At ground temperature and typical licensed operating pressures, the release may be dense at ambient conditions. At higher operating temperatures or lower pressures, the release may become buoyant. The initial release is identified with a subscript i and the effective or average release with a subscript a . The input temperature T_I is converted to T_o in absolute units (K):

$$T_o = T_I + 273.15 \quad (5.1)$$

The initial gauge pressure P_I (kPa g) input by the user is converted to P_o (kPa abs):

$$P_o = P_I + P_A \quad (5.2)$$

The initial density (kg/m^3) of the material in the pipeline is:

$$\rho_I = 1000 \frac{P_o}{Z_o R_s T_o} \quad (5.3)$$

Similarly for licensed conditions, the input temperature T_I is converted to T_L in absolute units (K):

$$T_L = T_I + 273.15 \quad (5.4)$$

The licensed gauge pressure P_I (kPa g) input by the user is converted to P_o (kPa abs):

$$P_L = P_I + P_{REF} \quad (5.5)$$

The initial density (kg/m^3) of the material in the pipeline is:

$$\rho_L = 1000 \frac{P_L}{Z_L R_s T_L} \quad (5.6)$$

Initially Z_o and Z_L are set to 1.0 and the ideal gas values are used to estimate inputs to AERFLASH. AERFLASH then provides the real gas predictions which are used in subsequent calculations. A subscript g stands for the ideal gas guess of the parameter to be input to the AERFLASH program. The pressure at the exit plane (kPa), assuming ideal gas choked flow is:

$$P_{Eig} = P_o \left(\frac{2}{k_I + 1} \right)^{\frac{k_I}{k_I - 1}} \quad (5.7)$$

The temperature at the exit plane (K), assuming ideal gas choked flow is:

$$T_{Eig} = T_o \left(\frac{2}{k_I + 1} \right) \quad (5.8)$$

The ratio of specific heats k_I , is not constant for a real gas. The ideal gas values of P_{og} , P_{Eg} and T_{Eg} are the first guesses in the iterative solution performed by the real fluids program AERFLASH (see Appendix 1).

AERFLASH solves for the initial and average exit conditions by guessing until the flow, energy and entropy conditions are satisfied. The initial entropy and enthalpy inside the pipe before the rupture depends on the specified temperature and pressure. The program determines the initial exit pressure under isentropic expansion from the initial pressure such that the total energy at the exit under critical, choked flow conditions is equal to the initial enthalpy h_o (J/kg or m²/s²):

$$h_o = h_{Ei} + \frac{c_{Ei}^2}{2} \quad (5.9)$$

The average entropy and enthalpy upstream of the exit depends on a guessed pressure upstream of the exit and the initial enthalpy. The program determines the average exit pressure under isentropic expansion from the initial enthalpy such that the total energy at the exit under critical, choked flow conditions is equal to the initial enthalpy h_o (J/kg or m²/s²):

$$h_o = h_{Ea} + \frac{c_{Ea}^2}{2} \quad (5.10)$$

An isenthalpic blowdown of the pipeline is modelled. Then it checks if the critical mass flux at the average exit pressure P_{Ea} that satisfies the above equation is equal to the specified mass flux (kg/ (s·m²)):

$$\frac{\dot{m}_E}{A_E} = c_{Ea} \cdot \rho_{Ea} \quad (5.11)$$

It then updates the guessed average upstream pressure P_{Ia} with an isentropic compression up to the initial enthalpy and repeats the calculations until the critical mass flux equals the calculated mass flux. The average mass flux at the exit \dot{m}_E / A_E is calculated from the initial conditions, as described in subsequent sections.

The ratio of specific heats k_I for the real gas is required for transient mass release rate and extra mass calculations to predict the properties as pressure changes. Initially the polytropic exponent for the isentropic expansion at the initial flow rate was proposed to account for k_I changing with pressure in a real

gas. It was discovered that k_i could be less than 1 for high H₂S sour gas, resulting in questionable predictions. To be consistent with the quasi-ideal assumptions used in the formulation of the release rate and extra mass equations, k_i is calculated from the real gas isentropic expansion as follows:

$$k_i = 2 \frac{T_o}{T_{Ei}} - 1 \tag{5.12}$$

This is consistent with the assumption that the ratio of compressibility factors Z_o/Z_E is constant.

5.1.2 Transient Mass Release Rate

As described in Appendix 2, a double-exponential blowdown model is used to define the time varying mass release rate, from a pipe segment blowing down from one direction:

$$\dot{m}_e = \left(\frac{1}{1 + \alpha} \right) \left[\dot{m}_{ei} \exp\left(\frac{-t}{\alpha^2 \beta} \right) + \frac{M_i}{\beta} \exp\left(\frac{-t}{\beta} \right) \right] \tag{5.13}$$

Alternately, this can be expressed as:

$$\frac{\dot{m}_e}{\dot{m}_{ei}} = \left(\frac{1}{1 + \alpha} \right) \left[\exp\left(\frac{-t}{\alpha^2 \beta} \right) + \alpha \exp\left(\frac{-t}{\beta} \right) \right] \tag{5.14}$$

At the moment of the release, $t = 0$, the initial mass flow rate (kg/s) for one jet is \dot{m}_{ei} . The mass flow rate rapidly decreases until the total mass released (kg) from one direction is M_i . The total flow rate and mass released is double the above to account for the two jets, one from each segment direction.

A release can occur anywhere between the ESD valves resulting in the pipeline blowing down from both the upstream and downstream directions. The upstream and downstream valves close at different times, depending on the distance to the valve. For a guillotine rupture, the flows are independent of each other, and based on the analysis in Appendix 2, it can be shown that the total mass released is independent of the rupture location.

The release is modelled as if it occurs at the mid-point and depends on the hole size defined by the ratio of release area to pipe area. A logarithmic-like range of hole sizes are modelled to determine the hazard distances. The default inputs to determine the hazard distances are:

Gas Pipeline Release Hole Size Fraction, Ae/AP $\frac{A_{Total}}{A_p}$	Range 0.01 to 2.0	Default searches for value to give largest hazard distances starting at 2.0 for guillotine rupture then 1.0, 0.8, 0.5, 0.3, 0.2, 0.1, 0.08, 0.05, 0.02, 0.01
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The user can select a specific hole size fraction to review intermediate calculations. The hole size is given by:

$$\frac{A_E}{A_P} = \frac{A_{Total}}{A_P} \cdot \frac{1}{2} \quad (5.15)$$

= ratio of effective hole area to pipe area for flow from one direction, one half of flow from both directions.

$$A_E = \frac{A_{Total}}{A_P} \cdot \frac{1}{2} \cdot A_P \cdot c_c \quad (5.16)$$

= effective hole area (m²), including c_c , the jet exit contraction coefficient. For a guillotine break, A_{Total}/A_P is 2 and c_c is 1, therefore $A_E = A_P$ for one jet.

$$A_P = \frac{\pi}{4} D^2 \quad (5.17)$$

= pipeline cross-section area (m²) for pipe where:

$$D = \frac{D_o - 2t}{1000} \quad (5.18)$$

= inside diameter D (m) is pipeline outside diameter D_o (mm) less twice the wall thickness t (mm) with a unit conversion.

Note for pipelines with a liner, the wall thickness t is the pipe thickness plus the liner thickness.

The final time constant, β , (s) is:

$$\beta = \frac{2}{3} \frac{\rho_l A_P}{B_A \dot{m}_{ei}} \left(\left(1 + B_A L_{eff} \right)^{\frac{2}{3}} - 1 \right) \quad (5.19)$$

ρ_l and A_P are defined above. \dot{m}_{ei} is defined in (5.22) or (5.23). B_A , a constant, is defined in Equation (5.27). L_{eff} , the effective pipe segment length (m) is defined by (5.24) and derived in Appendix

2. The initial time constant (s) is:

$$\alpha^2 \beta = \frac{M_i^2}{\beta \dot{m}_{ei}^2} \quad (5.20)$$

The time adjustment factor, α , is:

$$\alpha = \frac{M_i}{\beta \dot{m}_{ei}} \quad (5.21)$$

M_i , the total mass released (kg) is calculated in the following sections and is defined by (5.24). The initial ideal gas mass flow rate \dot{m}_{ei} (kg/s) for one jet is:

$$\dot{m}_{ei} = K_{inertial} \left(\frac{Z_E}{Z_o} \left(\frac{2}{k_I + 1} \right) \right)^{\frac{k_I + 1}{2(k_I - 1)}} \left(\frac{k_I}{Z_o R_S T_o} \right)^{\frac{1}{2}} P_o A_E \quad (5.22)$$

The specific heat ratio k is ideal gas value k_I for the first pass then the real gas value is used. The compressibility factors Z_E and Z_o are set to one for the initial estimate of \dot{m}_{ei} . Then for the real gas, it is calculated from:

$$\dot{m}_{ei} = K_{inertial} c_{Ei} \rho_{Ei} A_E \quad (5.23)$$

The AER default inertial delay factor as recommended by the Wilson report in Appendix 2 is:

Inertial delay factor $K_{inertial}$	0.5
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The total mass release rate for both directions is double the value calculated for one jet.

5.1.3 Effective Length

The effective length, L_{eff} (m), is needed to calculate the time constants for the double exponential blowdown equation. As given in Appendix 2, the effective length, L_{eff} , of the blowdown from one direction is:

$$L_{eff} = L_{ESD} \cdot \left(1 + \frac{L_{extra}}{L_{ESD}} \right) \quad (5.24)$$

The term in the brackets was called the extra mass factor in GASCON2 (1990). GASCON2 mistakenly used L_{ESD} instead of L_{eff} in the calculation of the time constant β . For a mid-segment rupture, L_{ESD} , the distance (m) to the ESD valve is:

$$L_{ESD} = \frac{S_{ESD}}{2} \quad (5.25)$$

where the segment length (m), S_{ESD} , is the distance between adjacent ESD valves input by the user. The extra length ratio is:

$$\frac{L_{extra}}{L_{ESD}} = \left[1 + \left(\frac{1}{B_A L_{ESD}} \right) \right] \left[\frac{1}{3} \left(\frac{P_o}{P_{ESD}} \right)^2 + \frac{2}{3} \left(\frac{P_{ESD}}{P_o} \right) - 1 \right] \quad (5.26)$$

The constant B_A (1/m) is defined for a release exit area, pipe diameter and properties by:

$$\begin{aligned}
 B_A &= \left(\frac{2}{k+1} \right)^{\frac{k+1}{k-1}} \left(\frac{K_{inertia} A_e}{A_p} \right)^2 \left(\frac{Z_e}{Z_{oi}} \right) \frac{kf}{D} \\
 &= \frac{\dot{m}_{ei}^2 f}{\rho_{oi} D P_{oi} A_p^2}
 \end{aligned}
 \tag{5.27}$$

The first equation is the quasi-ideal gas derivation; the second equation uses the real gas initial flow rate and density. The Moody friction factor f for turbulent flow (which is 4 times the Fanning friction factor given in Eq 17-17, GPSA 2016) is:

$$f = 4 \left(4 \log \left(\frac{3.7D}{\varepsilon} \right) \right)^{-2}
 \tag{5.28}$$

The AER default absolute surface roughness ε is for commercial steel pipe (Fig. 17-3, GPSA 2016):

Absolute surface roughness, ε	0.05 mm
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For pipelines with a liner, the liner absolute surface roughness is selected by the user. Plastic liners are smoother than steel pipe thus L_{extra} for an unlined pipeline is less than for a lined pipeline.

The compressibility factors Z_E and Z_O are set to one and the ideal gas value of k_I are used for the initial ideal gas estimate of B_A , and then the real gas values calculated in AERFLASH are used. A very important input in the extra length equation is the ESD valve pressure ratio P_{ESD}/P_O to initiate the valve closure.

5.1.4 ***ESD Valve Settings to Reduce the Release***

The pressure ratio at the ESD valve when it finally closes depends on when valve closure is initiated and on the valve closure time. Three methods are commonly used to initiate valve closure: low pressure (LP, kPa), pressure rate of change (PROC, kPa/s) and manual or remote (MANUAL at t_{manual} , minutes).

Pressure is continuously monitored at the ESD valve. During normal operation the pressure at the valve will increase and decrease with flow rate and operating strategy. The pressure should never be above the maximum licensed pressure of the pipeline P_I . If a release occurs, the pressure at the valve will decrease substantially. The LP set point pressure is input as P_{ESD} (kPa gauge). If the pressure drops below the LP set point, the valve begins to close.

Some valves are also equipped to record the pressure and calculate the pressure change between the current reading and a previous reading. The time between readings is called the sampling time. The change in pressure divided by the sampling time is the slope dP/dt . The time between calculations is called the polling time t_{poll} and there may be several sampling cycles until the final decision to close is

made, N_{poll} . During normal operation the pressure at the valve will increase and decrease slowly with time so dP/dt is a small positive or negative number. When a release occurs, the pressure drops rapidly and dP/dt is a large negative number. For convenience, PROC is defined as a positive number $(dP/dt)_{set}$. If the calculated dP/dt at the polling time is greater than the $(dP/dt)_{set}$, the valve begins to close after the time it takes (N_{poll} times t_{poll}) to verify the decision to close.

The above describes when a valve is triggered and begins to close. As the valve closes flow through the valve is reduced and the pressure continues to drop. At the valve closure time t_{close} , the valve will be fully closed. The valve is assumed to close instantaneously at one half of the valve closure time to determine the pressure ratio when the valve closes.

Pipeline releases are mitigated through the ESD valve settings. The AER requires ESD valves on sour gas pipelines with over 10 mol/kmol of H₂S to be equipped with automatic LP closure. Sour gas pipelines with less than or equal to 10 mol/kmol of H₂S may not have automatic ESD valves but rely on manual closure. Most sour gas pipelines do not currently use PROC to trigger the valve closure. Some operators install additional pressure sensors between valves that can trigger on LP or PROC. All ESD valves can be closed manually, and some can be closed remotely. The time for manual or remote closure is from the initial release and includes the detection, notification, travel and field verification time. The range of values and the default input are provided below:

Table 5-1: Gas Pipeline ESD Mitigation Range of Values and Default Values

Source Mitigation Parameter	With Mitigation	No Mitigation
ESD Valve Closure Time, <i>t_{close}</i>	1 to 60 s	60 s
ESD Valve Low Pressure (LP) Trigger, <i>P_{ESD}</i>	0.1* P_i to 0.9* P_i kPa	0.1* P_i kPa
ESD Valve Pressure Rate of Change (PROC) Trigger, (dP/dt)_{set}	1 to P_i kPa/s	P_i kPa/s
ESD Valve Pressure Rate of Change (PROC) Sampling Time <i>t_{poll}</i>	1 to 3600 s	3600 s
Number of Sampling Cycles until Final Decision <i>N_{poll}</i>	1 to 100	3
Time from initial release until ESDs manually or remotely closed, <i>t_{manual}</i>	60 to 360 minutes	360 minutes
Time from initial release until ignition or stop flow <i>t_{ignition}</i>	60 to 360 minutes	360 minutes

The default valve closure time and sampling time are set at the maximum range value. The default LP trigger is set to a low value for pipelines without ESD valves. The AER recommends a minimum setting of 50% of the expected maximum operating pressure. The default PROC trigger is set to a high value based on the initial pipeline pressure P_i . The sampling time with the lowest dP/dt value is the input PROC set point. These default values result in larger hazard zones and encourage the operator to optimize their system to reduce the EPZ without shutting down the pipeline due to false triggers. Note that the operation of the pipeline dictates how sensitive the ESD valve closure can be to changes in pressure.

The time for manual or remote closure is from the initial release and includes the detection, notification, travel and field verification time. The maximum is the longest reasonable time to arrive at a remote site and to close the valve. After 6 hours (360 minutes) the dispersion of the release is in equilibrium and the predicted concentrations will not change for the modelled stability class and wind speed. Ignition times of less than the maximum exposure time of 3 hours (180 minutes) are required reduce the hazard zones.

These inputs are used to calculate the pressure ratio when the valve closes for the three methods of closure.

5.1.5 ESD Valve Closure on Low Pressure

Equation (5.26) requires the P_{ESD}/P_o based on absolute pressures when the valve is closed and is determined from the input LP trigger point of P_{ESDg} and the atmospheric pressure P_A .

$$\frac{P_{ESD}}{P_o} = \frac{P_{ESDg} + P_A}{P_i + P_A} \quad (5.29)$$

Following the Wilson report's inertia-less approach of Appendix 2, the mass that escapes from the release up to the time the ESD valve closes can be determined from:

$$M_{escaped} = \rho_o A_p \int_0^{x_{wave}} \left(1 - \frac{\rho}{\rho_o}\right) dx \quad (5.30)$$

With the quasi-ideal gas assumption, the density ratio is proportional to the pressure ratio. When the above equation is integrated:

$$M_{escaped} = \frac{\rho_o A_p}{B_A} \left[\frac{1}{3} \left(\frac{P_o}{P_{ESD}} \right)^2 (1 + B_A L_{ESD}) + \frac{2}{3} \left(\frac{P_{ESD}}{P_o} \right) (1 + B_A L_{ESD})^{-1/2} - 1 \right] \quad (5.31)$$

B_A has been defined in Equation (5.27). This assumes the ESD valve closes instantly the pressure ratio equals P_{ESD}/P_o . Equation (5.14) gives the mass flow from the release and it can be integrated to solve for the time t_{ESD} the pressure equals P_{ESD} .

$$\begin{aligned}
 M_{escaped} &= \int_0^{t_{ESP}} \dot{m}_e dt \\
 &= \frac{\dot{m}_{ei} \alpha \beta}{1 + \alpha} \left[(1 + \alpha) - \alpha \exp\left(\frac{-t_{ESD}}{\alpha^2 \beta}\right) - \exp\left(\frac{-t_{ESD}}{\beta}\right) \right]
 \end{aligned} \tag{5.32}$$

Using (5.31), the escaped mass, $M_{escaped}$, can be calculated with the known physical properties of the pipeline and valve setting for P_{ESD}/P_o . Note the α (5.21) and β (5.19) dependence on L_{eff} (5.24) for a given pressure ratio as defined by (5.26). These represent a closed set of equations that are solved iteratively.

When the pressure drops to $(P_{ESD}/P_o)_{set}$ the ESD valve triggers on LP and starts to close. The corresponding time t_{set} is solved for. The time at which the valve starts to close at the $(P_{ESD}/P_o)_{set}$ is t_{set} , and can be solved using an iterative numerical method using (5.32) and the known $M_{escaped}$ (5.31). Mass can no longer escape past the valve once it is defined as shut. The valve is defined as shut at one half of t_{close} and the ESD valve instantly closes.

$$t_{shut} = t_{set} + \frac{1}{2}t_{close} \tag{5.33}$$

Initially, when the release starts P_{ESD}/P_o is 1. P_{ESD}/P_o stays at one until the density wave arrives and the pressure starts to decrease, ($t_{arrival}$). Similar to the calculation for t_{set} , the arrival time of the density wave at the ESD valve can be determined by calculating the mass escaped for a pressure ratio of $P_{ESD}/P_o=1$, using (5.31), then solving for $t_{arrival}$, using (5.32). Note that $t_{arrival}$ is consistent with the inertia-less flow approach and is not the same as the travel time of the wave (L_{ESD}/c_o).

5.1.6 ESD Valve Closure on Pressure Rate of Change

Following the Wilson report's inertia-less approach of Appendix 2, the pressure in the pipe at any time and location is given by:

$$\frac{P(t)}{P_o} = \left(\frac{\dot{m}_{e,x}(t)}{\dot{m}_{ei}} \right) (1 + B_A x)^{1/2} \tag{5.34}$$

The change in pressure in time at a location is obtained by taking the derivative:

$$\frac{1}{P_o} \frac{dP_x}{dt} = (1 + B_A x)^{1/2} \frac{d}{dt} \left(\frac{\dot{m}_{e,x}(t)}{\dot{m}_{ei}} \right) \tag{5.35}$$

The derivative of the mass flow rate (5.14) is:

$$\frac{d}{dt} \left(\frac{\dot{m}_e}{\dot{m}_{ei}} \right) = \frac{-1}{1 + \alpha} \left[\frac{1}{\alpha^2 \beta} \exp\left(\frac{-t}{\alpha^2 \beta}\right) + \frac{\alpha}{\beta} \exp\left(\frac{-t}{\beta}\right) \right] \tag{5.36}$$

Combining these two equations, the dP/dt at the ESD valve is (note negative sign is removed as PROC is input as a positive, even though it is a drop in pressure with time):

$$\frac{dP_{ESD}}{dt} = (1 + B_A L_{ESD})^{1/2} \frac{P_o}{1 + \alpha} \left[\frac{1}{\alpha^2 \beta} \exp\left(\frac{-t_{arrival}}{\alpha^2 \beta}\right) + \frac{\alpha}{\beta} \exp\left(\frac{-t_{arrival}}{\beta}\right) \right] \quad (5.37)$$

Note that at time $t_{arrival}$ after the rupture the pressure ratio is P_{ESD}/P_o defined in the previous section. Thus, α and β are changing with the P_{ESD}/P_o at the ESD. To be conservative and consistent with the previous assumptions of the emissions model, the rupture is assumed to occur midway between the ESD valves.

PROC can be calculated using (5.37) and $t_{arrival}$ that was calculated in the previous section. PROC measurement techniques use a polling time and an integer number of polls (N_{poll}). To be conservative, the earliest time that PROC could trigger the closing of the valve is:

$$t_{PROC} = t_{arrival} + N_{poll} t_{poll} \quad (5.38)$$

Where ($N_{poll}=2$). This assumes that last polling time just missed the arrival of the density wave and change of pressure at the valve. Using (5.37), the PROC can be calculated at the time that the ESD valve closes as a result of the LP setting, $PROC_{trigger}$. The shut time for the ESD based upon PROC is determined if:

$$t_{shut} = \left(t_{PROC} + \frac{1}{2} t_{close} \right) \Big|_{\text{where } (t_{PROC} < t_{ESD}) \text{ and } (PROC > PROC_{trigger})} \quad (5.39)$$

The two equations for $M_{escaped}$, (5.31) and (5.32), can be equated to create a complex function f that provides the variation of P/P_o with time. This function must be solved numerically, and can be used to determine the P/P_o at t_{shut} as determined by the larger of (5.33) or (5.39), P/P_{o_calc} .

5.1.7 ESD Valve Closed Manually or Remotely

The time for manual or remote closure is from the initial release and includes the detection, notification, travel and field verification time. The maximum is the longest reasonable time to arrive at a remote site and to close the valve. After 6 hours (360 minutes) the dispersion of the release is in equilibrium and the predicted concentrations will not change for the modelled stability class and wind speed. Ignition times of less than the maximum exposure time of 3 hours (180 minutes) are required reduce the hazard zones.

The same set of equations, (5.31) and (5.32), may be solved P/P_{o_manual} at the time the valve is closed manually, t_{manual} . The valve will be closed manually if the pressure ratio ($P/P_{o_calc} < P/P_{o_manual}$) or if the time ($\max(t_{shut} (5.33) \text{ or } t_{shut} (5.39)) > t_{manual}$). Note that α and β depend on L_{eff} (5.24) which depends on P_{ESD}/P_o (5.26). This is an iterative solution to determine the unique time and pressure ratio pair for the release exit area and spacing between ESD valves.

5.1.8 *Effective Release Duration and Effective Steady Mass Release Rate*

Both the effective release duration and effective steady mass release rate are sensitive to the pipeline mitigation settings that control the ESD valves. For each hole size ratio, the LP, PROC and MANUAL valve closure times and pressure ratios are found. The maximum pressure ratio corresponds to the minimum valve closure time. The maximum pressure ratio is used to calculate the effective length using (5.26) in (5.24). The release continues after the ESD valve has closed so the effective duration should not be confused with the valve closure time.

For the hazard analysis of pipelines, a steady, constant mass release rate over a release duration is input to the dispersion model. Then the concentration predictions are scaled (as described in Section 7.2) to determine the time varying concentration exposure. From Appendix 2 (Chapter 4), the effective release duration is the sum of the two-time constants used in the double exponential blowdown equation:

$$t_{eff} = TSD_{\infty} = \beta + \alpha^2 \beta \quad (5.40)$$

This accounts for all the mass that is released if the blowdown continues to infinity in time. The source duration in AERSLAB, TSD is set to this, unless the release is ignited or the flow is stopped to reduce the duration, as discussed in the next sections. Releases from both the upstream and downstream direction have the same time constants, since a mid-point release is used. The total mass (kg) released from one direction is:

$$M_i = \rho_l A_p L_{eff} \quad (5.41)$$

The total mass released for both directions is twice the above. The effective mass release rate (kg/s) is the total mass released over the effective time:

$$\dot{m}_{eff} = 2 \frac{M_i}{TSD_{\infty}} \quad (5.42)$$

The factor of two accounts for the equal jets from each direction. However, for small hole size fractions, TSD_{∞} can be very large so \dot{m}_{eff} is less than the average flow rate that occurs until ignition occurs or the flow is stopped.

5.1.9 *Effect of Ignition or Stoppage of Flow on Duration and Rate*

The time until ignition or the flow is stopped $t_{ignition}$ (s) reduces the amount of gas that escapes:

$$M_{unignited} = \int_0^{t_{ignition}} \dot{m}_e dt \quad (5.43)$$

$$\frac{M_{unignited}}{M_i} = \frac{1}{1+\alpha} \left[(1+\alpha) - \alpha \exp\left(\frac{-t_{ignition}}{\alpha^2 \beta}\right) - \exp\left(\frac{-t_{ignition}}{\beta}\right) \right]$$

This is the fraction of mass that is released un-ignited. Note that the final α and β for the blowdown depend on the valve settings as described in the previous section. The exponential blowdown constants are set as if the release will continue to infinity in time. To account for the reduced release duration due to ignition, the effective release duration TSD_{∞} is reduced:

$$TSD_{ignition} = TSD_{\infty} \left(\frac{M_{unignited}}{M_i} \right) \quad (5.44)$$

The average steady mass release rate is based on $t_{ignition}$:

$$\dot{m}_{avg} = 2 \frac{M_{unignited}}{t_{ignition}} \quad (5.45)$$

For full ruptures of the pipeline, all the mass is released before ignition occurs and the effective release rate and duration are unchanged. For leaks, the effective release duration can be several days with only a small portion released within the default ignition time of 6 hours.

5.1.10 **Modelled Steady Mass Release Rate and Duration**

The modelled release duration TSD (s) is the minimum of:

$$TSD = \min(TSD_{ignition}, t_{ignition}) \quad (5.46)$$

The modelled steady mass release rate \dot{m}_E , (kg/s) is the maximum of:

$$\dot{m}_E = \max(\dot{m}_{eff}, \dot{m}_{avg}) \quad (5.47)$$

5.1.11 **Actual Volume of H₂S Released**

The AER has traditionally used the volume of H₂S to characterize sour gas releases. It depends on the density of the released gas with the expected gas composition, at reference conditions, assuming ideal gas behavior ($Z=1$).

$$\rho_{REF,E} = 1000 \frac{P_{REF}}{R_{S,E} T_{REF}} \quad (5.48)$$

The initial H₂S volume (m³ of H₂S at T_{REF} and P_{REF}) in a pipeline segment at expected maximum operating pressure (gauge plus atmospheric pressure), expected gas composition and expected minimum operating temperature is:

$$H_2S_{VOL,initial} = \frac{\rho_l A_p S_{ESD} w_{H_2S,E}}{\rho_{REF,E}} \quad (5.49)$$

The actual volume released (m³ of H₂S at T_{REF} and P_{REF}), accounting for the gas that flows by the ESD valves before they close is:

$$H_2S_{VOL,actual} = H_2S_{VOL,initial} \left(1 + \frac{L_{extra}}{L_{ESD}} \right) \quad (5.50)$$

The actual amount of H₂S released will be sensitive to when the ESD valve closes. The predicted hazard zones will depend on the H₂S concentration in the pipeline, the release rate and duration which determines the actual volume of H₂S released.

5.1.12 Gas Gathering System Equivalent Pipeline Lengths

The formulae for the gas pipeline gathering system equivalent length calculations are listed below. The BATCH page contains the Gas Gathering System - Pipeline Networking analysis feature.

ERCBH2S determined the mass of H₂S in each pipeline segment (determined using ideal gas properties and based on licensed maximums) and summed the total mass released based on whether the upstream and downstream nodes are Emergency Shut Down (ESD) valves or Check Valves (CV). This simplification ignored compressibility effects, and implicitly assumed the compressibility is the same for each segment.

AERH2S determines the volume of H₂S in each pipeline segment (determined using ideal gas properties and based on licensed maximums) normalized to reference conditions using a GVF (gas volume fraction) calculation. The results are identical to ERCBH2S and is based upon the same assumptions.

The volume and length of a pipeline segment are related by:

$$V_p = L_p \frac{\pi}{4} (D_o - 2t)^2 \quad (5.51)$$

Where:

V_p pipe segment volume, m³

L_p length of pipe segment, m

D_o outside diameter of pipe, m

t pipe wall thickness, m

The Gas Volume Factor, GVF_i , term is defined as:

$$GVF_i = \frac{\rho}{\rho_{ref}} = \frac{(P_i + P_{ref}) (T_{ref} + 273.15)}{P_{ref} (T_i + 273.15)} \quad (5.52)$$

Where:

GVF_i Gas volume fraction relative to reference conditions, unitless

P_i licensed maximum operating pressure of the pipeline segment, kPa (gauge)

T_i minimum temperature of pipeline segment, 5°C default

P_{ref} reference pressure, 101.325 kPa

T_{ref} reference temperature 15°C

The volume of H₂S initially in a segment is:

$$V_i = V_p GVF_i X_i \quad (5.53)$$

Where:

V_i H₂S volume of pipeline segment at reference conditions, m³

If we consider each pipeline segment having an upstream end and downstream end, then the Equivalent Segment Length between ESD valves is determined by the volume of the segment, plus all volume flow downstream into the upstream end of the segment, and all volume flow upstream into the downstream end of the segment:

$$S_{ESD} = \left(V_i + V_{du,i} + V_{ud,i} \right) \frac{L_p}{V_p} \quad (5.54)$$

Where:

S_{ESD} equivalent segment length between ESD valves, m

$V_{du,i}$ volume flowing downstream into upstream end of segment i , m³

$V_{ud,i}$ volume flowing upstream into the downstream end of segment i , m³

Note that L_p/V_p is A_p . If L_p has an ESD at each end ($V_{du,i}$ and $V_{ud,i}$ are 0), and $S_{ESD}=L_p$.

The Equivalent Cumulative Pipeline Volume between ESD valves is:

$$V_{ESD} = S_{ESD} A_p \quad (5.55)$$

Where:

V_{ESD} equivalent cumulative pipeline volume between ESD valves, m³

The volume flowing downstream into the upstream end of the segment is calculated by:

$$V_{du,i} = \begin{cases} = 0 & | \text{TYPE}_{u,i} = ESD \\ = \sum_{j=1}^{N \text{ Segments}} V_{uu,j} \{ \{ N_{u,j} = N_{u,i}; i \neq j \} \} + \sum_{j=1}^{N \text{ Segments}} V_{dd,j} \{ \{ N_{d,j} = N_{u,i}; i \neq j \} \} \end{cases} \quad (5.56)$$

Where:

$V_{dd,j}$ volume of H₂S flowing downstream into downstream node of segment j for all connections to that node, m³

$V_{uu,j}$ volume of H₂S flowing upstream into the upstream node of segment j for all connections to that node, m³

V_i volume of current segment must be removed because the previous summation would include the current segment, excluding if the current segment upstream node is a CV

The down flow out of the segment at the downstream node is calculated by:

$$V_{dd,i} = V_{du,i} + V_i \quad (5.57)$$

Where:

$V_{dd,i}$ total volume of H₂S flowing downstream at the downstream end of segment i, m³

The back-flow into segment i at the downstream end is calculated by:

$$V_{ud,i} = \begin{cases} = 0 & | \text{TYPE}_{d,i} = ESD \text{ or } \text{TYPE}_{d,i} = CV \\ = \sum_{j=1}^{N \text{ Segments}} V_{dd,j} \{ \{ N_{d,j} = N_{d,i}; i \neq j \} \} + \sum_{j=1}^{N \text{ Segments}} V_{uu,j} \{ \{ N_{u,j} = N_{d,i}; i \neq j \} \} \end{cases} \quad (5.58)$$

Where:

$V_{dd,j}$ volume of H₂S flowing downstream in the downstream end of segment j from all connects to that node, m³

$V_{ud,j}$ volume of H₂S back-flowing into the downstream end of segment i, m³

The backflow into segment i at the upstream end is calculated by:

$$V_{uu,i} = V_{ud,i} + V_i \tag{5.59}$$

Where:

$V_{uu,i}$ total volume of H₂S back-flowing upstream at upstream end of segment i , m³

The formulae are expressed using variables and are readily converted spreadsheet cell/columns/rows. This can be readily implemented in a spreadsheet using 17-Columns of data as documented below (using row 10 as example and generic column names). Row 10 on the BATCH page contains the formulae implemented for Pipeline Networks and can be copied rather than typing the formulae.

Generic Column	Equation	Variable	Excel Formula
A	–	D _{po}	user entry, pipe outside diameter, mm
B	–	t	user entry, pipe wall thickness, mm
C	–	P	user entry, maximum licensed pipeline pressure, kPa
D	–	X _{H2S}	user entry, maximum licensed H ₂ S concentration, %
E	–	T	user entry, pipeline temperature, °C
AA	–	N _u	user entry, upstream node name
AB	–	N _d	user entry, downstream node name
AC	–	TYPE _u	user entry, upstream node type (ESD, CV or other)
AD	–	TYPE _d	user entry, downstream node type (ESD, CV or other)
AE	–	L _p	user entry, pipe segment length
AF	(5.51)	V _p	=AE10*PI()*0.25*((A10-2*B10)*0.001)^2
AG	(5.52)	GVF	=(C10+101.325)/(101.325)*(273.15+E10)/(273.15+15)
AH	(5.53)	V _{H2S}	=AF10*AG10*D10
AI	(5.54)	S _{ESD}	=(AH10+AJ10+AL10)*AE10/AF10
AJ	(5.56)	V _{du}	=IF(AC10="ESD",0,SUMIFS(\$AL\$1:\$AL9,\$AB\$1:\$AB9,AA10)+SUMIFS(\$AL11:\$AL\$1048576,\$AB11:\$AB\$1048576,AA10)+SUMIFS(\$AN\$1:\$AN9,\$AA\$1:\$AA9,DE10)+SUMIFS(\$AN11:\$AN\$1048576,\$AA11:\$AA\$1048576,AA10))
AK	(5.57)	V _{dd}	=AH10+AK10
AL	(5.58)	V _{ud}	=IF(OR(AD10="CV",AD10="ESD"),0,SUMIFS(\$AL\$1:\$AL9,\$AB\$1:\$AB9,AB10)+SUMIFS(\$AL11:\$AL\$1048576,\$AB11:\$AB\$1048576,AB10)+SUMIFS(\$AN\$1:\$AN9,\$AA\$1:\$AA9,AB10)+SUMIFS(\$AN11:\$AN\$1048576,\$AA11:\$AA\$1048576,AB10))
AM	(5.59)	V _{uu}	=AH10+AL10

5.1.13 Gas Pipeline Licensed H2S Volume

The licensed H₂S volume (m³ of H₂S at T_{REF} and P_{REF}) in a gas pipeline segment at licensed maximum operating pressure and H₂S concentration is:

$$H_2S_{VOL,licensed} = GVF \cdot A_p S_{ESD} w_{H_2S,L} \quad (5.60)$$

The licensed H₂S volume between ESD valves (assuming the valves close instantaneously) was previously used by the ERCB for determining the EPZ from a nomograph. It is also currently used to determine the level classification of the pipeline for determining the land use setbacks. The licensed H₂S volume corresponding to Level designations are given in *Directive 056*. ERCBH₂S and AERH₂S account for the gas released until the valves close and the pipeline drains to determine the EPZ.

The equivalent segment length between ESD valves (S_{ESD}), was calculated in the previous section. The licensed H₂S concentration (mol fraction) is $w_{H_2S,L}$.

The Gas Volume Factor GVF (m³/m³) is the ratio of released gas volume at standard conditions to the volume at the licensed MOP and the lowest expected temperature TL (the default is the ground temperature), as given below:

$$GVF = \frac{\rho_{LIC}}{\rho_{ref}} \quad (5.61)$$

The density includes real gas effects such as the compressibility factor. The licensed volume of H₂S between ESD valves in oil effluent pipelines with gas to liquid ratio (GLR) greater than 1000 for the setback determination are based on the equations above. The gas fraction (GF) is now assumed to be 1.0 for gas pipelines in AERH₂S. ERCBH₂S estimated the fraction of the pipe occupied by gas in oil effluent pipelines and it was greater than 0.95 for high GLR and typical licensed pressures. AERH₂S will predict slightly higher volumes than ERCBH₂S.

Note that for these pipelines the EPZ is based on gas pipeline hazard zone modelling described in this section. The liquids are ignored in the modelling of the jet release as they have less mass than the gas and are assumed to fallout.

5.2 Gas Well

The GAS WELL page performs the release calculations for a well blowout that typically result in a release that exits at sonic conditions. The steady release rate and duration are defined directly by user inputs described in Section 2.4.

5.2.1 *Steady Mass Release Rate*

In ERCBH2S the user entered the hydrogen sulphide release rate H_2S_{RR} (Rm^3/s) and expected maximum hydrogen sulphide concentration $EH2S\%$ (%) to calculate the Absolute Open Flow Rate (AOF , $10^3\text{Rm}^3/\text{d}$). However, the user calculates the H_2S_{RR} from the AOF and $EH2S\%$ and occasionally users adjusted the H_2S_{RR} and $EH2S\%$ independently from the AOF for input to the model. This resulted in unbelievable values of the AOF for the well. In AERH2S the user now enters the AOF and the $EH2S\%$ to calculate the H_2S_{RR} .

The H_2S release rate input for sour wells is based on *Directive 056* requirements. To properly assess the sub-surface release conditions requires detailed well-bore inflow modelling that is beyond the scope of AERH2S. The *H_2S Release Rate Assessment and Audit Forms* (CAPP, 2012) referenced in *Directive 056*, provides the methods to assess the maximum AOF and maximum $EH2S\%$ for each zone to determine the H_2S release rate.

For releases from multiple zones such as during drilling through open zones or commingled production, the cumulative gas release rate and the flow weighted average H_2S concentration must be input. The MULTIZONE page determines the required inputs.

The steady mass release rate (kg/s) is defined by:

$$\dot{m}_E = \rho_{REF} \frac{H_2S_{RR}}{m_{H_2S,E} (1 - w_{H_2O,E})} \quad (5.62)$$

where $m_{H_2S,E}$ ($=EH2S\%/100$), $w_{H_2O,E}$ is molar fraction of H_2O , and ρ_{REF} is the reference density (kg/m^3) of the release was given earlier in Equation (5.48).

The exit area A_E (m^2) depends on the tubing or casing internal diameter D (mm) entered and is:

$$A_E = \frac{\pi}{4} \left(\frac{D}{1000} \right)^2 \quad (5.63)$$

The mass flux at the exit \dot{m}_E/A_E (kg/s/m^2) is an important input to AERFLASH. It is calculated from the ratio of equations (5.62) and (5.63).

5.2.2 *Initial and Exit Conditions*

Initial conditions for a well release are at the wellhead, just upstream of the exit. The initial pressure P_O is estimated from the calculated \dot{m}_E/A_E and sour gas properties.

The wellhead stagnation temperature T_O includes the static temperature and the temperature rise due to kinetic energy, if the flow was stopped. As the release rises from the reservoir it will cool due to expansion and transfer heat through the well-bore. Typical Alberta reservoir and ground temperatures are

80 and 5 °C, respectively. The calculated wellhead stagnation temperature during a blowout is typically less than ground temperature due to the cooling as the pressure drops. It is independent of the ambient conditions but strongly dependent on the flow rate.

The default wellhead stagnation temperature is the ground temperature of 5 °C.

Gas Well Stagnation Temperature T_I	Default Ground temperature of 5°C	°C
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The stagnation temperature T_o is converted to absolute units (K) for input as the initial temperature in K:

$$T_o = T_I + 273.15 \quad (5.64)$$

In the following equations, a subscript g stands for the initial ideal gas solution which is used as a guess of the value to be solved for in the AERFLASH program using real fluid behaviour. The temperature at the exit plane (K), assuming ideal gas choked flow is:

$$T_{Eg} = T_o \left(\frac{2}{k_I + 1} \right) T_E \quad (5.65)$$

The pressure at the exit plane (kPa), assuming ideal gas choked flow is:

$$P_{Eg} = \frac{1}{1000} \frac{\dot{m}_E}{A_E} \left(\frac{Z_E R_S T_{Eg}}{k_I} \right)^{\frac{1}{2}} \quad (5.66)$$

The average mass flux at the exit \dot{m}_E / A_E is calculated from the initial conditions, as described in the next section. The compressibility factor Z_E , is a function of the exit pressure but is set to 1.0 for an ideal gas.

The initial upstream source pressure (kPa), assuming ideal gas choked flow is:

$$P_{og} = P_{Eg} \left(\frac{k_I + 1}{2} \right)^{\frac{k_I}{k_I - 1}} \quad (5.67)$$

The ratio of specific heats k_I , is not constant for a real gas. The ideal gas values of P_{og} , P_{Eg} and T_{Eg} are the first guesses in the iterative solution performed by the real fluids program AERFLASH (see Appendix 1). If the flow is not choked, the sonic velocity c_E is replaced by the exit V_E .

AERFLASH solves for the initial pressure and exit conditions by guessing until the flow, energy and entropy conditions are satisfied. The mass flux at the exit \dot{m}_E / A_E is calculated from user inputs. The initial entropy and enthalpy upstream of the exit depends on the guessed upstream pressure and user specified temperature. The program determines the exit pressure under isentropic expansion from the

initial pressure such that the total energy at the exit under critical, choked flow conditions is equal to the initial enthalpy h_o (J/kg or m^2/s^2):

$$h_o = h_E + \frac{c_E^2}{2} \tag{5.68}$$

Then AERFLASH checks if the critical mass flux at the exit pressure that satisfies the above conditions is equal to the specified mass flux ($kg/(s \cdot m^2)$):

$$\frac{\dot{m}_E}{A_E} = c_E \rho_E \tag{5.69}$$

It then updates the guessed initial pressure with an isentropic compression up to the initial temperature and repeats the calculations until the critical mass flux equals the user-specified mass flux. If the flow is not choked, the sonic velocity c_E is replaced by the exit V_E .

5.2.3 Release Duration before Ignition or Stop Flow

The duration of the release before ignition or the flow is stopped is a source mitigation variable that has a default value, or the user can input an alternate value. Early ignition of the H₂S release converts it to an SO₂ release and will reduce the size of the H₂S hazard distances. The range of acceptable values and the default inputs are:

Table 5-2: Gas Well Mitigation Range of Settings and Default Settings

Source Mitigation Parameter	With Mitigation	No Mitigation
Is Surface Controlled Sub Surface Safety Valve Installed?	For Producing wells with SCSSSV 3 minutes	360 minutes
Time from initial release till ignition or stop flow, TSD	For manned Drilling and Servicing 15 to 360 minutes For Manned Producing (onsite) 10 to 360 minutes For un-manned Producing 60 to 360 minutes	360 minutes

For manned operations, the minimum of 15 minutes is based on simulations and represents the shortest time to evacuate and safely ignite a release for typical crews with allowances for problems (extreme weather, man-down, etc.). For manned production operations onsite, where protocols are well established

and the site is well organized, the minimum time is 10 minutes. For un-manned operations, the minimum of 60 minutes is from the initial release and includes the detection, notification, travel and field verification time. For producing wells with a Surface Controlled Sub-Surface Safety Valve (SCSSSV) a short release duration of 3 minutes is used.

The maximum is the longest reasonable time to arrive at a remote well site and to ignite the release. After 6 hours (360 minutes) the dispersion of the release is in equilibrium and the predicted concentrations will not change for the modelled stability class and wind speed. Ignition times of less than the maximum exposure time of 180 minutes are required reduce the hazard zones.

5.2.4 Gas Well Licensed H₂S Release Rate

The licensed H₂S release rate (m³/s of H₂S at T_{REF} and P_{REF}) from a gas well is based on the *H₂S Release Rate Assessment and Audit Forms* (CAPP, 2012) referenced in *Directive 056*. provides the methods to assess the maximum AOF and maximum EH₂S% to determine the H₂S release rate for each phase of operation are provided.

The licensed H₂S release rate was previously used by the ERCB for determining the EPZ from a simplified power law equation. ERCBH₂S and AERH₂S account for the gas released until the release is ignited or the valves are closed to determine the EPZ.

The licensed H₂S release rate is also used to determine the level classification of the well for determining the land use setbacks during producing, injecting or suspended phases of operation. The licensed H₂S release rate corresponding to Level designations are given in *Directive 056*.

AERH₂S uses the AOF and maximum EH₂S% for emergency response and planning zone calculations. It does not use the H₂S release rate.

5.3 Liquid Pipeline or Liquid Well

The LIQUID page performs the release calculations for sour liquid pipelines or wells. The steady release rate and duration are defined directly by user inputs described in Section 2.5. A liquid pool source model is now used to model the dispersion of H₂S in AERH₂S rather than a ground level jet source that was used in ERCBH₂S.

5.3.1 Steady Mass Release Rate

The Gas to Liquid Ratio (*GLR*) must be less than or equal to 1000 for the release to be modelled as a liquid.

$$GLR = \frac{\text{standard m}^3 \text{ Gas}}{\text{stock tank m}^3 \text{ Liquid}} \quad (5.70)$$

Note that the *GLR* is at reference conditions of 15 °C and 101.325 kPa. When the $GLR \leq 1000$, the mass flow rate of liquids is approximately greater than the mass flow rate of gas, as given by:

$$\frac{\text{mass Gas (kg)}}{\text{mass Liquid (kg)}} = GLR \left(\frac{\text{m}^3_{\text{gas}}}{\text{m}^3_{\text{liquid}}} \right) \frac{WMS_E \left(\frac{\text{kg}}{\text{kmol}} \right)}{\rho_{\text{liquid}} \left(\frac{\text{kg}}{\text{m}^3} \right)} \left(\frac{1}{23.645 \left(\frac{\text{m}^3}{\text{kmol}} \right)} \right) \quad (5.71)$$

In ERCBH2S the liquid well hydrogen sulphide release rate H_2S_{RR} (m³/s) was directly entered by the user. For the pool source model now used for liquid wells and liquid pipelines in AERH2S, the hydrogen sulphide release rate H_2S_{RR} (m³/s) is calculated from the user inputs of Q_{LIQUID} (m³/d of oil and water at 15 °C and 101.325 kPa), the *GLR* (m³ gas/m³ liquid) and the maximum expected *EH2S%*:

$$H_2S_{RR} = \frac{Q_{LIQUID} GLR (EH2S\%/100)}{24 \cdot 3600} \quad (5.72)$$

H_2S_{RR} was an important factor in historical hazard zone air dispersion modelling using mass release models. Contemporary hazard models use the total flow (AOF) and gas composition to determine the exit conditions, thermodynamics and dispersion. The *H₂S Release Rate Assessment and Audit Forms* (CAPP, 2012) provides the methods to assess the AOF and *EH2S%* for wells. Note that the maximum expected *H₂S* concentration and gas flow rate is used for the zone(s) the gas is flowing from. For releases from multiple zones such as during drilling through open zones or commingled production, the cumulative gas release rate and the flow weighted average *H₂S* concentration must be input. The MULTIZONE page determines the required inputs.

The steady mass release rate (kg/s) of the solution gas is then given by Equation (5.73) for wells, repeated below:

$$\dot{m}_E = \rho_{REF} \frac{H_2S_{RR}}{m_{H_2S,E} (1 - w_{H_2O,E})} \quad (5.73)$$

where $m_{H_2S,E}$ (= *EH2S%*/100) and $w_{H_2O,E}$ and the reference density (kg/m³) of the release was given earlier in Equation (5.48).

The exit area A_E (m²) depends on the pipe outside diameter D_o (mm) and wall thickness t (mm) entered and is:

$$A_E = \frac{\pi}{4} \left(\frac{D_o - 2t}{1000} \right)^2 \quad (5.74)$$

The mass flux at the exit \dot{m}_E/A_E (kg/s/m²) is calculated from the above equations and is an important input to AERFLASH. The H_2S_{RR} corresponding to Level designations are given in Directive 056.

5.3.2 Initial and Exit Conditions

The initial temperature input is:

Expected Minimum Liquid Temperature	Range	Default
T_o (°C)	0 to 200	5

The model uses the stagnation temperature and since the velocity of flow in a pipeline is low, the kinetic energy can be ignored, and the stagnation temperature equals the static temperature. A stagnation temperature of 5 °C, a typical Alberta ground temperature at pipeline depths, is the default. This conservatively assumes the liquid in the pipeline has cooled to the ground temperature before a release. At ground temperature and typical licensed operating pressures, the release is usually lighter than air at ambient conditions. At higher operating temperatures the release is more buoyant. The initial temperature T_I is converted to absolute units (K):

$$T_o = T_I + 273.15 \quad (5.75)$$

The following equations are the same as for Gas Wells. A subscript g stands for the initial ideal gas solution which is used as a guess of the value to be solved for in the AERFLASH program using real fluid behaviour. The temperature at the exit plane (K), assuming ideal gas choked flow is:

$$T_{Eg} = T_o \left(\frac{2}{k_I + 1} \right) \quad (5.76)$$

The pressure at the exit plane (kPa), assuming ideal gas choked flow is:

$$P_{Eg} = \frac{1}{1000} \frac{\dot{m}_E}{A_E} \left(\frac{Z_E R_S T_{Eg}}{k_I} \right)^{\frac{1}{2}} \quad (5.77)$$

The compressibility factor Z_E , is a function of the exit pressure but is set to 1.0 for an ideal gas. The initial upstream source pressure (kPa), assuming ideal gas choked flow is:

$$P_{og} = P_{Eg} \left(\frac{k_I + 1}{2} \right)^{\frac{k_I}{k_I - 1}} \quad (5.78)$$

The ratio of specific heats k_i , is not constant for a real gas. The ideal gas values of P_{0g} , P_{Eg} and T_{Eg} are the first guesses in the iterative solution performed by the real fluids program AERFLASH (see Appendix 1). For liquid releases, the initial pressure P_O is often near atmospheric pressure so choked flow conditions may not exist.

AERFLASH solves for the initial pressure and exit conditions by guessing until the flow, energy and entropy conditions are satisfied. The mass flux at the exit \dot{m}_E/A_E is calculated from user inputs. The initial entropy and enthalpy upstream of the exit depends on the guessed upstream pressure and user specified temperature. The program determines the exit pressure under isentropic expansion from the initial pressure such that the total energy at the exit under critical, choked flow conditions is equal to the initial enthalpy h_o (J/kg or m^2/s^2):

$$h_o = h_E + \frac{1}{2} c_E^2 \quad (5.79)$$

Then it checks if the critical mass flux at the exit pressure that satisfies the above conditions is equal to the specified mass flux ($kg/(s \cdot m^2)$):

$$\frac{\dot{m}_E}{A_E} = c_E \rho_E \quad (5.80)$$

It then updates the guessed initial pressure with an isentropic compression up to the initial temperature and repeats the calculations until the critical mass flux equals the user-specified mass flux. If the flow is not choked, the sonic velocity c_E is replaced by the exit V_E .

Note in the liquid hazard zone pool modelling, the momentum of the liquids is ignored as the liquids pool on the ground. The gas that comes out of solution flashes from the liquid pool surface. The area of the pool is selected so the vapour velocity leaving the pool is the same as the liquid velocity in the pipe.

For liquid wells and liquid pipelines C_D is set so the velocity of the vapour leaving the pool $V_R (=V_{vap})$ is the same as the velocity of the liquid within the piping before the liquid enters the pool $V_Q (=V_{liq}$ in pipe). Based on the guessed density at the exit, the guessed vapour flow rate can be calculated.

$$\rho_{Eg} = 1000 \frac{P_{Eg}}{R_s T_{Eg}}$$

$$Q_{Eg} = \frac{\dot{m}_E}{\rho_{Eg}}$$

The superficial velocity at the exit of the vapour and liquid can then be determined at actual operating conditions:

$$V_{Eg} = \frac{Q_{Eg}}{A_E}$$

$$V_{Liquid} = \frac{Q_{Liquid}}{A_E}$$

These velocities are used to estimate the required drag coefficient in the Drag Zone.

5.3.3 Release Duration before Shut-In or Ignition

The duration of the release before stopping the flow or ignition is a source mitigation variable that has a default value, or the user can input an alternate value. Stopping the flow by shutting valves and/or turning off pumps will reduce the size of the H₂S hazard distances. The range of acceptable values and the default inputs are:

Table 5-3: Liquid Well or Liquid Pipeline Mitigation Range of Values and Default Settings

Source Mitigation Parameter	With Mitigation	No Mitigation
Are Automated Safety Valves Installed?	<p>For Producing wells with SCSSSV 3 minutes</p> <p>For Pipelines with ESD valves 0.25 minute</p>	360 minutes
Time from initial release till manually stop flow (valves closed) or ignition, TSD	<p>For manned Drilling and Servicing Wells 10 to 360 minutes</p> <p>For un-manned Producing Wells and Pipelines 60 to 360 minutes</p>	360 minutes

For un-manned operations, the minimum of 60 minutes is from the initial release and includes the detection, notification, travel and field verification time. For producing wells with a Surface Controlled Sub-Surface Safety Valve (SCSSSV) a short release duration of 3 minutes is used.

The maximum is the longest reasonable time to arrive at a remote well site and to ignite the release. After 6 hours (360 minutes) the dispersion of the release is in equilibrium and the predicted concentrations will not change for the modelled stability class and wind speed. Ignition times of less than the maximum exposure time of 180 minutes are required reduce the hazard zones.

5.3.4 Oil Well Licensed H₂S Release Rate

The licensed H₂S release rate (m³/s of H₂S at T_{REF} and P_{REF}) from a liquid well is based on the *H₂S Release Rate Assessment and Audit Forms* (CAPP, 2012) referenced in *Directive 056*. provides the methods to assess the maximum AOF and maximum EH₂S% to determine the H₂S release rate for each phase of operation are provided.

The licensed H₂S release rate was previously used by the ERCB for determining the EPZ from a simplified power law equation. ERCBH₂S and AERH₂S account for the gas released until the release is ignited or the valves are closed to determine the EPZ.

The licensed H₂S release rate is also used to determine the level classification of sour oil wells for determining the land use setbacks during producing, injecting or suspended phases of operation. The licensed H₂S release rate corresponding to Level designations are given in *Directive 056*.

5.3.5 Liquid Gathering System Equivalent Pipeline Lengths

The formulae for the pipeline gathering system equivalent length calculations are listed below. The BATCH page contains the Liquid Gathering System - Pipeline Networking analysis feature. It determines the mass of H₂S mass in each pipeline segment (determined using ideal gas properties and based on the gas to liquid ratio) and sums the total mass released based on whether the upstream and downstream nodes are Emergency Shut Down (ESD) valves or Check Valves (CV). This simplification ignores compressibility effects, but implicitly assumes the compressibility is the same for each segment.

The volume and length of a pipeline segment are related by:

$$V_p = L_p \frac{\pi}{4} (D_o - 2t)^2 \quad (5.81)$$

Where:

V_p pipe segment volume, m³

L_p length of pipe segment, m

D_o outside diameter of pipe, m

t pipe wall thickness, m

The volume of H₂S initially in the segment is:

$$V_i = V_p GVF_i GF X_i \quad (5.82)$$

Where:

V_i H₂S volume of pipeline segment at reference conditions, m³

The Gas Volume Factor GVF (m³/m³) is the ratio of released gas volume at standard conditions to the volume at MOP and the user input for lower temperature limit, TL , for the pipeline segment, as given below:

$$GVF_i = \frac{\rho}{\rho_{ref}} = \frac{(P_i + P_{ref}) (T_{ref} + 273.15)}{P_{ref} (T_i + 273.15)} \quad (5.83)$$

Where:

GVF_i Gas volume fraction relative to reference conditions, unitless

P_i licensed maximum operating pressure of the pipeline segment, kPa (gauge)

T_i minimum temperature of pipeline segment, 5°C default

P_{ref} reference pressure, 101.325 kPa

T_{ref} reference temperature 15°C

The simplified gas fraction, GF , for oil effluent pipelines (from Directive 026) is calculated using the Gas to Liquid Ratio, GLR :

$$GF = \frac{GLR}{GLR + GVF} \quad (5.84)$$

The licensed maximum concentration of H₂S in the segment is X_{H2S} .

If we consider each pipeline segment having an upstream end and downstream end, then the Equivalent Segment Length between ESD valves is determined by the volume of the segment, plus all volume flow downstream into the upstream end of the segment, and all volume flow upstream into the downstream end of the segment:

$$S_{ESD} = (V_i + V_{du,i} + V_{ud,i}) \frac{L_p}{V_p} \quad (5.85)$$

Where:

S_{ESD} equivalent segment length between ESD valves, m

$V_{du,i}$ volume flowing downstream into upstream end of segment i , m³

$V_{ud,i}$ volume flowing upstream into the downstream end of segment i , m³

Note that L_p/V_p is A_p . If L_p has an ESD at each end ($V_{du,i}$ and $V_{ud,i}$ are 0), and $S_{ESD}=L_p$.

The Equivalent Cumulative Pipeline Volume between ESD valves is:

$$V_{ESD} = S_{ESD} A_p \quad (5.86)$$

Where:

V_{ESD} equivalent cumulative pipeline volume between ESD valves, m³

The volume flowing downstream into the upstream end of the segment is calculated by:

$$V_{du,i} = \begin{cases} = 0 & | \text{TYPE}_{u,i} = ESD \\ = \sum_{j=1}^{N \text{ Segments}} V_{uu,j} \left\{ N_{u,j} = N_{u,i}; i \neq j \right\} + \sum_{j=1}^{N \text{ Segments}} V_{dd,j} \left\{ N_{d,j} = N_{u,i}; i \neq j \right\} \end{cases} \quad (5.87)$$

Where:

$V_{dd,j}$ volume of H₂S flowing downstream into upstream node of segment j for all connections to that node, m³

$V_{uu,j}$ volume of H₂S flowing upstream into the upstream node of segment j for all connections to that node, m³

V_i volume of current segment must be removed because the previous summation would include the current segment, excluding if the current segment upstream node is a CV

The down flow out of the segment at the downstream node is calculated by:

$$V_{dd,i} = V_{du,i} + V_i \quad (5.88)$$

Where:

$V_{dd,i}$ total volume of H₂S flowing downstream at the downstream end of segment i, m³

The backflow into segment i at the downstream end is calculated by:

$$V_{ud,i} = \begin{cases} = 0 & | \text{TYPE}_{d,i} = ESD \text{ or } \text{TYPE}_{d,i} = CV \\ = \sum_{j=1}^{N \text{ Segments}} V_{dd,j} \left\{ N_{d,j} = N_{d,i}; i \neq j \right\} + \sum_{j=1}^{N \text{ Segments}} V_{uu,j} \left\{ N_{u,j} = N_{d,i}; i \neq j \right\} \end{cases} \quad (5.89)$$

Where:

$V_{dd,j}$ volume of H₂S flowing downstream in the downstream end of segment j from all connects to that node, m³

$V_{ud,j}$ volume of H₂S back-flowing into the downstream end of segment i, m³

The backflow into segment i at the upstream end is calculated by:

$$V_{uu,i} = V_{ud,i} + V_i \tag{5.90}$$

Where:

$V_{uu,i}$ total volume of H₂S back-flowing upstream at upstream end of segment i , m³

The formulae are expressed using variables and are readily converted spreadsheet cell/columns/rows. This can be readily implemented in a spreadsheet using 17-Columns of data as documented below (using row 10 as example and generic column names). Row 10 on the BATCH page contains the formulae implemented for Liquid Gathering System Pipeline Networking and can be copied rather than typing the formulae.

Generic Column	Equation	Variable	Excel Formula
A	–	D _{po}	user entry, pipe outside diameter, mm
B	–	t	user entry, pipe wall thickness, mm
C	–	GLR	user entry, Gas to Liquid Ratio, GLR
D	–	X _{H2S}	user entry, maximum licensed H ₂ S concentration, %
E	–	T _L	user entry, pipeline lower limit temperature, °C
F	–	P _{MOP}	user entry, pipeline maximum licensed pressure, kPa gauge
AA	–	N _u	user entry, upstream node name
AB	–	N _d	user entry, downstream node name
AC	–	TYPE _u	user entry, upstream node type (ESD, CV or other)
AD	–	TYPE _d	user entry, downstream node type (ESD, CV or other)
AE	–	L _p	user entry, pipe segment length
AF	(5.81)	V _p	=AE10*PI()*0.25*((A10-2*B10)*0.001)^2
AG	(5.83)	GVF	=((F10+Pref)/Pref)*(Tref+273.15)/(TL+273.15))
AH	(5.84)	GF	=C10/(C10+AG10)
AI	(5.82)	V _{H2S}	=AF10*AG10*AH10*(D10*0.01)
AJ	(5.85)	S _{ESD}	=(AI10+AK10+AM10)/AI10*AE10
AK	(5.87)	V _{du}	=IF(AC10="ESD",0,SUMIFS(\$AL\$1:\$AL9,\$AB\$1:\$AB9,AA10)+SUMIFS(\$AL11:\$AL\$1048576,\$AB11:\$AB\$1048576,AA10)+SUMIFS(\$AN\$1:\$AN9,\$AA\$1:\$AA9,DE10)+SUMIFS(\$AN11:\$AN\$1048576,\$AA11:\$AA\$1048576,AA10))
AL	(5.88)	V _{dd}	=AI10+AK10
AM	(5.89)	V _{ud}	=IF(OR(AD10="CV",AD10="ESD"),0,SUMIFS(\$AL\$1:\$AL9,\$AB\$1:\$AB9,AB10)+SUMIFS(\$AL11:\$AL\$1048576,\$AB11:\$AB\$1048576,AB10)+SUMIFS(\$AN\$1:\$AN9,\$AA\$1:\$AA9,AB10)+SUMIFS(\$AN11:\$AN\$1048576,\$AA11:\$AA\$1048576,AB10))
AN	(5.90)	V _{uu}	=AI10+AM10

5.3.6 **ERCBH2S Oil Pipeline Licensed H2S Volume**

Setback volume calculations are only done for oil effluent pipelines with a gas to liquid ratio (GLR) less than or equal to 1000, not for other liquid pipelines. The licensed H₂S volume (m³ of H₂S at T_{REF} and P_{REF}) in an oil effluent pipeline segment is:

$$V_{H2S,LIC} = S_{ESD} A_p GVF GF X_{H2S} \quad (5.91)$$

ERCBH2S assumed all the gas was out of solution (as it is assumed that the liquid contains no gas), with the fraction of the pipe containing gas depending on the GLR and GVF.

The volume is used to determine the level classification of oil effluent pipelines for determining the land use setback. The licensed H₂S volume corresponding to Level designations are given in Directive 056.

The licensed H₂S volume between ESD valves (assuming the valves close instantaneously) was previously used by the ERCB for determining the EPZ from a nomograph. It is also currently used to determine the level classification of the pipeline for determining the land use setbacks. The licensed H₂S volume corresponding to Level designations are given in *Directive 056*. ERCBH2S and AERH2S account for the gas released until the valves close and the pipeline drains to determine the EPZ.

The Gas Volume Factor *GVF* (m³/m³) is the ratio of released gas volume at standard conditions to the volume at the licensed MOP and the lowest temperature TL (the default is the ground temperature) (m³/m³), as given below:

$$GVF = \frac{\rho_{LIC}}{\rho_{ref}} \quad (5.92)$$

The density includes real gas effects such as the compressibility factor.

The simplified gas fraction is calculated below for oil effluent pipelines (originally from Directive 026):

$$GF = \frac{GLR}{(GLR + GVF)} \quad (5.93)$$

The equivalent segment length between ESD valves (*S_{ESD}*), was calculated in the previous section. The licensed H₂S concentration (mol fraction) is $X_{H2S} = w_{H2S,L}$.

5.3.7 **AERH2S Oil Pipeline Licensed H2S Volume**

A modified approach using the ERCBH2S equations was used for AERH2S which is more realistic. As demonstrated by Behr (2003), as the pressure in the pipeline drops below the bubble point, gas will start coming out of solution as free gas phase while the rest of the gas remains captive in solution. First properties are determined that allow the bubble point, oil formation volume factor and then the total gas within the pipe segment the MOP can be estimated.

Vasquez & Beggs (1980) regressions are based upon correcting the gas gravity for a standard separator condition at 100 psig.

$$\gamma_{gs} = \gamma_{gp} \left[1 + (5.912 \times 10^{-5}) \text{API} \cdot T \log \left(\frac{p}{114.7} \right) \right] \quad (5.94)$$

Where

- γ_{gs} = gas gravity (air=1) that would result from separator conditions of 100 psig
- γ_{gp} = gas gravity obtained at separator conditions of p and T
- p = actual separator pressure, psia
- T = actual separator temperature, °F
- API = oil gravity, °API

Vasquez & Beggs (1980) dissolved gas ratio, R_s , is based upon dividing the oil gravity into two groups, above and below 30 °API. The regression is based on 5,008 measured data points, where $p=MOP$,

$$R_s = a_1 \gamma_{gs} p^{a_2} \exp \left(\frac{a_3 \text{API}}{T + 460} \right) \quad (5.95)$$

Where

	API ≤ 30	API >30
a_1	0.0362	0.0178
a_2	1.0937	1.1870
a_3	25.7240	23.9310

The gas bubble point can be computed by re-arrangement of the equation for dissolved solution gas at bubble point which is the $R_s=GOR$,

$$p_b = \left(\frac{GOR}{a_1 \gamma_{gs} \exp \left(\frac{a_3 \text{API}}{T + 460} \right)} \right)^{1/a_2} \quad (5.96)$$

Vasquez & Beggs (1980), the oil formation volume factor for saturated oil, $B_o(p < p_b)$ is a function correlated as a function of the dissolved gas,

$$B_o = 1 + a_1 R_s + (a_2 + a_3 R_s) (T - 60) \frac{\text{API}}{\gamma_{gs}} \quad (5.97)$$

Where

	API ≤ 30	API >30
a ₁	4.677×10 ⁻⁴	4.670×10 ⁻⁴
a ₂	1.751×10 ⁻⁵	1.100×10 ⁻⁵
a ₃	-1.811×10 ⁻⁸	1.337×10 ⁻⁹

5.3.8 AERH2S Salt Water Pipeline Licensed H2S Volume

Like the AERH2S Oil Pipelines, a modified approach using the ERCBH2S equations was used for AERH2S which is more realistic. As demonstrated by Behr (2003), as the pressure in the pipeline drops below the bubble point, gas will start coming out of solution as free gas phase while the rest of the gas remains captive in solution.

The Gas-Water ratio can be estimated using Ahmed (1989) based upon the salt content of the water.

$$R_{sw,H2O} = A + B p + C p^2 \quad (5.98)$$

Where

$$\begin{aligned} A &= 2.12 && +3.45 \times 10^{-3} T - 3.59 \times 10^{-5} T^2 \\ B &= 0.0107 && -5.25 \times 10^{-5} T + 1.48 \times 10^{-7} T^2 \\ C &= -8.75 \times 10^{-7} && +3.9 \times 10^{-9} T - 1.02 \times 10^{-11} T^2 \end{aligned}$$

In units of scf/bbl. The gas to water ratio is corrected for salinity,

$$\begin{aligned} R_{sw,brine} &= K R_{sw,H2O} \\ K &= 1 - (7.53 \times 10^{-2} - 1.73 \times 10^{-4} T) [\% \text{NACL}] \end{aligned} \quad (5.99)$$

With a ranges

$$\begin{aligned} 100 &< T < 250^\circ F \\ 1000 &< P < 5000 \text{ psi} \end{aligned}$$

The water formation volume factor is used to correct the volume of water for the dissolved gas (Ahmed 1989),

$$B_{ow,H2O} = A + B p + C p^2 \quad (5.100)$$

For pressures below the bubble pressure

$$\begin{aligned}
 A &= 0.9911 + 6.35 \times 10^{-5} T + 8.5 \times 10^{-7} T^2 \\
 B &= -1.093 \times 10^{-6} - 3.497 \times 10^{-9} T + 4.57 \times 10^{-12} T^2 \\
 C &= -5.0 \times 10^{-11} + 6.429 \times 10^{-13} T - 1.43 \times 10^{-15} T^2
 \end{aligned}$$

In units of bbl/bbl or m³/m³. The volume factor is corrected for salinity,

$$B_{o,brine} = K B_{o,H2O} \tag{5.101}$$

Where,

$$K = 1 + \left(A + B(T - 60) + C(T - 60)^2 \right) [\%NACL]$$

$$\begin{aligned}
 A &= 5.1 \times 10^{-8} P \\
 B &= 5.47 \times 10^{-6} - 1.95 \times 10^{-10} P \\
 C &= -3.23 \times 10^{-8} + 8.5 \times 10^{-13} P
 \end{aligned}$$

With a ranges

$$\begin{aligned}
 100 &< T < 250 \text{ } ^\circ F \\
 1000 &< P < 5000 \text{ } psi \\
 0 &\leq \% NACL < 25
 \end{aligned}$$

5.3.9 Pipeline Free Gas Volume

Based on Behr's work, the free gas can be estimated using, $p=MOP$,

$$V_{free} = V_{pipe} \left(\frac{GLR_p}{GLR_p + GVF} \right) GVF \tag{5.102}$$

$$GLR_p = \frac{(GLR - R_s)}{B_o} \tag{5.103}$$

$$GVF = \frac{\rho_p}{\rho_{ref}} \tag{5.104}$$

The captive solution gas remaining in the liquid at a pressure p can be estimated using,

$$V_{sol} = V_{pipe} \left(\frac{(R_s/B_o)}{GLR_p + GVF} \right) GVF \tag{5.105}$$

The sum of V_{free} and V_{sol} is the total gas that comes out of solution. The setback volume is the portion of the total gas that is H₂S.

6 JET EXPANSION - INITIAL BEHAVIOUR OF RELEASE

The approach used to determine the dispersion model inputs are like that used in *GASCON2* (ERCB 1990), as illustrated below. Jet expansion calculations progress from the initial conditions to the exit or E plane, to the pressure equalization zone defined at the Q plane, then to the Drag zone, and stops at the R plane. Equations for the E, Q, and Drag zone to R plane are based on mass, momentum and energy balances and are solved accounting for real fluid behaviour.

The E plane can be horizontal, (as shown) or vertical. The Q plane is parallel to the E plane. Drag may result in a change in direction in the D zone, thus the R plane can be vertical, as shown, or horizontal for a liquid pool. The R plane is the input to the un-ignited H₂S dispersion model. Liquids may be present as an aerosol, if determined by the flash calculation at any of the planes. The SLAB dispersion model allows for air entrainment. There is no air entrainment until after the R plane.

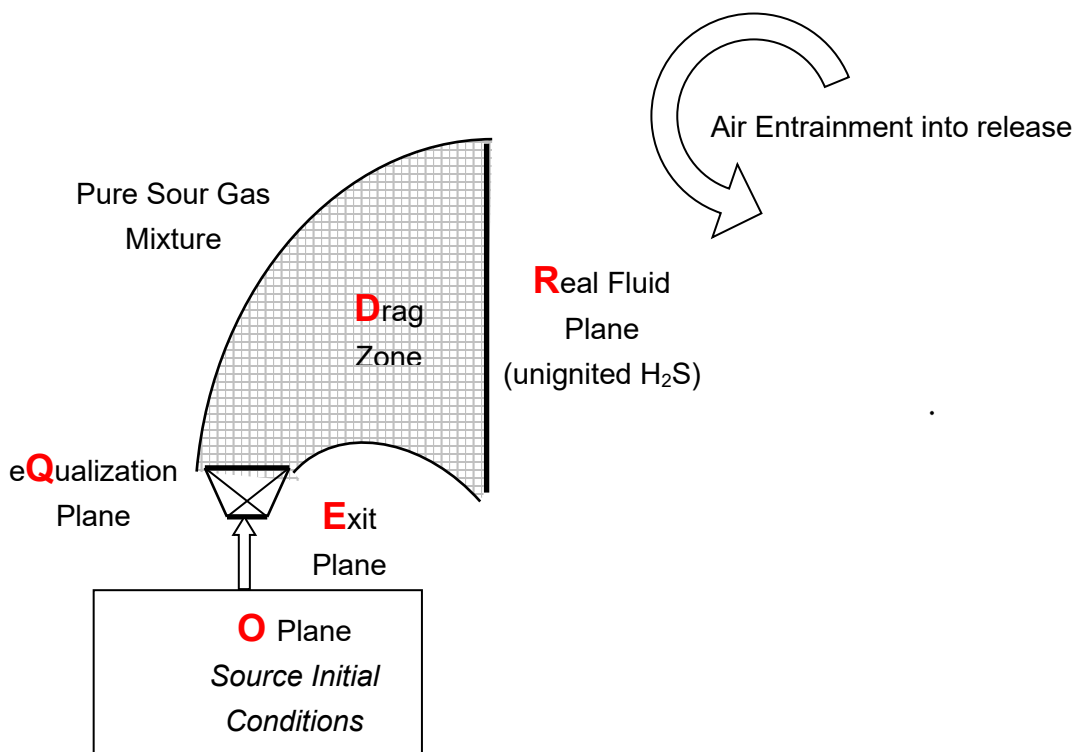


Figure 6-1 Jet Expansion Regions showing the Source Modelling Planes

6.1 E Plane

The initial and exit conditions were provided in the previous section for choked flow when the exit velocity V_E (m/s) is equal to the speed of sound c_E (m/s) at the exit.

$$V_E = c_E \quad (6.1)$$

If the flow is not choked, P_E is set to P_A and V_E and the other properties are solved for in AERFLASH, as described in Appendix 1.

6.2 Q Plane

At the equalization or Q plane the release expands to atmospheric pressure P_A (kPa), so P_Q is equal to P_A . Since there is no air entrainment, $\dot{m}_Q = \dot{m}_E$ (kg/s). From the conservation of momentum, the velocity V_Q (m/s) increase from the exit velocity V_E :

$$V_Q = V_E + 1000 \frac{P_E - P_A}{\rho_E V_E} \quad (6.2)$$

The free expansion from the exit pressure to atmospheric pressure is not isentropic since not all the available energy is converted to kinetic energy. V_Q may exceed the sonic velocity. The exit is a poorly designed nozzle with energy losses. The free expansion is not isenthalpic unless $P_E = P_A$. From the conservation of energy, the enthalpy h_Q (J/kg) at the Q plane is:

$$h_Q = h_o - \frac{1}{2} V_Q^2 \quad (6.3)$$

With the enthalpy and pressure defined, the required real fluid properties are determined in AERFLASH for subsequent calculations. The temperature decreases from the exit, thus the fraction of material present as a condensed liquid increases.

6.3 D Zone to R Plane

The Drag zone allows the release to lose momentum due to changes in direction or impingement with the ground or structures. The drag coefficient cannot be measured and is set to be realistic yet cautiously conservative. Appendix 3 discusses the selection of the drag coefficient. The release exits the drag zone at

the R plane. Since there is no air entrainment yet, $\dot{m}_R = \dot{m}_D = \dot{m}_Q$ (kg/s). From conservation of momentum, the velocity at the D plane V_D (m/s) is:

$$V_D = V_R = V_Q \left(\frac{1 - C_D}{1 + C_D} \right) \quad (6.4)$$

The fluid dynamic force to slow down and change the direction of a release is significant (see calculation on the GAS WELL or GAS PIPELINE page). For an unrestricted jet, C_D is zero, and the Q plane properties are equal to the R Plane properties.

The default inputs are:

Drag Coefficient C_D	Range 0.0 to 1.0	Default 0.5 for a drilling or servicing gas well, 0.25 for a producing gas well, 0.5 for a gas pipeline, calculated for liquid well or pipeline
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During drilling or servicing of a gas well the rig is an obstacle that can slow down and change direction of the release. For a gas pipeline, the release impinges on the crater, removing soil and slowing down the release. A C_D of 0.5 results in the velocity at the R plane V_R being 1/3 of the velocity at the Q plane V_Q (2/3 of the momentum is lost). For a producing gas well, an obstacle is not as likely, so C_D is set to 0.25 (V_R is 3/5 of V_Q with 2/5 of the momentum lost).

For liquid wells and liquid pipelines C_D is set so the velocity of the vapour leaving the pool V_R (V_{Eg}) is the same as the velocity of the liquid within the piping before the liquid enters the pool V_Q (V_{Liquid}):

$$C_D = \frac{(V_{Eg} - V_{Liquid})}{(V_{Eg} + V_{Liquid})}$$

All the kinetic energy is recovered which is the stagnation conditions with $h_R = h_O$. Although momentum may be lost, but energy is conserved with the enthalpy at the R plane h_R (J/kg):

$$h_R = h_o - \frac{1}{2} V_D^2 \quad (6.5)$$

With the enthalpy and pressure defined, the rest of the real fluid properties are determined in AERFLASH. A low velocity at the R plane due to drag results in less dilution due to air entrainment as the release is slowed down to the wind speed.

6.4 R Plane Inputs to AERSLAB

Real fluid calculations allow for the correction of the ideal, perfect gas assumptions used in AERSLAB. AERFLASH provides flash calculations based on conservation of energy and real fluid behaviour from the initial T_O and P_O , to determine R plane conditions. The R plane initial liquid mass fraction is set to the AERSLAB variable, $CMEDO$:

$$CMEDO = LF_R \quad (6.6)$$

The source density calculated within AERSLAB is:

$$\rho_{R,SLAB} = \frac{RHOSL \cdot rhos}{CMEDO \cdot rhos + (1 - CMEDO) \cdot RHOSL} \quad (6.7)$$

based on the input flashed liquid density (kg/m^3), $RHOSL$, calculated in AERFLASH and the source vapour density (kg/m^3) as calculated in AERSLAB from:

$$rhos = 1000 \frac{P_A}{R_S T_R} \quad (6.8)$$

The R plane densities calculated by AERFLASH and AERSLAB are typically within a few percent. From conservation of mass and momentum, the adjusted R plane area A_R (m^2) is:

$$A_R = \frac{\dot{m}_E}{\rho_{R,SLAB} V_R} \quad (6.9)$$

Calculation of the heat capacities, densities and saturation pressure constants of the liquids that may form at the R plane is discussed in Appendix 1. AERSLAB treats the multi-component mixture as a single pseudo-component with a constant boiling point and composition. T_{DEW} is the temperature (K) at atmospheric pressure that the first liquid drops condense from the vapour as the temperature is reduced. Note T_{DEW} is greater than T_R for a multi-component mixture in the phase envelope. The real fluid liquid and vapour compositions vary from T_R to T_{DEW} as the various components boil away or evaporate. The boiling point of the release T_{BP} (K) is the minimum of T_{DEW} and T_R .

The specific heat of the vapour CPS ($\text{J}/(\text{kg} \cdot \text{K})$) is constant in AERSLAB; in reality it varies by a few percent with temperature. AERFLASH determines CPS at the final temperature which is the maximum of (T_A , T_{DEW}).

AERSLAB requires the heat of vapourization DHE (J/kg) as an input. ERCBH2S calculated DHE in three ways and the maximum value was used. This created problems when the liquids fraction variable in the denominator approached zero. To avoid this, DHE_C in AERH2S is now calculated consistent with SLAB using the Clapeyron equation with the Saturation Pressure constant slope SPB and mixture gas constant R_S :

$$DHE_c = \frac{SPB}{R_s} \quad (6.10)$$

The release starts at a height and angle defined by the user (the centre of the E plane is placed at this height and orientation). The default inputs are:

Source height <i>h_s</i>	Range 0.0 to 10.0 m	Default 0.0 m for pipeline 1.0 m for well
Release angle	Range horizontal or vertical	Default horizontal for gas pipeline, gas well and liquid pipeline/well

7 DISPERSION METEOROLOGY

Meteorological parameters affect the dispersion of the released source material in the atmosphere.

Recalling that:

- **User inputs are in regular font in bold boxes**,
- **Default inputs are in bold font in shaded boxes**, and
- **Ranges of inputs are in bold font in bold boxes**.

The inputs and the default parameters are defined below.

Table 7-1: Meteorological and Environmental Range of Values and Default Settings

Parameter	Range	Default
Average ERP Elevation, Z_{ASL}	0 to 3000 m	User
Ambient temperature, T_A	-50 to 50 °C	3.56°C
Relative humidity, RH	0 to 100 %	60%
Surface roughness height, Z_o	0.0001 to 10.0 m	0.1 m
Ambient measurement height, Z_A	3 to 30 m	4 m
Ambient Wind Speed at measurement height, U_{ref}	1 to 30 m/s	3.63 m/s
Stability Class (A=1, B=2, C=3, D=4, E=5, F=6)	1 to 6	F=6

7.1 Stability Class, Wind Speed and Temperature Screening Matrix

Dispersion conditions are defined by the wind speed, stability class and temperature. The wind speed affects the plume rise and transport velocity. Higher wind speeds result in more dilution but lower plume rise.

The stability class is used to classify atmospheric turbulence, which results in dilution of the plume. During unstable conditions (Stability Classes A, B, and C), atmospheric turbulence is enhanced due to the rising motion of air as it is heated near the ground during the daytime. As cloud cover increases the stability class changes from A (strong solar radiation) to B (moderate solar radiation) to C (slight solar radiation).

During stable conditions (Stability Classes E and F), atmospheric turbulence is suppressed due to the settling of air as it is cooled near the ground surface during the nighttime. As cloud cover increases the stability class changes from F (< 3/8 cloud cover), to E (> 4/8 cloud cover).

During overcast conditions or at higher wind speeds (> 20 km/h), the convective motions are overcome by the horizontal mechanical turbulence resulting in neutral conditions (Stability Class D). The ‘mixing height’ defines the lowest layer of the atmosphere that is directly affected by surface heating or cooling and the turbulence caused by wind. The mixing height prevents the plume from dispersing upward and can increase ground level concentrations if the plume approaches it.

Higher temperatures during the day reduce the plume rise but the dispersion turbulence is enhanced. Lower temperatures at night increase the plume rise of a buoyant release but the dispersion turbulence is dampened resulting in higher predictions and larger hazard zones during stable conditions.

In the Advanced User Selected Case section, the user can input the wind speed, stability class and ambient temperature for a single case of interest. The default wind speed of 2 m/s, stability class value of 6 (Stability Class F for very stable) and temperature of -1.59°C typically yields the largest EPZ for a ground-based source.

AERH2S searches for the worst-case dispersion conditions that produce the largest ERP Zone by running the standard regulatory screening conditions (54 combinations of stability class and wind speed) provided in the following table, along with the ambient temperature. The probability of the dispersion conditions occurring in Alberta are provided to allow responders to make informed decisions during an event.

Notice that a few cells are struck through in Table 7-2, as these conditions are modelled for the hazard zones, but the results are not considered representative of measured turbulence. Moderately stable Class F (STAB=6) with wind speeds of 1 and 1.5 m/s and slightly stable Class E (STAB=5) with wind speeds of 1 m/s occur in the Alberta meteorological data sets but due to the reduced turbulence used by dispersion models during low wind speed conditions, the ERP Zones are over-predicted during these conditions as the effect of meandering on ground based H₂S releases is underestimated in the SLAB dispersion model. Minimum turbulence is further discussed in Section 7.5.

The Canadian Weather Energy and Engineering Datasets (CWEEDS) was used to provide enhanced meteorology representative of Alberta. 100 stations (was 6 before), with more than 10 years of data (was 5 before) were compiled to determine the following matrix of meteorology probability of occurrence for dispersion conditions defined by the stability class, windspeed and average temperature in Alberta.

Table 7-2: Alberta Averaged Meteorology and Observed Probability of Occurrence

PG Stability Class		Wind Speed (m/s)	Ambient Temperature (°C)	Probability (met)
Stability Class A	A	1	20.89	0.002460
	A	1.5	20.98	0.003688
	A	2	20.85	0.003330
	A	2.5	19.48	0.000000
	A	3	19.48	0.000000
Stability Class B	B	1	9.32	0.017316
	B	1.5	11.08	0.016354
	B	2	11.95	0.015281
	B	2.5	20.55	0.004586
	B	3	20.59	0.005073
	B	3.5	20.54	0.004554
	B	4	20.51	0.004001
	B	4.5	20.50	0.003262
Stability Class C	C	1	5.40	0.009512
	C	1.5	6.47	0.006192
	C	2	7.93	0.008429
	C	2.5	9.99	0.019314
	C	3	10.10	0.021700
	C	3.5	10.20	0.020358
	C	4	10.32	0.018879
	C	4.5	10.43	0.016534
	C	5	19.38	0.008038
	C	8	17.44	0.000635
Stability Class D	D	10	14.76	0.000121
	D	1	1.16	0.024660
	D	1.5	2.90	0.015107
	D	2	3.33	0.014894
	D	2.5	3.54	0.013307
	D	3	3.47	0.015009
	D	3.5	3.22	0.014122
	D	4	3.01	0.012609
	D	4.5	2.86	0.010144
	D	5	5.41	0.091588
	D	8	5.85	0.084914
Stability Class E	D	10	6.17	0.032125
	D	15	5.78	0.007683
	D	20	4.62	0.001248
	E	4	0.00	0.015676
	E	1.5	1.59	0.008860
	E	2	2.16	0.008354
	E	2.5	2.59	0.007020
	E	3	2.85	0.007337
Stability Class F	E	3.5	-0.03	0.044078
	E	4	0.13	0.038624
	E	4.5	0.13	0.029893
	E	5	0.41	0.029202
	F	4	-3.72	0.090626
	F	1.5	-2.12	0.048315
	F	2	-1.59	0.045115
Stability Class F	F	2.5	-1.13	0.038246
	F	3	-0.87	0.041416
	F	3.5	-0.87	0.000000
	F	4	-0.87	0.000000
	Average	D	3.63 m/s	3.56 °C

7.2 Site Elevation and Atmospheric Pressure

The atmospheric pressure is calculated from the site elevation input by the user. The concentration predictions (ppm) change slightly with the atmospheric pressure. Lower pressures occur at higher elevations resulting in higher predicted concentrations and larger hazard zones. An average elevation for an ERP area can be input for multiple sour gas facilities (wells and pipelines) in an ERP area.

7.3 Relative Humidity

The observed relative humidity given in the default input table above varies with the time of day and temperature. The early morning observations at 0600 h are about when the daily minimum temperature is observed and the afternoon observations at 1500 h are about when the daily maximum temperature is observed. If the released sour gas is cold, moisture in the entrained air may condense forming fog, making the release visible and denser. As air continues to be entrained, the liquid water evaporates, and the fog disappears within several hundred metres. ERP hazard zone predictions are not sensitive to the relative humidity. A default relative humidity of 60% will be used for Alberta.

7.4 Surface Roughness

The surface roughness height is a measure of the influence of surface features on the generation of turbulence as the wind blows over the surface. Rougher surfaces result in more mechanically generated turbulence and for a ground-based release, a lower prediction of concentration for a wind speed.

A surface roughness of 0.01 m is for flat or sloped open terrain with obstructions several centimetres in height (e.g. prairie grassland, cultivated fields, young agricultural crops). A surface roughness of 0.1 m is for flat or sloped open terrain or gently rolling terrain covered by vegetation a few metres in height (e.g. mature agricultural crops with scattered obstructions of various sizes like wind breaks and buildings). A surface roughness of 1.0 m is for flat or sloped open terrain or rolling terrain covered by obstructions several tens of metres in height (e.g. forest, cities, process plants). The default value of 0.1 is representative of rural areas.

7.5 Minimum Turbulence

RWDI AIR Inc. (RWDI 2006) was retained by the ERCB to review meteorological conditions that can be regarded as *worst case* in terms of determining emergency response hazard zones for sour gas facilities in Alberta. A summary of their report follows.

The ERCB (1990) conducted a Field Measurement Program (FMP) to measure dispersion under low wind stable conditions at a location about 20 km to the east of Calgary. Concentrations of tracer gas releases to represent a well blowout were made along downwind distance arcs of 700 m, 1400 m and 2100 m on 33 evenings between October and December 1998. At 700 m, 313 and 262 concentration traverses were obtained for surface and elevated releases, respectively. At 1400 m, 33 and 220 concentration traverses were obtained for surface and elevated releases, respectively. At 2100 m, 18 traverses for elevated releases were obtained. Concurrent meteorological measurements (as 3 minute and 30 minute averages) were made at four levels on an instrumented 25 m platform (ERCB 1990).

The 3- and 30-minute meteorological data from the FMP were analyzed to determine turbulence trends with wind speed and atmospheric stability. This updated analysis differs from the ERCB (1990) and Davies et al (1991) analysis that did not delineate trends with respect to stability class, and differs from the Leahey et al (1994) analysis that did not examine averaging periods other than 30 minutes or measurement levels other than 10 m. The updated analysis examines the 30-minute meteorological data from the 4, 10, 16 and 25 m levels; and the 3-minute meteorological data from the 10 m level.

A comparison of the FMP turbulence values with those associated with the PG stability class values indicates:

- The 3-minute FMP σ_v and D values are more consistent with the PG values than the 30-minute FMP values. The PG values for σ_v , and hence σ_θ and σ_y , are more consistent with the 3 minute averaging time than the usually assumed one hour average assumption.
- Reasonable agreement between the FMP and PG class values occurs when the PG values are adjusted for the appropriate surface roughness Z_o .
- For low wind speeds (i.e., for 0 to 2 m/s) the use of the PG values will understate the turbulence levels.
- For wind speeds greater than 3 m/s, there is reasonable agreement between the FMP and PG stability class values.

There are wide ranges of turbulence levels in the atmosphere, the lowest occur during extremely stable conditions that typically occur during the night. The turbulence parameters measured by the FMP are consistent with those measured elsewhere. In contrast to the fundamental approaches adopted by dispersion models, the lowest dilution levels do not occur under low wind speed conditions. For low wind speeds less than 2 m/s, the PG dispersion coefficients will understate turbulence levels and over predict

ambient concentrations. At the minimum, the continuing use of the reference PG F2 condition is recommended.

7.6 Ambient Measurement Height

The typical ambient measurement height for wind speed is the standard 10 m anemometer tower height. Wind speeds are referenced to this height. The wind speed data in Section 7.1 is based on measurements at 10 m. Closer to the ground, below the reference height, wind speeds decrease depending on the surface roughness and stability class. Above the reference height wind speeds increase.

Through testing of AERH2S it was observed that the SLAB model is very sensitive to the ambient measurement height. In the limiting case of a trace gas release where all dense gas effects are negligible, SLAB was supposed to yield a cloud concentration, width and height that correspond to the values estimated by the standard dispersion curves when the concentration averaging time is 15 minutes. In SLAB, the turbulence parameters are referenced to the ambient wind velocity at 4 m, thus the ambient measurement height Z_A was set to the reference height of 4 m. With $Z_A = 4$ m, the turbulence formulations for SLAB give approximately the same dispersion parameters as the US EPA SCREEN3 and ISC3 dispersion models (as discussed in the SLAB manual).

8 AERSLAB - RELEASE DISPERSION MODELLING

AERSLAB, an enhanced version of SLAB (Ermak, 1990) is used to model the dispersion of H₂S. First the inputs to AERSLAB are summarized and then the improvements to SLAB are discussed. Recalling that:

- **AER Default inputs are in bold font in shaded boxes**, and
- Calculated values from user inputs are in regular font in regular boxes.

8.1 AERSLAB Inputs

Inputs to AERSLAB are summarized below. The variable name, type, units and the Default values are provided. *New to SLAB Inputs are in italic font in shaded boxes with **. Inputs are either calculated from the user inputs or are defaulted and cannot be changed by the user.

Table 8-1: AERSLAB Input Variables

AERSLAB VARIABLE	Description	Gas Wells	Gas Pipelines	Liquid Pipelines or Wells	Units
Source Type and Numerical Parameter (default)					
<i>IDSPL</i>	Spill source type	Horizontal jet-2	Horizontal jet-5	Pool-1	
<i>NCALC</i>	Numerical sub-step parameter - fixed	1	1	1	
<i>iHOPT*</i>	<i>Plume rise calculation option 0=SLAB, 1=ISC, 2=Briggs</i>	2	2	0	
Source Properties (calculated from User Inputs)					
<i>WMS</i>	Molar mass of source material	<i>WMS/1000</i>	<i>WMS/1000</i>	<i>WMS/1000</i>	kg/mole
<i>CPS</i>	Vapour heat capacity at constant pressure	<i>CPS</i>	<i>CPS</i>	<i>CPS</i>	J/(kg·K)
<i>TBP</i>	Boiling point temperature	<i>min(T_R, T_{DEW})</i>	<i>min(T_R, T_{DEW})</i>	<i>min(T_R, T_{DEW})</i>	K
<i>CMEDO</i>	Initial liquid mass fraction	<i>CMEDO</i>	<i>CMEDO</i>	<i>CMEDO</i>	
<i>DHE</i>	Heat of vapourization	<i>DHE</i>	<i>DHE</i>	<i>DHE</i>	J/kg
<i>CPSL</i>	Liquid heat capacity	<i>CPSL</i>	<i>CPSL</i>	<i>CPSL</i>	J/(kg·K)
<i>RHOSL</i>	Liquid density of source material	<i>RHOSL</i>	<i>RHOSL</i>	<i>RHOSL</i>	kg/m ³
<i>SPB</i>	Saturation pressure constant	<i>SPB</i>	<i>SPB</i>	<i>SPB</i>	
<i>SPC</i>	Saturation pressure constant	<i>SPC</i>	<i>SPC</i>	<i>SPC</i>	K
Exposure Characteristics (default except as noted)					

AERSLAB VARIABLE	Description	Gas Wells	Gas Pipelines	Liquid Pipelines or Wells	Units
<i>xxAlpha</i> *	<i>Time Factor</i>	-1.0	α	-1.0	
<i>xxBeta</i> *	<i>Time Constant</i>	-1.0	β	-1.0	s
<i>QSi</i> *	<i>Initial release rate for transients (same as QS for wells and liquids)</i>	\dot{m}_E	\dot{m}_{E_i}	\dot{m}_E	kg/s
<i>TN</i> *	<i>Concentration Exponent for Toxic Load</i>	3.5	3.5	3.5	
<i>TKL</i> *	<i>Toxic Load Factor to account for Fluctuations</i>	K_L	K_L	K_L	
<i>TACH</i> *	<i>Building air changes per hour</i>	3.0	3.0	3.0	1/h
<i>TH2S</i> *	<i>Percent H2S in source mixture</i>	$100 * W_{H2S,E}$	$100 * W_{H2S,E}$	$100 * W_{H2S,E}$	Mole%
<i>TCPL</i> *	<i>Toxic Load Endpoint for Planning steady ppm for 3 minutes</i>	235	235	235	ppm
<i>TCRE</i> *	<i>Toxic Load Endpoint for Response steady ppm for 3 minutes</i>	306	306	306	ppm
<i>TMAXEX</i> *	<i>Maximum Exposure Time</i>	10800	10800	10800	s
<i>TIGN</i> *	<i>Time to ignition or mitigation</i>	21600	21600	21600	s
Spill Parameters (calculated from User Inputs except as noted)					
<i>TS</i>	Temperature of source material	T_R	T_R	T_R	K
<i>QS</i>	Mass source rate	\dot{m}_E	\dot{m}_E	\dot{m}_E	kg/s
<i>AS</i>	Source area	A_R	A_R	A_R	m ²
<i>QTIS</i>	Instantaneous source mass -fixed at zero	0.0	0.0	0.0	kg
<i>TSD</i>	Continuous source duration	<i>TSD</i>	<i>TSD</i>	<i>TSD</i>	s
<i>HS</i>	Source Height	h_s	0	0	m
Field Parameters (default except as noted)					
<i>TAV</i>	Concentration averaging time	<i>TSD</i>	<i>TSD</i>	<i>TSD</i>	s
<i>XFFM</i>	Maximum downwind distance -fixed	30000	30000	30000	m
<i>ZP(1)</i>	Height of concentration calculation - fixed	0.0	0.0	0.0	m

Table 8-2: AERSLAB Meteorological Input Variables

Meteorological Parameters (default except as noted)			
AERSLAB VARIABLE	Type	All Sources	Units
ZO	Surface roughness height	0.1	m
ZA	Ambient measurement height	4.0	m
UA	Ambient wind speed	2.0 see Section 7.1	m/s
TA	Ambient temperature	$T_{amb}+273.15$ see Section 7.1	K
RH	Relative humidity	60	%
PA *	<i>Atmospheric pressure</i>	1000*PA	Pa
STAB	Stability class	6 see Section 7.1	

Table 8-3: AERSLAB Critical Parameters

Critical Parameters (default except as noted *)			
AERSLAB VARIABLE	Type	All Sources	Units
$L_{p,crit}$	Critical Richardson Number Buoyant	30.0000 See Section 8.2.2	--
$L_{p,dense}$	Critical Richardson Number Dense	1.0000 See Section 8.2.2	--
Ru	Gas Constant	8.3145	(kPa·m ³)/(K·kmol)
w_{ma}	Molar mass dry air	0.0290	kg/mole
cp_a	Specific Heat Dry Air (isobaric)	1004.2833	J/(kg·K)
g	Gravity	9.8067	m/s ²
w_{mw}	Molar mass water	0.0180	kg/mole
ρ_{wl}	Density Water Liquid	999.1020	kg/m ³
cp_{wv}	Specific Heat Water Vapour	1862.0000	J/(kg·K)
cp_{wl}	Specific Heat Water Liquid	4188.8000	J/(kg·K)
dH_w	Latent Heat Water	2466200.0000	J/kg
SPA_w	SPAW Intercept ln(atm local), T[K]	12.6456 * Local Elevation Specific	--
SPB_w	SPBW slope	4284.9300	--
SPC_w	SPCW correction	-30.1935	K

8.2 Enhancements to SLAB to Produce AERSLAB

The following changes were made to the SLAB program to create AERSLAB:

- 1) Constants and properties changed slightly as given in Section 3.
- 2) Now using site atmospheric pressure instead of reference pressure requiring new input variable and changes to saturation pressure constants for water (as given in Section 3.3).
- 3) IDSPL 1, flashing gas in solution from pool for steady liquid well/pipeline modelling.
IDSPL 2, horizontal jet release and IDSPL 3, vertical jet release for steady gas well modelling.
Added IDSPL 5, horizontal jet release and IDSPL 6, vertical jet release for transient gas pipeline modelling.
- 4) Set meteorological averaging time TAV to source duration TSD within code.
- 5) Revised Buoyancy Flux calculation to properly handle high speed jets with liquid droplets based on source inputs (see Section 8.2.1).
- 6) Limit plume rise to maximum value based on common relationships used in regulatory models. A lift-off criterion is used to determine if buoyant plumes rise. Dense releases are not allowed to rise and a Richardson number criterion is used to stop dense plumes from dropping (see Section 8.2.2).
- 7) Allowed for air entrainment while vertical buoyant releases are rising (see Section 8.2.3).
- 8) Corrected error in vertical dense release plume rise (see Section 8.2.4).
- 9) Included kinetic energy term in energy conservation equation for high-speed jet. This results in the temperature increasing (and the density decreasing) as the jet slows down allowing the release to rise, if it is lighter than air (see Section 8.2.5).
- 10) Revised solution for pool modelling to prevent inconsistent results (see Section 8.2.6)
- 11) Corrected modelling of air entrainment into high speed jets and dispersion parameter (see Section 8.2.7)
- 12) Gas pipeline blowdowns are modelled as short-term duration steady release. Steady concentration predictions are transformed to transient predictions (see Section 8.3).
- 13) Outdoor toxic load calculation accounts for concentration fluctuations about the average prediction for the exposure time (see Section 9.1).
- 14) Indoor concentrations are predicted from the outdoor predictions and then indoor toxic load is determined (see Section 9.2).

- 15) Created new output file to present outdoor and indoor exposure time averaged H₂S concentrations (ppm) and toxic load equivalent H₂S concentrations (ppm) for a 3-minute reference time, as a function of downwind distance. Interpolated distance to toxic load equivalent endpoints to define hazard zones (see Section 9.3).

8.2.1 *Buoyancy Flux in a High Velocity Jet with Droplet Evaporation*

The Wilson-Springer approach to determine the effective buoyancy flux of a high velocity jet with droplet evaporation was implemented in AERSLAB (see Chapter 3 of Appendix 2). The buoyancy flux is required to determine if a release will rise and behave as a neutrally buoyant or passive plume or drop and spread along the ground like a dense gas. The buoyancy flux (m⁴/s³) is given by:

$$F_B = \frac{g \dot{m}_E}{\pi \rho a} \left(\frac{CPS \cdot T_{OSS}}{cpaa \cdot T_A} - \frac{CPS}{cpaa} + \frac{wmae}{WMS} - 1 \right) \quad (8.1)$$

The variables have been previously defined, except T_{OSS} which is defined below. The first and second terms in the bracket are the ratio of the source to air stagnation enthalpy and specific heats, respectively. The third term is the ratio of the air to source molar mass. This expression reduces to the commonly used equation for hot releases from stacks by assuming the ratio of specific heats $CPS/cpaa$ and molar mass $wmae/WMS$ are equal to one.

T_{OSS} , the effective source temperature (K) accounting for the kinetic energy of the high-speed jet and the evaporation of liquid droplets is defined in the derivation of Equation 8.1:

$$T_{OSS} = T_R + \frac{1}{2} \frac{V_R^2}{CPS} - \frac{CMEDO}{CPS} DHE \quad (8.2)$$

In ERCBH2S, for releases with a high liquid fraction, T_{OSS} could be negative (which is physically impossible). This means that there is not enough sensible and kinetic energy in the release to evaporate the droplets; air must be added to provide additional energy. When nature does this the temperature does not drop below the boiling point of the evaporating mixture. In AERH2S, T_{OSS} is now calculated by using the isenthalpic flash stagnation temperature T_F and stagnation liquid mass fraction X_F :

$$T_{OSS} = \max \left(T_F - \frac{X_F dH_{spb}}{CPS}, T_{bp} \left(\text{component with highest mol fraction} \right) \right) \quad (8.3)$$

The boiling point of a mixture changes as the components with the lowest boiling point evaporate. Heavy hydrocarbons and water have higher boiling points than lighter compounds like H₂S, CO₂ and CH₄, thus they may form aerosol droplets at typical ambient temperatures when mixed with air. The boiling point of the compound with the highest mole fraction in the source mixture is assigned to the release.

The equivalent density (kg/m^3) of the release after it slows down and the liquids evaporate is:

$$\rho_{equiv} = \rho_{hoa} \left(\frac{CPS T_{OSS}}{cpaa T_A} - \frac{CPS}{cpaa} + \frac{wmae}{MWS} \right)^{-1} \quad (8.4)$$

A maximum limit is placed on ρ_{equiv} of $4 * \rho_{hoa}$ for very dense releases.

Releases with an equivalent density less than air result in a positive F_B and will rise due to buoyancy.

Releases with an equivalent density greater than air result in a negative F_B and will sink due to buoyancy.

A molar mass lighter than air does not mean the release will rise as it also depends on the ratio of the source to air stagnation enthalpy and specific heats.

The buoyancy flux as a function of downwind distance was added to the AERSLAB output to assist in the development. The flux depends on the downwind plume density ρ and mass fraction cm of the release that change with downwind distance:

$$F_B(x) = \frac{g}{\pi} \left(\frac{\rho_{hoa}}{\rho} - 1 \right) \frac{\dot{m}_E}{\rho_{hoa} \cdot cm} \quad (8.5)$$

This equation is only applicable to a plume, when AERSLAB switches to a puff mode the values produced are not applicable and should be ignored.

8.2.2 **Plume Rise Limits**

SLAB has no plume rise limits. In SLAB, a release with a molar mass lighter than air will eventually rise even if it starts out denser than air. Most sour gas releases are in this category (see above discussion).

Similarly, in SLAB, a release with a molar mass heavier than air will eventually sink to the ground even if it starts out lighter than air. For buoyant vertical releases, SLAB places them at the final rise and adjusted the temperature and specific heat to counteract the molar mass and make the release density the same as that of the air; however, eventually the release would rise again. The reason is that the momentum equations depend on the difference in density between the air and the plume. Far downwind there will always be a slight difference in density unless the molar mass of the source equals the molar mass of the air. This slight difference results in SLAB letting the plume continuing to rise if it has a molar mass lighter than air and continuing to sink if it has a molar mass heavier than air.

For releases that were vertical and initially buoyant, SLAB uses the Briggs (1984) plume rise relations (that included the ambient friction velocity) for the initial height of the release. For buoyant releases that were horizontal and initially buoyant the release would continue to rise if it had a molar mass less than air, but it would sink if the molar mass was greater than air. For releases that were vertical and initially dense, SLAB uses the Hoot, Meroney and Peterka (HMP 1973) relations for the initial height of the

release. For dense releases that were horizontal and initially dense the release would eventually rise if it had a molar mass less than air but it would sink if the molar mass was greater than air.

To overcome these problems, limits were placed on the plume rise in AERSLAB. For releases that have an equivalent density less than or equal to air, the simplified form of Briggs plume rise equations for buoyant plumes and momentum jets for each stability class, were used in AERSLAB (as provided in Table 4.1 of Chapter 4, Appendix 2). The final plume rise h_{prf} for a release is calculated and the profile centre height Z_C is not allowed to exceed the source height plus the final rise (h_s+h_{prf}). A horizontal release rises to this limit before the profile centre height is reset to this height.

Note that the height used to calculate the wind speed for plume rise has been changed to the maximum of the reference anemometer height Z_A and the source height h_s , to be consistent with the regulatory modelling approach. This change results in lower predicted rise.

However, the release may not rise at all if the internal plume turbulent energy due to buoyancy forces cannot overcome the ambient atmospheric turbulent energy (Post, 1994). If the release is grounded and the lift-off parameter L_p is greater than a critical value, the profile centre height Z_C is permitted to rise:

$$L_p = g \frac{(\rho_{oa} - \rho)}{\rho_{oa}} \frac{h}{u_*^2} \quad (8.6)$$

where $h(x)$ is the box height (m) and $\rho(x)$ is the density (kg/m^3) of the release-air mixture at each calculation plane. A release is grounded if $Z_C < h/2$. The box height increases as air is entrained and the release slows down to the wind speed. The friction velocity u_* is a measure of ambient turbulence and depends on the wind speed and stability class. Thus, a buoyant grounded release may be allowed to rise during low wind speeds but is held to the source height at higher wind speeds. Or, a buoyant release may be allowed to rise during stable conditions but is held to the source height during neutral and unstable conditions.

ERCBH2S used a critical value $L_{PCRIT}=L_p = 20$ from Post (1994). AERH2S sets L_p at 30 based on Meroney (1979) which showed a range of $9 \leq L_p \leq 30$. There is considerable uncertainty in L_p (Meroney 1979, Briggs 1973, Post 1994) with uncertainty being a factor of two to a factor of four. AERH2S has adopted a conservative approach using the upper limit of Meroney (1979), $L_{PCRIT}=L_p=30$. This may prevent sour gas releases from rising and thus increase ERP hazard zones.

The final plume rise h_{prf} for a dense horizontal release is zero and the profile centre height Z_C is not allowed to exceed the initial height h_s . The profile centre height may decrease but it is not allowed to increase. The local cloud Richardson number is used to define the ratio of density to ambient turbulence effects:

$$R_{i*} = L_{p,DENSE} = g \frac{(\rho - \rho_{oa})}{\rho_{oa}} \frac{h}{u_*^2} \quad (8.7)$$

The Richardson number is compared to a critical value of $L_{p,DENSE} = 1.0$. For dense plumes only, the plume center height is held constant once R_{i^*} is less than $L_{p,DENSE}$.

8.2.3 Vertical Buoyant Release Air Entrainment and Source Conditions

SLAB starts a buoyant vertical release horizontally at the final rise height with the input source conditions (no air entrainment is accounted for). This was modified in AERSLAB to match the approach used in SLAB for a dense vertical release. In a dense vertical release, SLAB starts the plume at the peak rise and downwind distance to peak rise with air added to match the predicted concentration at the peak rise. The source properties are recalculated at the reduced mass fraction of the release, changing the temperature, liquid fraction, density and dimensions.

Air entrainment while a buoyant release is rising is now accounted for using the methods of Wilson (1994) to determine the reduced mass fraction cm_o of the release after it has risen h_{pr} and is travelling horizontally at the wind speed U_c at the final rise.

$$cm_o = \left(1 + \frac{U_c}{V_R} \left(\frac{\beta_e h_{pr}}{\sqrt{A_R/\pi}} \right)^2 \right)^{-1} \quad (8.8)$$

where V_R is the initial vertical velocity from the source with area A_R . The effective entrainment constant β_e is given by:

$$\beta_e = 0.6 \left(\frac{1 + 0.015 M_S^2}{1 + 0.04 M_S^2} \right) \quad (8.9)$$

where M_S depends on the R plane density and velocity and the air density and wind speed:

$$M_S = \frac{V_R}{U_C} \sqrt{\frac{\rho_R}{rhoa}} \quad (8.10)$$

The distance to final rise is calculated according to the equations used in the USEPA dispersion model ISCST3.

In AERSLAB the vertical buoyant plumes are started at the downwind distance to final rise at the height of the final rise travelling at the wind speed at the final rise with the properties calculated at the reduced mass fraction cm_o . At these revised source conditions, the temperature and density are approaching those of the ambient air and the plume dimensions are much larger.

8.2.4 Correction to Vertical Dense Release Plume Rise

For vertical releases that have an equivalent density greater than air, the corrected HMP plume rise equations for dense jets with momentum were used in AERSLAB. In Equation (45) of the SLAB manual and in the computer code (Ermak 1990), the Froude number F_r is incorrectly defined and does not match the original HMP equations. HMP specifically point out that they defined the Froude number differently from the normal convention by normalizing the density difference between the source and air with the source density $(\rho_s - \rho_a)/\rho_s$. SLAB incorrectly uses the air density to normalize $(\rho_s - \rho_a)/\rho_a$, as done in the definition of F_B . The corrected equation (45) used in AERSLAB is:

$$F_R = W_s \left(g D_s (\rho_s - \rho_a) / \rho_s \right)^{-1/2} \quad (8.11)$$

The source density ρ_s is the R plane density. The minimum value of the Froude number is set to zero to allow for initially buoyant releases that are dense in the far field.

8.2.5 Kinetic Energy in Energy Conservation Equation

Most uncontrolled releases of sour gas are at sonic velocity, choked flow conditions. The Wilson-Springer buoyancy flux approach demonstrates the importance of allowing for the conversion of kinetic energy into sensible energy for high-speed jets. In SLAB, the kinetic energy is lost by not accounting for it. The release temperature only increases due to the addition of air and the density changes slowly, extending the downwind distance to final rise beyond several kilometres. By allowing for the conversion of kinetic energy to sensible energy in AERSLAB, the resulting temperature increase reduces the density, and the release rises within several 100 m, if it is buoyant.

AERSLAB includes this important effect in the solution of the governing dispersion equations. The kinetic energy of the entrained air is neglected. SLAB Equation (3) now includes the kinetic energy term ($U^2/2$) on the left-hand side of the equation and on the second line of the right-hand side of the equation:

$$\left[\rho U B h \left(C_p T + \frac{U^2}{2} \right) \right] = \rho_a (V_e h + W_e B) C_{pa} T_a + \rho_s U_s B_s C_{ps} T_s + f_{pc} + f_t + \rho_s U_s B_s \frac{U_s^2}{2} \quad (8.12)$$

SLAB Equation (3c) now includes the kinetic energy term on the second line of the right-hand side of the equation:

$$E = R \cdot (1 - m) \cdot C_{pa} \cdot T_a + R \cdot m \cdot C_{ps} \cdot T_s + R \cdot (1 - m) \cdot m \cdot \frac{U_s^2}{2} \quad (8.13)$$

SLAB Equation (41) now includes the kinetic energy term as the last term on the first and second line of the numerator of the right-hand side of the equation:

$$T = \frac{\left[\begin{aligned} &(1-m) \cdot C_{paa} \cdot T_a + m \cdot C_{ps} \cdot T_s + (1-m) \cdot m \cdot \frac{U_s^2}{2} \\ &+ R_o/R \cdot \left(C_{po} \cdot T_o - (1-m_o) \cdot C_{paa} \cdot T_a - m_o \cdot C_{ps} \cdot T_s - (1-m_o) \cdot m_o \cdot \frac{U_s^2}{2} \right) \\ &+ F_t/R + E_{pc} \end{aligned} \right]}{C_p} \quad (8.14)$$

8.2.6 Pool Modelling

Liquid wells and pipelines are now modelled as pool sources. Liquid wells and pipelines were modelled as jets which often resulted in EPZs decreasing with increasing H₂S release rate. They are now modelled as a flashing gas release from a pool of liquid. H₂S release volumes may change which may impact setback.

Pool modelling was attempted in the development of ERCBH2S but the SLAB model did not always solve and provide consistent results. AERSLAB solving routine was adjusted to provide reasonable results.

8.2.7 Air Entrainment due to High Speed Jets

Air is entrained into the release due to the jetting effect when the release is travelling faster than the wind and due to atmospheric turbulence. Near the source jetting effects dominate, further away once the release has slowed down atmospheric dispersion dominates. Jetting and dispersion coefficient corrections in SLAB were revised.

For atmospheric turbulence a square root of 3 factor was missing in the vertical entrainment term and has been added. The original jetting term was wrong because SLAB kept this term constant with distance whereas jetting turbulence should decrease as jet slows down as air is entrained. Therefore, atmospheric turbulence now becomes dominant sooner closer to the source. A high velocity choked flow release is now only at a high velocity for a couple hundred metres. Some of the extreme zone sizes (>30 km) for sour gas pipelines have been reduced because of this correction.

8.3 Steady to Transient Transformation

Pipelines are modelled at a steady effective release rate for the equivalent steady release duration. The steady release rate dispersion model predictions can be transformed to allow for time-varying release and plume rise (see Chapters 4 and 5 of Appendix 2). The time varying mass release rate is \dot{m}_e (small e) while the modelled steady mass release rate from the exit is \dot{m}_E (large E). The time varying mass release rate \dot{m}_e can be calculated from the modelled effective steady release rate \dot{m}_E using the double exponential blowdown equation provided earlier. The Wilson report approach was adjusted to use the effective release rate \dot{m}_E concentration predictions instead of the initial release rate \dot{m}_{ei} concentration predictions. The method used depends on whether the release is classified as being neutrally buoyant or denser than air.

8.3.1 Neutral and Buoyant Releases

If the equivalent density of the release is less than the air density, the release is considered neutral or buoyant.

8.3.1.1 ERCSLAB Methodology

Steady state concentration predictions are transformed to transient predictions using the following based on the approach given in Chapter 4 of Appendix 2. $C_{oE,steady,withrise}$ is the outdoor H₂S concentration calculated by ERCBSLAB for the effective release rate conditions. $C_{oE,steady,no rise}$ is calculated by forcing the plume center height to zero while maintaining the other plume properties. The ratio of the no rise and with rise concentration predictions is a function of downwind distance:

$$R_E = \frac{C_{oE,steady,no rise}}{C_{oE,steady,withrise}} = \exp\left(\frac{h^2}{2\sigma_Z^2}\right) \quad (8.15)$$

$C_{o,transient,\dot{m}_e,h}$ is the transformed H₂S concentration as a function of time through the dependence on \dot{m}_e and plume rise h and is:

$$C_{o,transient,\dot{m}_e,h} = \frac{\dot{m}_e}{\dot{m}_E} \left(R_E^{1-(h/h_E)^2} \right) C_{oE,steady,withrise} \quad (8.16)$$

The plume rise function for purely buoyant plumes (negligible vertical momentum) in transitional rise is:

$$\left(\frac{h}{h_E} \right)_{buoyant} = \left(\frac{\dot{m}_e}{\dot{m}_E} \right)^b \quad (8.17)$$

The plume rise function for vertical momentum jets in transitional rise is:

$$\left(\frac{h}{h_E}\right)_{momentum} = \left(\frac{\dot{m}_e}{\dot{m}_E}\right)^m \quad (8.18)$$

The exponents b and m are from Table 4.2 of Chapter 4 Appendix 2. The combined momentum and buoyancy rise is based on the square root of the sum of the squares of each contribution and depends on whether final rise has been reached yet.

8.3.1.2 AERSLAB Methodology

The Appendix 2 methodology often created inconsistent or erroneous results. Instead, the transient concentration can be determined from the steady plume results by calculating the expected plume rise for each state and then adjusting the z-term of the Gaussian dispersion model equation. Transitional plume rise can be calculated using Briggs (1975):

$$\Delta h = \left(\frac{3F_m x}{\beta^2 U^2} + \frac{3F_b x^2}{2\beta^2 U^3}\right)^{1/3} \quad (8.19)$$

Where $\beta=0.6$ for a horizontal plume, $\beta=0.11$ (Briggs 1975, Houtt and Wiel 1972) for vertical buoyant plumes and β is represented by the expression below for horizontal jet plumes (Briggs 1975, 1984)

$$\beta = 0.4 + 1.2 \frac{U_a}{U_s} \quad (8.20)$$

Where U_a is the ambient wind speed and U_s is the source horizontal speed.

Define a height ratio using the transitional rise calculated for transient and for the steady release,

$$hhi = \frac{h}{h_i} = \frac{\Delta h_{transient} + H_s}{\Delta h_{steady} + H_s} \quad (8.21)$$

Where H_s is the source height. When the plume height is greater than the source height,

$$z_{adj} = H_s + (z_p - H_s) hhi \quad (8.22)$$

And when the plume height is below the source height,

$$z_{adj} = \min(H_s, z_p hhi) \quad (8.23)$$

The z-term in AERSLAB Gaussian dispersion equation can be calculated using,

$$fczi = \exp\left(-\frac{z_a^2}{2}\right) + \exp\left(-\frac{z_b^2}{2}\right) \quad (8.24)$$

Where,

$$z_a = \frac{z + z_{adj}}{\sigma_p(k)}, \quad z_b = \frac{z - z_{adj}}{\sigma_p(k)}$$

Using this method, AERSLAB calculates the concentration using the steady f_x , f_y along with the updated f_z terms based for the transient at each x location using the saved terms for the steady plume. Neither Appendix 2 nor AERSLAB accounts for changes in the f_x term for the plume averaged velocity, entrainment or friction effects for the transient.

8.3.2 Dense Releases

If the equivalent density of a horizontal release is greater than the air density, the release is considered dense. Steady state concentration predictions are transformed to transient predictions using the following approach from Chapter 5 of Appendix 2:

$$(C_{o,transient})_{dense\ at\ \dot{m}_e} = \left(\frac{\dot{m}_e}{\dot{m}_E} \right) \left(\frac{F_N(\phi)}{F_N(\phi_E)} \right)^2 (C_{o,steady})_{dense\ at\ \dot{m}_E} \quad (8.25)$$

$(C_{o,steady})_{dense\ at\ \dot{m}_E}$ is the outdoor H_2S concentration calculated by AERSLAB for the effective release rate conditions and $(C_{o,transient})_{dense\ at\ \dot{m}_e}$ is the transformed H_2S concentration as a function of time because of the dependence on \dot{m}_e . $F_N(\phi)$ and $F_N(\phi_E)$ are defined below and because ϕ depends only on source release rate, density difference and wind speed, the functions are independent of x ; all dependence on downwind distance comes from the predicted steady-state dense gas concentration.

$$\phi = \left(g_O^2 \frac{\dot{m}_e}{\rho_{equiv} \cdot UA^5} \right)^{\frac{1}{5}} \quad (8.26)$$

with UA the wind speed (m/s) at the reference height and:

$$g_O \equiv g \left(\frac{\rho_{equiv} - \rho_{air}}{\rho_{air}} \right) \quad (8.27)$$

$$F_N = \frac{F(\phi)}{F(\phi=0)} = \frac{1 + 6.0\phi^3 e^{-4(\phi-0.1)^2}}{(1 + 0.05\phi^6)^{0.1}} \quad (8.28)$$

The above equations are for a dense horizontal release. Vertical dense releases are transformed using the buoyant release formulations for neutral stability class. This is because the final rise for a vertical dense

release has the same exponent of 1.0 as for a vertical buoyant release; both are directly proportional to the mass release rate.

8.4 Transition from Continuous to Puff Mode

Once the release has stopped at time TSD , SLAB switches from a continuous plume mode to a puff mode. The puff mode allows for alongwind dispersion that reduces the predicted concentration but increases the duration that a receptor is exposed to the release. For steady releases, the increase in duration is accounted for in SLAB by the cloud duration t_{cld} (s) variable that conserves mass passing over a receptor. The minimum value of t_{cld} is TSD . For transient releases, the steady to transient transformations of the previous section are adjusted by changing the time adjustment factor α used in the double exponential blowdown equation to conserve mass with the increasing effective duration t_{cld} . The final time constant β is held constant; the initial time constant $\alpha^2\beta$ is changed through α_{new} as follows:

$$\alpha_{new} = \sqrt{\frac{t_{cld}}{\beta} - 1} \quad (8.29)$$

The new initial mass flow rate (kg/s) is:

$$\dot{m}_{einew} = \dot{m}_{ei} \frac{\alpha}{\alpha_{new}} \quad (8.26)$$

As t_{cld} increases, the initial mass flow may become less than the modelled effective mass flow rate. The frozen mass release rate profile assumption may no longer be valid as the cloud has been smeared in the along wind direction.

8.5 Parallel Airflow or Complex Terrain?

Egan (1976) summarized that in complex terrain there are several effects which tend to increase dispersion and the dilution of the plume. One is wind shear due to the variation of wind speed and direction with height above the terrain. Another is the distortion of the plume as it flows over and around the terrain. There are significant distortions of airflow in complex terrain. Flow separation, which occurs when the airflow streamlines no longer follow the shape of an obstacle, may take place. Separation tends to be less severe for flow around an isolated three-dimensional object such as a hill than for flow normal to an object which is effectively two dimensional such as a ridge. Separation is more pronounced for

unstable or neutral conditions than for stable conditions, which tend to suppress it. The difference between complex and parallel airflow terrain in respect of stability is most marked for stable conditions. Stable stratification is liable to produce shearing motions and thus to promote turbulence. The effect of terrain on turbulence is less pronounced for unstable and neutral conditions. In valleys there tends to be local variations of wind direction and velocity. Typically there are upslope winds during the day (due to the air at the surface being heated and rising) and down-slope winds at night (due to the air at the surface being cooled and falling). Two issues of concern in complex terrain are the impingement of a plume from an elevated source on the ground and episodes of low dilution in stagnant regions.

Ramsay (1994) noted that a dispersing dense gas release forms a ground-based cloud that is sensitive to the effects of both man-made and natural obstructions. Variations in the elevation of the ground the cloud flows over will influence the buoyancy driven motion of the gas. Topography in the form of a general slope, isolated hill or complex terrain, will alter or divert the cloud. The topography may enhance plume dilution and divert the cloud away from elevated terrain. Alternatively, the dense cloud may be channeled into low-lying areas and then be protected from the diluting influence of the ambient flow.

Davies (2001) noted that complex terrain can have adverse and beneficial effects on dispersion of elevated plumes. Adverse effects produce ground-level concentrations that would be larger than those expected under parallel airflow terrain conditions and include:

- a) Vertical plume trajectory modification that can lead to decreased plume heights and the increased potential for plumes to impact directly on elevated terrain. Direct impingement is most likely under stable conditions when the plume trajectory cannot lift over the elevated feature.
- b) Horizontal plume trajectory modification that can lead to plumes either being steered around an elevated terrain feature or being confined within a limited area. For example, the width and depth of the valley may limit the mixing and increase ground-level concentrations.
- c) Persistence due to channeling leading to extended periods of high exposure beyond that associated with the persistence of above-valley winds. Specifically, the plume may remain in a narrow sector for days.

Beneficial terrain-related factors that can lead to reduced concentrations include:

- a) Light winds that tend to occur in complex terrain areas can result in greater plume heights above the stack base.
- b) Increased turbulence due to the presence of terrain features results in greater dilution of the plume.
- c) Increased turbulence levels due to the presence of a forest canopy can lead to greater dilution when compared to flat, non-forest canopy surfaces.

The overall effect of terrain on ambient air quality depends on competing adverse and beneficial effects.

AERSLAB maintains the airflow parallel to the ground and in a steady wind direction (neither are changed by terrain). Most accidental releases are dense and thus ground based. A review of the AERSLAB model output shows that for sour gas releases, that the liquid aerosol drops that may be present at the exit are quickly evaporated ($cmv=cm$, usually within metres of the exit) before the water drops that condense in the cold plume are evaporated ($cmwv=cmw$, usually within tens of metres of the exit). Soon the density ρ of a dense release approaches the air density ρ_a ; at this point the cloud is passive and is carried by the wind. Thus, topography effects on a dense gas release are not a factor at the distances that define the EPZ. A buoyant release may rise if the lift-off criterion is satisfied.

Parallel airflow modelling describes passive flow, except the release may not travel in a straight line, as assumed in the model. During unstable and neutral conditions, it may flow over or across an obstacle. During moderate wind speed stable conditions, it may also flow over or across an obstacle, however at lower wind speeds it may be diverted by the obstacle and flow around a hill or into a valley. The shortest distance between a source and a receptor is the straight line modelled, the longer path taken by a cloud diverted by terrain results in increased dilution.

9 H₂S EXPOSURE

This section discusses how the downwind H₂S concentrations are determined. SLAB provides the time-averaged volume fraction of the released material in the plume (m³ of release per m³ of plume, not m³ H₂S per m³ of plume) at the specified location and time, $\overline{C}(x, y, z, t)$. The H₂S concentration (ppm) at a downwind (x), centreline ($y = 0$) and ground-level ($z = 0$) location is used to determine the maximum outdoor concentration (at $t = t_{peak}$) from:

$$\overline{C}_O(x, 0, 0, t_{peak}) = \overline{C}(x, 0, 0, t_{peak}) \cdot w_{H_2S} \cdot 10^6 = \overline{C}_O \tag{9.1}$$

AERSLAB’s additional output file provides predictions of the H₂S concentration in parts per million (ppm) for the event meteorological averaging time. \overline{C}_O will be used as the shorthand notation for the outdoor H₂S concentration for the event meteorological averaging time TAV . The response and planning endpoints are based on the toxic load.

9.1 Outdoor Concentration Fluctuations

Dispersion models can only predict the average concentration. Concentration fluctuations about the average are accounted for using the methods of the Wilson report (Chapter 6, Appendix 2) to determine the toxic load factor. The meteorological averaging time for the concentration prediction is equal to the source duration (Wilson 1995). The average toxic load is calculated using the average concentration for the exposure time:

$$TAV = TSD \tag{9.2}$$

The total intensity i is a measure of the concentration fluctuations and represents the standard deviation of the instantaneous concentrations divided by the mean concentration. It is a function of the averaging time TAV . The intensity changes with averaging time as follows:

$$i = \left(\left(\frac{TAV}{TAV_{ref}} \right)^{0.2} (i_{ref}^2 + 1) - 1 \right)^{\frac{1}{2}} \tag{9.3}$$

The AER default reference intensity and averaging time are:

Reference intensity i_{ref}	0.25	
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Reference intensity averaging time TAV_{ref}	3	minutes
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For averaging times less than 3 minutes, i is set to i_{ref} . The total intensity i includes time periods when the concentration is zero. The conditional intensity i_p removes the zero periods of concentrations and is given by:

$$i_p = \frac{i}{\left(1 + \left(\frac{i}{1.5}\right)^3\right)^{\frac{1}{3}}} \tag{9.4}$$

The intermittency factor γ denotes the non-zero fraction of concentrations:

$$\gamma = \frac{1 + i_p^2}{1 + i^2} \tag{9.5}$$

For H₂S, concentration fluctuations increase the toxic load above the value calculated from the predicted average concentration by the factor K_L :

$$K_L = K_{fluctuation}^n = \gamma^{\frac{(n-1)(n-2)}{2}} \left(1 + i^2\right)^{\frac{n(n-1)}{2}} \tag{9.6}$$

n is the exponent in the toxic load model. K_L increases with the exposure time offsetting the decrease in concentration due to averaging time.

9.1.1 **Steady Outdoor Load**

For gas wells and liquid wells and pipelines, the outdoor concentration-time profile resembles a step function: zero concentration until the plume arrives, then the maximum concentration given above for the cloud duration time, and then zero concentration once the plume passes by. For a steady outdoor exposure, the exposure duration is equal to the cloud duration, and the integration simplifies to:

$$\overline{L}_O = \frac{t_{cld}}{60} \cdot K_L \cdot \overline{C}_O^n \tag{9.7}$$

where:

\overline{L}_O = average outdoor toxic load (ppmⁿ·min)

t_{cld} = cloud duration (s)

n = exponent in the toxic load model

The AER maximum exposure time is 180 minutes (3 hours).

9.1.2 *Transient Outdoor Load*

For a gas pipeline blowdown, the receptor is exposed to a time varying concentration and the average toxic load for an outdoor exposure is:

$$\overline{L}_O = \frac{K_L}{60} \int_0^{t_{\max}} (\overline{C}_O)^n dt \quad (9.8)$$

The integration is done numerically in time units of seconds and is adjusted to minutes. The AER maximum outdoor exposure time, t_{\max} , is set at 10,800 s (180 minutes or 3 hours).

9.2 Transient Indoor Concentrations

These calculations are performed in AERSLAB with results presented in the new output file. Indoor concentrations are estimated based on a pollutant mass balance within the building (Wilson 1979, Wilson and Zelt, 1990), which gives the differential equation:

$$\tau_b \cdot \frac{d\overline{C}_i}{dt'} + \overline{C}_i = \overline{C}_o(t') \quad (9.9)$$

The general solution for any time varying outdoor concentration is given by:

$$\overline{C}_i(t') = \exp\left(\frac{-t'}{\tau_b}\right) \cdot \int_0^{t_{\max}} \overline{C}_o(t') \cdot \exp\left(\frac{t'}{\tau_b}\right) dt' \quad (9.10)$$

where:

\overline{C}_i = the indoor ‘well-stirred’ average H₂S concentration (ppm)

$\overline{C}_o(t')$ = time varying outdoor H₂S concentration (ppm) for averaging time

$$\tau_b = 3600 / ACH \quad (9.11)$$

= building time constant (s)

ACH = Air Changes per Hour of building

t' = time after plume arrives at building (s)

t_{max} = AER maximum indoor exposure time is set at 10,800 s

The default air changes per hour have increased from 0.5 used in ERCBH2S to 0.86 in AERH2S:

Building air changes per hour, <i>ACH</i>	Range 0.1 to 5.0	Default 0.86
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There are several methods to determine the building air infiltration. The Wilson/Walker method created in Alberta is the AIM(2.0) model, which measures the infiltration over a range and then reports the ACH4 (delta pressure=4 Pa) which represents the natural air change levels. Another common method is the LBL (Lawrence Berkely Labs) method developed by Max Sherman, which pressurizes the house to 50 Pa and determines the air infiltration rate, ACH50. The LBL method was adopted for the ASHRAE standard. This is the accepted approach to determine the air infiltration rate for energy efficiency. There are differences between the details, but AIM appears to be better for Canada because it accounts for such things as a furnace flue.

The ACH50 can be related to the ACH4 using:

$$ACH_4 = ACH_{50} \left(\frac{4}{50} \right)^n \tag{9.12}$$

Where AIM uses $n=2/3$

In AERSLAB the code from the SHELTER/EXPOSURE model is used to estimate the meteorological effects of wind speed and temperature on the ACH4 to create the ACHn (ACH natural or local value). This is based upon the AIMS (2.0) model.

From the Ismaiel et al (2019, 2022) studies, the ACH4 can be calculated based upon the large data set of ACH50 for homes in Canada (73,450), and looking at only Alberta, the plot below shows the variation with age for various dwelling types.

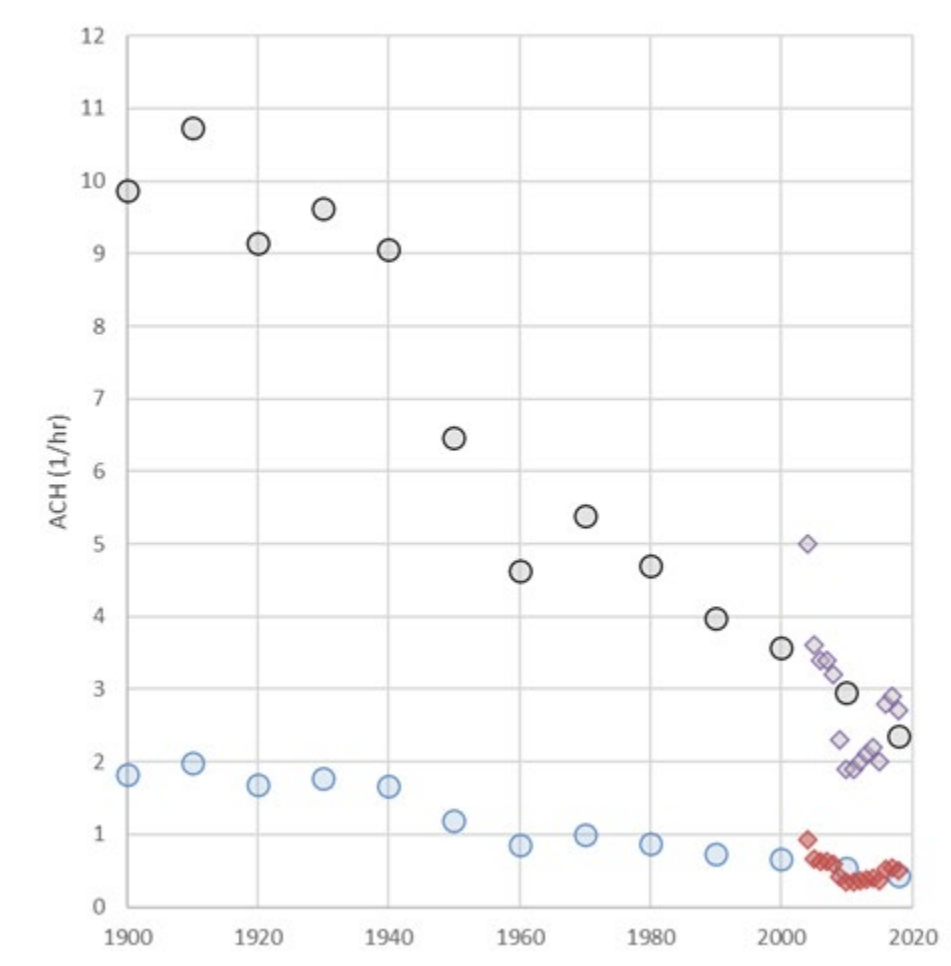


Figure 9-1: Variation with Age for Various Dwelling Types, Ismaiel et al (2019, 2022)

Most of the dwellings in Alberta are single detached homes (dark grey circles), so likely safe to use above ACH50 for all dwellings. By combining the Dwelling age and the ACH4, the estimated age weighted average ACH4=0.86.

Using the meteorology probabilities for wind speed and temperature, the meteorology weighted average is ACHn=1.1, with a minimum of ACHn=0.21, a 10% value of ACHn=.24 (Class A or F, 1.5 m/s), a 90% value of ACHn=2.1 (Class C or D, 8 m/s), and a maximum of ACHn=7.2 (D/20 m/s).

9.2.1 Indoor Load for Steady Outdoor Concentration

Steady outdoor concentrations for gas wells or liquid pipelines or wells are modelled with a step function to \bar{C}_o yielding a solution of the differential equation:

$$\bar{C}_i(t') = \bar{C}_o \cdot \left(1 - \exp\left(\frac{-t'}{\tau_b}\right) \right) \tag{9.13}$$

The maximum indoor concentration for a well release is obtained by substituting the cloud duration t_{cld} for t' . The average indoor toxic load is integrated numerically in time units of seconds and adjusted to minutes from:

$$\bar{L}_I = \frac{1}{60} \cdot \int_0^{t_{max}} \bar{C}_i^n(t') dt \quad (9.14)$$

Indoor concentration fluctuations are dampened and are not included in determining the toxic load within the building. The AER maximum indoor exposure time, t_{max} , is set at 10,800 s (3 hours).

9.2.2 Indoor Load for Transient Outdoor Concentration

For transient outdoor concentrations associated with a blowdown of a gas pipeline, it is necessary to integrate the general solution numerically (Wilson 1990) to obtain the indoor concentration:

$$\bar{C}_{i,j} = \bar{C}_{o,j} + (\bar{C}_{i,j-1} - \bar{C}_{o,j-1}) \cdot \exp\left(\frac{-\Delta t}{\tau_b}\right) - (\bar{C}_{o,j} - \bar{C}_{o,j-1}) \cdot \left(\frac{\tau_b}{\Delta t}\right) \left(1 - \exp\left(\frac{-\Delta t}{\tau_b}\right)\right) \quad (9.15)$$

with

$$\Delta t = t_j - t_{j-1} \quad (9.16)$$

Logarithmic time steps that approximate equal mass steps are used. The maximum indoor concentration for a pipeline release is also determined for each downwind location. The average toxic load is then obtained by numerically integrating the concentration in time units of seconds and then adjusting to minutes:

$$\bar{L}_I = \frac{1}{60} \cdot \sum_{j=1}^k \bar{C}_{i,j}^n (t_j - t_{j-1}) \quad (9.17)$$

The AER maximum exposure time, t_{max} , is set at 10,800 s (3 hours).

9.3 Hazard Distance Outputs

Plots of the predicted downwind concentrations and toxic load equivalent concentration predictions are provided in AERH2S-inputs workbook and allow the size of the hazard zone to be determined. The hazard zone is the distance to the exposure endpoint. Exposure endpoints relate how long a person can be exposed to a concentration before undesired effects occur. Several endpoints may be specified to provide

varying degrees of response actions planned for in the event of an uncontrolled release of sour gas. This section describes how the endpoints are used in AERH2S.

The selection of endpoints for protecting public safety from exposure to H₂S is discussed in *Volume 2: Emergency Response Planning Endpoints* (Volume 2). Two types of H₂S exposure endpoints are determined in AERSLAB; the traditional threshold average concentration for an averaging time and the toxic load during the exposure duration. Both are defined by concentration-time pairs ($C_{ENDPOINT}$, $t_{ENDPOINT}$).

The planning endpoint specifies the steady H₂S concentration (ppm) for an exposure time (minutes) that defines a toxic load (min ppmⁿ) by:

$$L_{ENDPOINT} = (C_{ENDPOINT})^n \cdot t_{ENDPOINT} \quad (9.18)$$

where n is the toxic load exponent. The endpoint is converted to a toxic load equivalent steady concentration for a reference 3-minute exposure time using:

$$C_{ENDPOINT,3} = C_{ENDPOINT} \cdot \left(\frac{t_{ENDPOINT}}{3} \right)^{\frac{1}{n}} \quad (9.19)$$

This is the steady H₂S concentration over the reference time of 3 minutes that yields the endpoint toxic load defined by ($C_{ENDPOINT}$, $t_{ENDPOINT}$). The average toxic load calculated in AERSLAB includes concentration fluctuations about the average concentration and the transient nature of the predicted concentrations. AERSLAB converts the outdoor and indoor toxic loads as a function of downwind distance to a steady H₂S concentration (ppm) for a reference 3-minute exposure time using:

$$C_{STEADY,3} = \left(\frac{\bar{L}}{3} \right)^{\frac{1}{n}} \quad (9.20)$$

AERH2S determines the distance to both the response and planning toxic load endpoints set by the AER as default inputs.

A horizontal release that is dense results in a ground-based release with the predicted concentrations continually decreasing as the distance from the source increases. The maximum concentration occurs near the source and is often the source H₂S concentration. The distance to the $C_{ENDPOINT,3}$ concentration endpoint is searched for starting from the source.

For a horizontal release that is buoyant and exceeds the lift-off criteria, the predicted concentrations initially decrease from a maximum value as the distance from the source increases. The primary distance to the $C_{ENDPOINT,3}$ concentration endpoint is searched for starting from the source. As the plume travels downwind, it rises and grows in the vertical direction resulting in the predicted ground level

concentrations increasing to a secondary maximum, which may exceed the endpoint. The secondary distance to the $C_{ENDPOINT,3}$ concentration endpoint is searched for starting from the maximum distance and moving towards the source.

In other words, two searches are performed for the distance to the desired endpoint, the primary one from the source to increasing distances (left to right) and the secondary one from the maximum distance modelled to the source (right to left). If the secondary hazard zone does not equal the primary hazard zone, the difference is identified in the AERH2S workbook for emergency response planning considerations.

AERH2S provides the distance to H₂S endpoints for each case in the meteorological matrix (as a function of stability class and wind speed) with a graphical summary.

9.4 H2S Exposure Endpoints

Volume 2 Emergency Response Planning Endpoints defines the default exponent and endpoint pairs for planning hazard zones and are summarized below:

Concentration exponent for toxic load lethality endpoint, n	Default 3.5
Response Endpoint - Toxic Load Equivalent Concentration for Exposure Duration	Default (100 ppm for 150 minutes) which is equivalent to (306 ppm for 3 minutes)
Planning Endpoint - Toxic Load Equivalent Concentration for Exposure Duration	Default (100 ppm for 60 minutes) which is equivalent to (235 ppm for 3 minutes)

The application of the toxic load model with an exponent based on lethality is not valid for exposures to low concentrations of H₂S.

10 SENSITIVITY OF PREDICTIONS TO INPUTS

The sensitivity of AERH2S predictions to the user and AER default inputs will be demonstrated. An Example case for a gas pipeline, gas well and liquid well or liquid pipeline is defined based on typical user inputs. The range of variation in each parameter from the example case is provided below. Default input parameters can be classified into three categories: source, meteorology and exposure parameters. One variable at a time is varied over the range of acceptable inputs for that variable.

10.1 User Inputs

These inputs are on the INPUTS page of AERH2S-inputs. An Example case with the sensitivity range is defined in the following tables. First the sensitivity to inputs that define gas well, gas pipeline and liquid pipeline or liquid well releases are demonstrated and then the composition is changed.

AER Default inputs are in bold font in shaded boxes

10.1.1 Elevation

Parameter/Variable	Units	Sensitivity Range	Example
Average EPZ Elevation, Z_{ASL}	m (ASL)	0 – 3000	1000

10.1.2 Gas Pipeline

Parameter/Variable	Units	Sensitivity Range	Example
Licensed Maximum Operating Pressure, P_l	kPa (gauge)	9930	9930
Expected Maximum Operating Pressure, P_E	kPa (gauge)	1400 – 9930	9930
Pipeline outside diameter, D	mm	114 – 324	168.3
Pipeline wall thickness, t	mm	STD pipe	7.1
Equivalent Segment length between ESD valves, S_{ESD}	m	100 – 30000	3000
Expected and Licensed Maximum H ₂ S, $LH_2S\%=EH_2S\%$	% (dry, mole fraction)	0.01 – 30	10
Minimum Gas Temperature, T_i	°C	-5 – 35	5
ESD Valve Closure Time, t_{close} (done at example LP & PROC sampling time and trigger=1)	s	1 – 60	1

ESD Valve LP Trigger, P_{esd} (done at default PROC)	kPa	993 – 8937	4965
ESD Valve PROC Trigger, dP/dt (done at example LP & PROC sampling time=1)	kPa/s	1–9930	9930
ESD Valve PROC Sampling Time, t_{sample} (done at example LP & PROC trigger=1)	s	1–3600	3600
Manual or Remote Trigger (done at example LP & default PROC)	minutes	60-720	720
Ignition Time (done at example LP & default PROC and manual=60)	minutes	60-720	720

10.1.3 Gas Well

Parameter/Variable	Units	Sensitivity Range	Example
Casing or tubing inside diameter, D	mm	41.4 – 331.2	165.6
Maximum Expected H_2S , $EH_2S\%$ (with choked flow diameter)	% (dry, mole fraction)	1 – 30	10.0
H_2S release rate, H_2S_{RR} (with choked flow diameter)	m^3/s at T_{REF} and P_{REF}	0.01 – 24	2.0
Release Time Before Ignition, TSD	minutes	15 – 720	720

10.1.4 Liquid Pipeline/Well

Parameter/Variable	Units	Sensitivity Range	Example
Maximum Licensed Operating pressure, P_i	kPa (gauge)	1400	1400
Oil and Water Production Capacity, Q_{LIQUID}	m^3/d	1-10000	100
Pipeline outside diameter, D	mm	60 – 406	168.3
Pipeline wall thickness, t	mm	STD pipe	7.1
Equivalent Segment length between ESD valves, S_{ESD}	m	1000	1000
Gas to Liquid Ratio, GLR	m^3/m^3	1-1000	100
Expected and Licensed Maximum H_2S , $H_2S\%$	% (dry, mole fraction)	0.01 – 30	10.0
Expected Minimum Liquid Temperature, T_i	$^{\circ}C$	-5 – 35	5
Release Time Before Flow Shut-in, TSD	minutes	60 - 720	720

10.1.5 Sour Gas Composition

The Example is based on the average compositions for sour gas wells in Alberta. The H_2S concentration will be varied and the program will adjust the composition for the example, methane based and acid gas.

Component mole fractions	Example	Methane Based	Acid Gas
H ₂	0.0000		
He	0.0006		
N ₂	0.0283		
CO ₂	0.0427		1-(%EH2S/100)
H ₂ S	0.0259	(%EH2S/100)	(%EH2S/100)
CH ₄	0.8137	1-(%EH2S/100)	
C ₂ H ₆	0.0488		
C ₃ H ₈	0.0208		
i-C ₄ H ₁₀	0.0036		
n-C ₄ H ₁₀	0.0065		
i-C ₅ H ₁₂	0.0020		
n-C ₅ H ₁₂	0.0021		
n-C ₆ H ₁₄	0.0020		
n-C ₇ H ₁₆ ⁺	0.0030		
Total	1.0000	1.0000	1.0000

10.2 ERCB Default Inputs

The sensitivity testing to default source, meteorology and exposure parameters is summarized in the following tables.

10.2.1 Source Parameters

Gas Pipeline	Units	Sensitivity Range	Example
Release Angle		Horizontal, Vertical	Horizontal
D Plane Drag Coefficient, C_d		0.0 – 1.0	0.5
Released Gas Water Content W	mg/m ³ at T_{REF} and P_{REF}	0 – 10 ⁴	0
Gas Pipeline Release Height, h_s	m	0.0 – 2.0	0.0
Pipe Absolute Roughness, ϵ	mm	0.02 – 0.1	0.05
Blowdown Inertial Delay Factor, K_i		0.25 – 0.75	0.5

Gas Well	Units	Sensitivity Range	Example
Release Angle		Horizontal, Vertical	Horizontal
D Plane Drag Coefficient, C_d		0 – 1	0.5
Released Gas Water Content W	mg/m ³ at T_{REF} and P_{REF}	0 – 10 ⁴	0
Stagnation Temperature, T_i	°C	-50 – +50	-22.86
Gas Well Release Height, h_s	m	0 – 10	1.0

Liquid Pipeline/Well	Units	Sensitivity Range	Example
Released Gas Water Content W	mg/m ³ at T_{REF} and P_{REF}	0 – 10 ⁴	0

10.2.2 Meteorology

Parameter/Variable	Units	Sensitivity Range	Example
Ambient Temperature, T_A	°C	-35 - 35	5.0
Relative Humidity, RH	%	0 - 100	60
Ambient Measurement Height, Z_a	m	3-30	4.0
Surface Roughness Height, Z_o	m	0.0001 - 10.0	0.1

Fifty-four combinations of wind speed and stability class are used, as listed in Section 7.1.

10.2.3 Exposure

Parameter/Variable	Units	Sensitivity Range	Example
Planning Endpoint, $TCPI$ ($TCPI$ =Toxic Load Equivalent Concentration)	H2S ppm	100	100
Planning Endpoint Duration	minutes	3 – 180	60
Concentration Exponent for Toxic Load, n		2.5 – 3.5	3.50
Response Endpoint, $TCRe$ ($TCRe$ =Toxic Load Equivalent Concentration)	H2S ppm	100	100
Response Endpoint Duration	minutes	3 – 180	150
Building Air Changes per Hour, ACH	1/h	0.2 – 5.0	0.50
Maximum Exposure Time	s	3600 – 10800	10800
Reference Total Fluctuation Intensity, i_{ref}		0.1 – 0.5	0.25

10.3 Gas Pipeline Sensitivity

Variable Changed from Example with Example in Bold	IIZ Initial Isolation Zone	PAZ Protective Awareness Zone	EPZ Emergency Planning Zone	ERCBH2S EPZ Emergency Planning Zone
User Inputs	km	km	km	km
Gas Pipeline Example	0.86	2.30	2.86	2.5
Expected Maximum Operating Pressure 1400 kPa (gauge)	0.28	0.80	0.97	0.76
Expected Maximum Operating Pressure 3000 kPa (gauge)	0.44	1.25	1.55	1.17
Expected Maximum Operating Pressure 6000 kPa (gauge)	0.69	2.00	2.49	1.84
Expected Maximum Operating Pressure 9930 kPa (gauge)	0.86	2.30	2.86	2.5
Equivalent Segment Length between ESDs 100 m	0.72	2.15	2.68	2.3
Equivalent Segment Length between ESDs 300 m	0.77	2.16	2.7	2.34
Equivalent Segment Length between ESDs 1000 m	0.81	2.20	2.75	2.37
Equivalent Segment Length between ESDs 3000 m	0.86	2.30	2.86	2.5
Equivalent Segment Length between ESDs 10000 m	0.95	2.68	3.24	3.03
Equivalent Segment Length between ESDs 30000 m	1.03	4.52	5.38	3.75
Pipe Diameter 4"	0.36	0.95	1.17	1.05
Pipe Diameter 6"	0.62	1.63	2.01	1.73
Pipe Diameter 8"	0.86	2.30	2.86	2.5
Pipe Diameter 10"	1.14	3.17	3.98	3.46
Pipe Diameter 12"	1.40	4.09	5.14	4.46
Expected H2S 0.01%	0.00	0.00	0.01	0.01
Expected H2S 0.03%	0.00	0.01	0.01	0.03
Expected H2S 0.1%	0.01	0.02	0.02	0.11
Expected H2S 0.3%	0.02	0.07	0.1	0.26
Expected H2S 1%	0.07	0.34	0.45	0.59
Expected H2S 3%	0.29	0.97	1.22	1.17
Expected H2S 10%	0.86	2.30	2.86	2.5
Expected H2S 30%	1.69	4.79	5.86	5.4
Gas Temperature -5C	0.83	2.23	2.76	2.72
Gas Temperature +5C	0.86	2.30	2.86	2.5
Gas Temperature +15C	0.96	2.73	3.37	2.45
Gas Temperature +25C	0.95	2.74	3.42	2.4
Gas Temperature +35C	0.92	2.69	3.37	2.2
ESD Closure Time 1 s	0.44	1.07	1.29	1.34
ESD Closure Time 10 s	0.44	1.08	1.29	1.35
ESD Closure Time 30 s	0.44	1.09	1.3	1.37

Variable Changed from Example with Example in Bold	IIZ Initial Isolation Zone	PAZ Protective Awareness Zone	EPZ Emergency Planning Zone	ERCBH2S EPZ Emergency Planning Zone
ESD Closure Time 60 s	0.44	1.10	1.31	1.42
ESD Low Pressure Trigger 993 kpa (gauge)	1.07	4.90	6.15	3.95
ESD Low Pressure Trigger 1986 kpa (gauge)	1.07	3.64	4.55	3.78
ESD Low Pressure Trigger 2979 kpa (gauge)	1.07	3.07	3.85	3.35
ESD Low Pressure Trigger 3972 kpa (gauge)	0.86	2.70	3.36	2.92
ESD Low Pressure Trigger 4965 kpa (gauge)	0.86	2.30	2.86	2.5
ESD Low Pressure Trigger 5958 kpa (gauge)	0.79	2.07	2.56	2.19
ESD Low Pressure Trigger 6951 kpa (gauge)	0.65	1.78	2.2	1.94
ESD Low Pressure Trigger 7944 kpa (gauge)	0.56	1.49	1.84	1.69
ESD Low Pressure Trigger 8937 kpa (gauge)	0.44	1.19	1.48	1.48
ESD Pressure Rate of Change Trigger 1 kPa/s	0.19	1.07	1.28	1.34
ESD Pressure Rate of Change Trigger 10 kPa/s	0.44	1.07	1.28	1.35
ESD Pressure Rate of Change Trigger 100 kPa/s	0.86	2.30	2.86	2.45
ESD Pressure Rate of Change Trigger 1000 kPa/s	0.86	2.30	2.86	2.49
ESD Pressure Rate of Change Trigger 9930 kPa/s	0.86	2.30	2.86	2.5
ESD Pressure Rate of Change Sampling Time 1 s	0.19	1.07	1.28	1.34
ESD Pressure Rate of Change Sampling Time 5 s	0.19	1.07	1.28	1.34
ESD Pressure Rate of Change Sampling Time 15 s	0.19	1.07	1.29	1.35
ESD Pressure Rate of Change Sampling Time 30 s	0.19	1.09	1.3	1.39
ESD Pressure Rate of Change Sampling Time 60 s	0.19	1.20	1.38	1.47
ESD Pressure Rate of Change Sampling Time 120 s	0.20	1.26	1.46	1.6
ESD Pressure Rate of Change Sampling Time 180 s	0.20	1.36	1.58	1.67
ESD Pressure Rate of Change Sampling Time 240 s	0.20	1.47	1.7	1.77
ESD Pressure Rate of Change Sampling Time 300 s	0.21	1.57	1.85	1.83
ESD Pressure Rate of Change Sampling Time 900 s	0.56	2.29	2.86	2.5
ESD Pressure Rate of Change Sampling Time 1800 s	0.86	2.30	2.86	2.5
ESD Pressure Rate of Change Sampling Time 3600 s	0.86	2.30	2.86	2.5
Manual ESD Closure Time 60 minutes	0.56	2.29	2.86	2.5
Manual ESD Closure Time 120 minutes	0.64	2.29	2.86	2.5
Manual ESD Closure Time 180 minutes	0.73	2.29	2.86	2.5
Manual ESD Closure Time 360 minutes	0.86	2.30	2.86	2.5
Manual ESD Closure Time 720 minutes	0.86	2.30	2.86	2.5
Ignition Time 60 minutes	0.56	2.29	2.85	2.5
Ignition Time 120 minutes	0.56	2.29	2.86	2.51
Ignition Time 180 minutes	0.56	2.29	2.86	2.5
Ignition Time 360 minutes	0.56	2.29	2.86	2.5

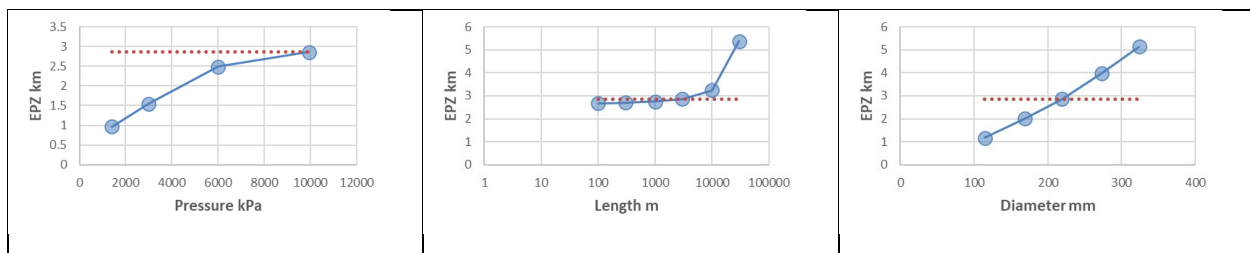
Variable Changed from Example with Example in Bold	IIZ Initial Isolation Zone	PAZ Protective Awareness Zone	EPZ Emergency Planning Zone	ERCBH2S EPZ Emergency Planning Zone
Ignition Time 720 minutes	0.56	2.29	2.86	2.5
Elevation 0 m	0.81	2.15	2.67	2.35
Elevation 1000 m	0.86	2.30	2.86	2.5
Elevation 2000 m	0.93	2.45	3.06	2.68
Elevation 3000 m	0.99	2.66	3.32	2.91
Drag Coefficient 0.0	0.68	1.84	2.28	2.54
Drag Coefficient 0.1	0.73	1.96	2.44	2.54
Drag Coefficient 0.2	0.77	2.16	2.68	2.54
Drag Coefficient 0.3	0.78	2.23	2.77	2.54
Drag Coefficient 0.4	0.84	2.29	2.84	2.52
Drag Coefficient 0.5	0.86	2.30	2.86	2.5
Drag Coefficient 0.6	0.89	2.31	2.88	2.56
Drag Coefficient 0.7	0.90	2.34	2.94	2.6
Drag Coefficient 0.8	0.91	2.42	3.07	2.62
Drag Coefficient 0.9	0.95	2.62	3.3	2.6
Drag Coefficient 1.0	1.13	3.05	3.74	2.55
Ambient Temperature -35C	0.89	2.34	2.91	2.34
Ambient Temperature -25C	0.88	2.33	2.9	2.52
Ambient Temperature -15C	0.88	2.32	2.89	2.42
Ambient Temperature -5C	0.87	2.31	2.87	2.44
Ambient Temperature +5C	0.86	2.29	2.86	2.5
Ambient Temperature +15C	0.86	2.28	2.84	2.6
Ambient Temperature +25C	0.85	2.27	2.82	2.75
Ambient Temperature +35C	0.84	2.26	2.81	2.87
Relative Humidity 0%	0.87	2.31	2.88	2.49
Relative Humidity 20%	0.87	2.31	2.87	2.5
Relative Humidity 40%	0.87	2.30	2.87	2.5
Relative Humidity 60%	0.86	2.30	2.86	2.5
Relative Humidity 80%	0.86	2.28	2.85	2.49
Relative Humidity 100%	0.97	2.77	3.46	2.5
Anemometer Height 3 m	0.81	2.12	2.63	2.33
Anemometer Height 4 m	0.86	2.30	2.86	2.5
Anemometer Height 5 m	0.92	2.47	3.07	2.68
Anemometer Height 6 m	0.97	2.66	3.32	2.85
Anemometer Height 7 m	1.02	2.81	3.53	3.02
Anemometer Height 8 m	1.07	2.95	3.74	3.19

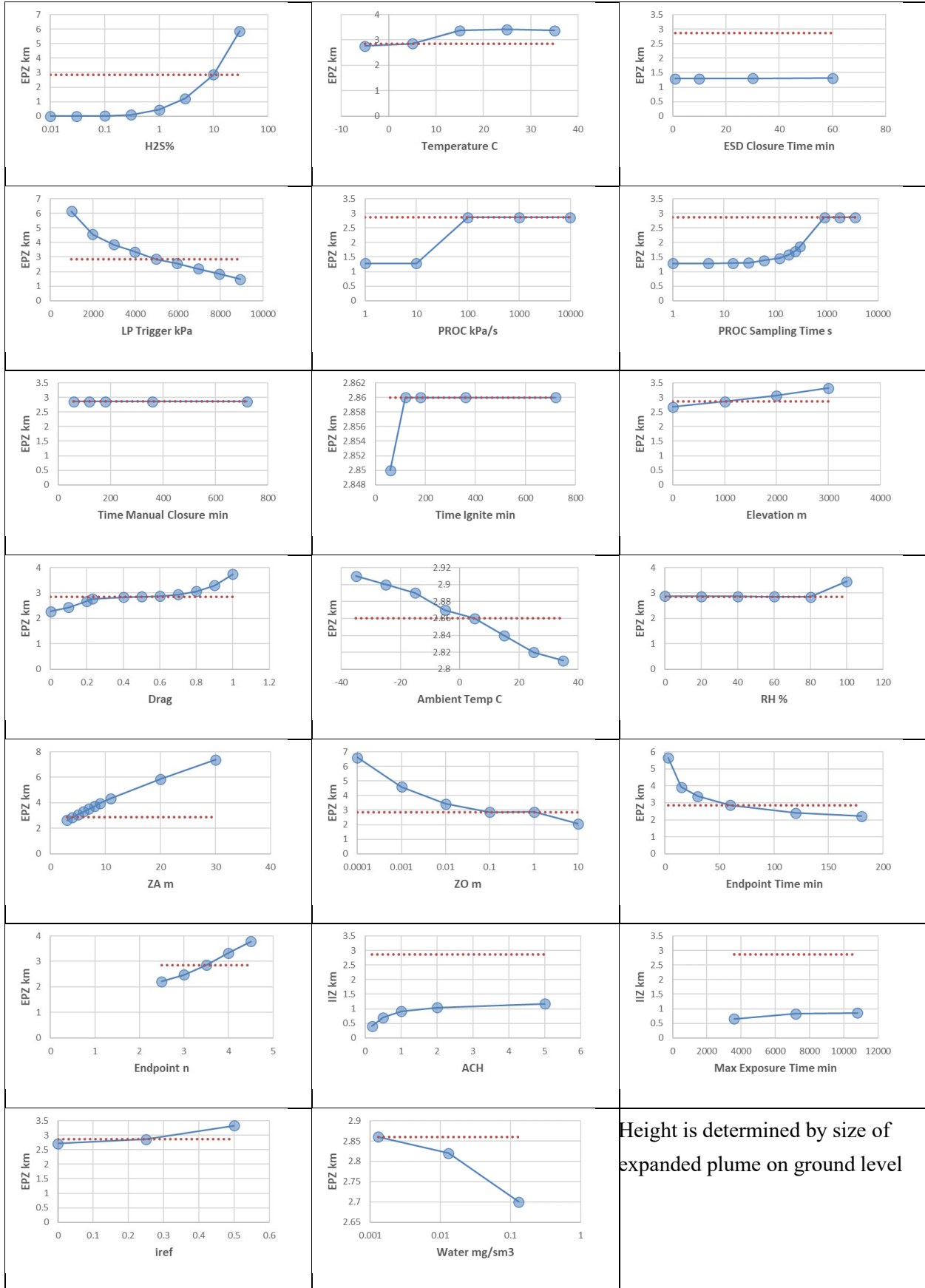
Variable Changed from Example with Example in Bold	IIZ Initial Isolation Zone	PAZ Protective Awareness Zone	EPZ Emergency Planning Zone	ERCBH2S EPZ Emergency Planning Zone
Anemometer Height 9 m	1.12	3.11	3.97	3.34
Anemometer Height 10 m	1.21	3.40	4.34	3.5
Anemometer Height 20 m	1.51	4.55	5.85	5.02
Anemometer Height 30 m	1.75	5.68	7.38	6.07
Surface Roughness 0.0001 m	1.75	5.27	6.61	6.97
Surface Roughness 0.001 m	1.29	3.65	4.59	4.54
Surface Roughness 0.01 m	1.00	2.76	3.44	3.27
Surface Roughness 0.1 m	0.86	2.30	2.86	2.5
Surface Roughness 1 m	1.02	2.41	2.88	2.06
Surface Roughness 10 m	0.64	1.81	2.06	1.39
Endpoint Duration 3 minutes	5.65	1.80	5.65	4.28
Endpoint Duration 15 minutes	3.92	1.22	3.92	3.19
Endpoint Duration 30 minutes	3.39	1.03	3.39	2.83
Endpoint Duration 60 minutes	2.86	0.86	2.86	2.5
Endpoint Duration 120 minutes	2.40	0.73	2.4	2.24
Endpoint Duration 180 minutes	2.21	0.65	2.21	2.1
Exponent 2.5	0.95	1.62	2.21	1.99
Exponent 3	0.90	1.93	2.48	2.25
Exponent 3.5	0.86	2.30	2.86	2.5
Exponent 4	0.84	2.75	3.33	2.78
Exponent 4.5	0.83	3.24	3.78	3.08
Air Changes per Hour 0.2	0.41	2.30	2.86	2.5
Air Changes per Hour 0.5	0.70	2.30	2.86	2.5
Air Changes per Hour 1	0.91	2.30	2.86	2.5
Air Changes per Hour 2	1.04	2.30	2.86	2.5
Air Changes per Hour 5	1.17	2.30	2.86	2.5
Maximum Exposure Time 3600 s	0.66	2.29	2.86	2.5
Maximum Exposure Time 7200 s	0.83	2.30	2.86	2.5
Maximum Exposure Time 10800 s	0.86	2.30	2.86	2.5
Fluctuation Intensity iref 0	0.86	2.19	2.71	2.41
Fluctuation Intensity iref 0.25	0.86	2.30	2.86	2.5
Fluctuation Intensity iref 0.5	0.86	2.68	3.33	2.79
Water Content 0.0000 (0 mg/m³)	0.86	2.30	2.86	2.5
Water Content 0.0013 (1000 mg/m³)	0.86	2.29	2.86	2.49
Water Content 0.0131 (10000 mg/m³)	0.85	2.27	2.82	2.49
Water Content 0.1312 (100000 mg/m³)	0.78	2.16	2.7	2.43

Variable Changed from Example with Example in Bold	IIZ Initial Isolation Zone	PAZ Protective Awareness Zone	EPZ Emergency Planning Zone	ERCBH2S EPZ Emergency Planning Zone
Pipeline Release Height 0 m	0.86	2.30	2.86	2.5
Pipeline Release Height 1 m	0.86	2.30	2.86	2.56
Pipeline Release Height 2 m	0.86	2.30	2.86	2.58
Release Angle 1 Horizontal	0.86	2.30	2.86	2.5
Release Angle 2 Vertical	0.81	1.92	2.34	2.24
Pipe Absolute Roughness 0.02 mm	0.88	2.51	3.13	2.62
Pipe Absolute Roughness 0.05 mm	0.87	2.43	3.04	2.5
Pipe Absolute Roughness 0.1 mm	0.86	2.30	2.86	2.44
Inertial Delay Factor Ki 0.25	0.86	2.34	2.91	2.52
Inertial Delay Factor Ki 0.5	0.86	2.30	2.86	2.5
Inertial Delay Factor Ki .75	0.87	2.38	2.95	2.52
Expected H2S 1% (rest CH4)	0.07	0.35	0.47	0.41
Expected H2S 3% (rest CH4)	0.34	1.20	1.51	0.83
Expected H2S 10% (rest CH4)	1.06	3.01	3.72	2.36
Expected H2S 30% (rest CH4)	2.07	5.87	6.81	5.23
Expected H2S 1% (rest CO2)	0.06	0.32	0.41	Err
Expected H2S 3% (rest CO2)	0.12	0.81	0.94	Err
Expected H2S 10% (rest CO2)	0.31	1.81	2.14	Err
Expected H2S 30% (rest CO2)	0.70	4.08	5.04	8.88

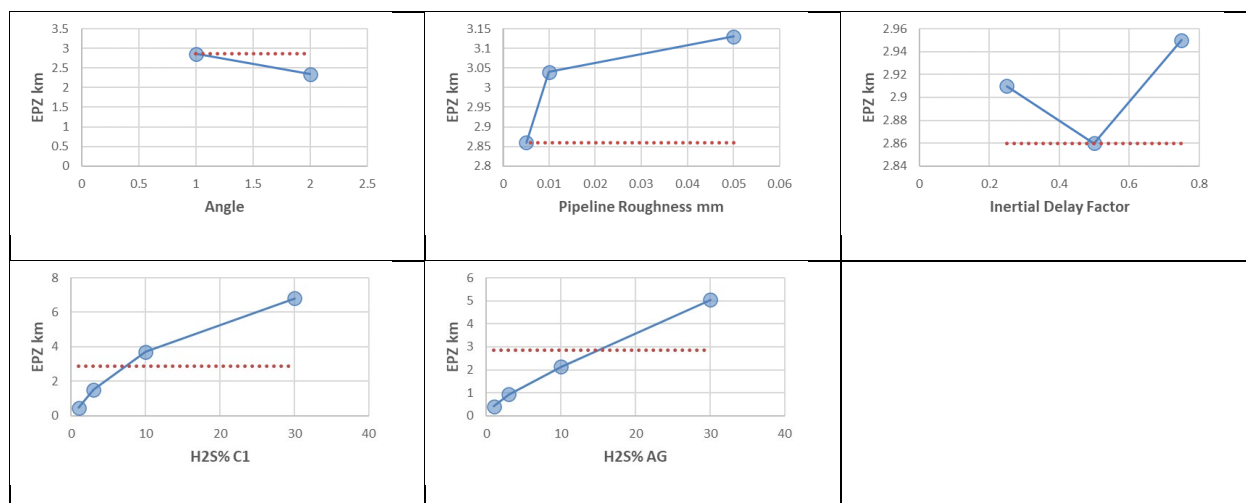
10.3.1 Gas Pipeline Sensitivity Figures

Figures show EPZ vs Sensitivity Parameter as per sensitivity ranges listed in Section 10.1 for gas pipelines. The red dotted line on each figure is the base case scenario EPZ (km).





Height is determined by size of expanded plume on ground level



10.4 Gas Well Sensitivity

Variable Changed from Example with Example in Bold	IIZ Initial Isolation Zone	PAZ Protective Awareness Zone	EPZ Emergency Planning Zone	ERCBH2S EPZ Emergency Planning Zone
User Inputs	km	km		km
Well Example (Base Drilling)	0.96	2.23	2.73	1.86
Servicing	0.96	2.23	2.73	1.86
Producing	0.84	2.27	2.83	0.91
0.25*Inside Diameter	0.94	2.33	2.88	2.09
0.5*Inside Diameter	0.98	2.41	2.97	2.01
Inside Diameter	0.96	2.23	2.73	1.86
1.5*Inside Diameter	1.04	2.34	2.85	1.85
2*Inside Diameter	1.05	2.22	2.66	1.86
Expected H2S 0.01% (choked flow diameter)	Err	Err	Err	0.31
Expected H2S 0.03% (choked flow diameter)	Err	Err	Err	0.34
Expected H2S 0.1% (choked flow diameter)	0.09	0.23	0.32	0.38
Expected H2S 0.3% (choked flow diameter)	0.11	0.45	0.66	0.56
Expected H2S 1% (choked flow diameter)	0.22	1.08	1.47	0.66
Expected H2S 3% (choked flow diameter)	0.56	1.57	1.99	0.86
Expected H2S 10% (choked flow diameter)	0.96	2.23	2.73	1.86
Expected H2S 30% (choked flow diameter)	1.39	2.91	3.5	2.08
H2S Release Rate 0.01 m ³ /s (choked flow diameter)	0.03	0.06	0.07	0.1

Variable Changed from Example with Example in Bold	IIZ Initial Isolation Zone	PAZ Protective Awareness Zone	EPZ Emergency Planning Zone	ERCBH2S EPZ Emergency Planning Zone
H2S Release Rate 0.1 m3/s (choked flow diameter)	0.16	0.32	0.38	0.36
H2S Release Rate 0.3 m3/s (choked flow diameter)	0.43	0.90	1.07	0.66
H2S Release Rate 1 m3/s (choked flow diameter)	0.75	1.73	2.09	1.33
H2S Release Rate 2 m3/s (choked flow diameter)	0.96	2.23	2.73	1.86
H2S Release Rate 6 m3/s (choked flow diameter)	1.98	4.74	5.85	1.61
H2S Release Rate 12 m3/s (choked flow diameter)	2.67	6.39	7.95	2.01
H2S Release Rate 24 m3/s (choked flow diameter)	4.71	12.22	15.47	2.64
Ignition Time 15 minutes	0.22	1.20	1.5	1.11
Ignition Time 30 minutes	0.40	1.45	1.79	1.31
Ignition Time 60 minutes	0.63	1.72	2.12	1.5
Ignition Time 120 minutes	0.87	2.02	2.47	1.71
Ignition Time 180 minutes	0.96	2.23	2.73	1.86
Ignition Time 360 minutes	0.96	2.23	2.73	1.86
Ignition Time 720 minutes	0.96	2.23	2.73	1.86
Elevation 0 m	0.90	2.07	2.53	1.72
Elevation 1000 m	0.96	2.23	2.73	1.86
Elevation 2000 m	1.02	2.39	2.92	1.99
Elevation 3000 m	1.11	2.61	3.19	2.15
Drag Coefficient 0.0	0.75	2.09	2.63	0.71
Drag Coefficient 0.1	0.75	2.11	2.66	0.74
Drag Coefficient 0.2	0.79	2.19	2.75	0.87
Drag Coefficient 0.3	0.90	2.34	2.91	1.8
Drag Coefficient 0.4	1.03	2.57	3.16	1.85
Drag Coefficient 0.5	0.96	2.23	2.73	1.86
Drag Coefficient 0.6	1.03	2.33	2.83	1.85
Drag Coefficient 0.7	1.18	2.51	3	1.85
Drag Coefficient 0.8	1.12	2.28	2.73	1.86
Drag Coefficient 0.9	0.64	1.22	1.44	0.87
Drag Coefficient 1.0	0.55	0.95	1.11	0.45
Ambient Temperature -35C	0.96	2.23	2.73	0.82
Ambient Temperature -25C	0.96	2.23	2.73	1.69
Ambient Temperature -15C	0.96	2.23	2.73	1.79
Ambient Temperature -5C	0.96	2.23	2.73	1.82
Ambient Temperature +5C	0.96	2.23	2.73	1.86
Ambient Temperature +15C	0.96	2.23	2.73	2.1
Ambient Temperature +25C	0.96	2.23	2.73	2.1

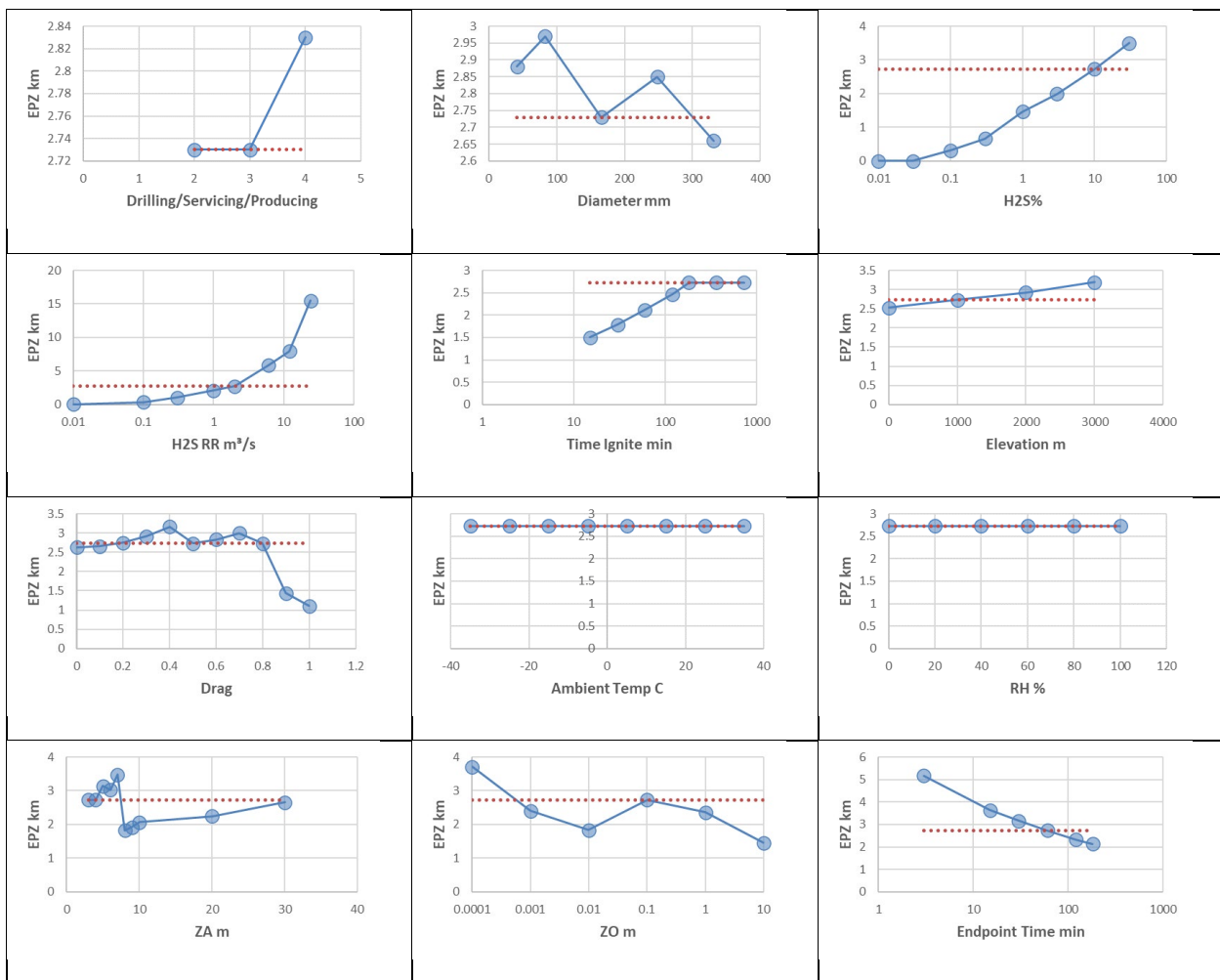
Variable Changed from Example with Example in Bold	IIZ Initial Isolation Zone	PAZ Protective Awareness Zone	EPZ Emergency Planning Zone	ERCBH2S EPZ Emergency Planning Zone
Ambient Temperature +35C	0.96	2.23	2.73	2.14
Relative Humidity 0%	0.96	2.23	2.73	1.86
Relative Humidity 20%	0.96	2.23	2.73	1.86
Relative Humidity 40%	0.96	2.23	2.73	1.86
Relative Humidity 60%	0.96	2.23	2.73	1.86
Relative Humidity 80%	0.96	2.23	2.73	1.86
Relative Humidity 100%	0.96	2.23	2.73	1.86
Anemometer Height 3 m	0.94	2.23	2.73	1.84
Anemometer Height 4 m	0.96	2.23	2.73	1.86
Anemometer Height 5 m	1.10	2.57	3.14	2.02
Anemometer Height 6 m	1.07	2.47	3.03	0.97
Anemometer Height 7 m	1.22	2.84	3.48	1.01
Anemometer Height 8 m	0.66	1.50	1.82	0.93
Anemometer Height 9 m	0.70	1.58	1.92	0.95
Anemometer Height 10 m	0.76	1.72	2.07	0.88
Anemometer Height 20 m	0.86	1.85	2.25	0.78
Anemometer Height 30 m	1.03	2.19	2.66	0.73
Surface Roughness 0.0001 m	1.40	3.03	3.71	0.66
Surface Roughness 0.001 m	0.93	1.99	2.4	0.8
Surface Roughness 0.01 m	0.67	1.52	1.83	0.87
Surface Roughness 0.1 m	0.96	2.23	2.73	1.86
Surface Roughness 1 m	0.98	1.94	2.36	1.53
Surface Roughness 10 m	0.60	1.20	1.46	0.86
Endpoint Duration 3 minutes	1.94	5.17	5.17	3.2
Endpoint Duration 15 minutes	1.34	3.64	3.64	2.38
Endpoint Duration 30 minutes	1.14	3.16	3.16	2.09
Endpoint Duration 60 minutes	0.96	2.73	2.73	1.86
Endpoint Duration 120 minutes	0.80	2.33	2.33	1.63
Endpoint Duration 180 minutes	0.72	2.14	2.14	1.52
Exponent 2.5	1.03	1.68	2.24	1.58
Exponent 3	0.99	1.92	2.43	1.69
Exponent 3.5	0.96	2.23	2.73	1.86
Exponent 4	0.94	2.56	3.03	2.03
Exponent 4.5	0.92	2.92	3.43	2.25
Air Changes per Hour 0.2	0.44	2.23	2.73	1.86
Air Changes per Hour 0.5	0.78	2.23	2.73	1.86

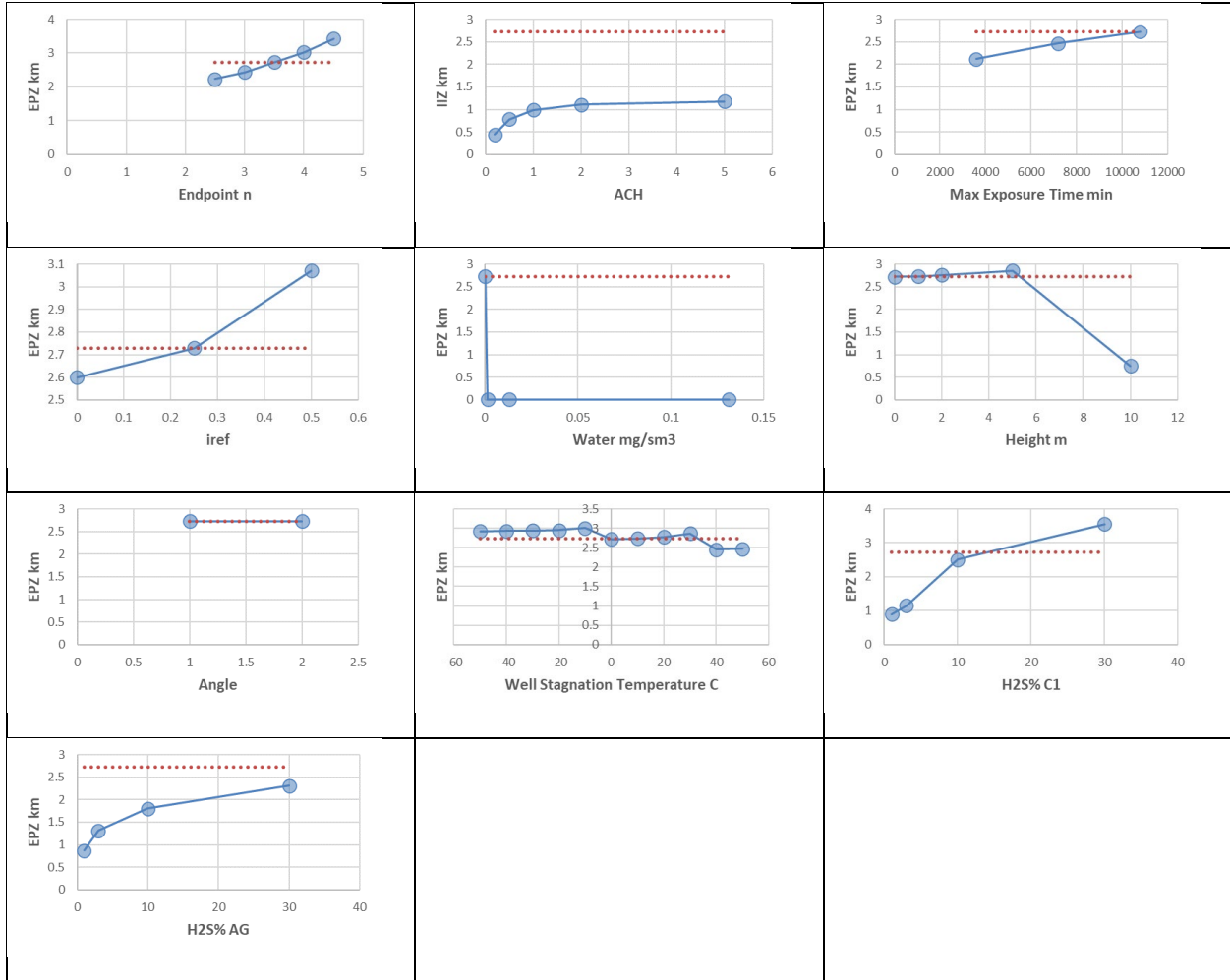
Variable Changed from Example with Example in Bold	IIZ Initial Isolation Zone	PAZ Protective Awareness Zone	EPZ Emergency Planning Zone	ERCBH2S EPZ Emergency Planning Zone
Air Changes per Hour 1	0.99	2.23	2.73	1.86
Air Changes per Hour 2	1.11	2.23	2.73	1.86
Air Changes per Hour 5	1.18	2.23	2.73	1.86
Maximum Exposure Time 3600 s	0.52	1.72	2.12	1.5
Maximum Exposure Time 7200 s	0.80	2.02	2.47	1.71
Maximum Exposure Time 10800 s	0.96	2.23	2.73	1.86
Fluctuation Intensity iref 0	0.96	2.13	2.6	1.78
Fluctuation Intensity iref 0.25	0.96	2.23	2.73	1.86
Fluctuation Intensity iref 0.5	0.96	2.52	3.07	2.05
Water Content 0.0000 (0 mg/m³)	0.96	2.23	2.73	1.86
Water Content 0.0013 (1000 mg/m³)	0.00	0.00	0.01	1.86
Water Content 0.0131 (10000 mg/m³)	0.00	0.00	0.01	1.86
Water Content 0.1312 (100000 mg/m³)	0.00	0.00	0.01	1.85
Well Release Height 0 m	0.96	2.22	2.72	1.85
Well Release Height 1 m	0.96	2.23	2.73	1.86
Well Release Height 2 m	0.98	2.26	2.76	1.87
Well Release Height 5 m	1.02	2.34	2.85	1.92
Well Release Height 10 m	0.30	0.63	0.75	0.5
Release Angle 1 Horizontal	0.96	2.23	2.73	1.86
Release Angle 2 Vertical	0.96	2.23	2.73	0.19
Well Stagnation Temperature -50C	0.99	2.37	2.92	2
Well Stagnation Temperature -40C	0.99	2.38	2.93	2
Well Stagnation Temperature -30C	0.99	2.39	2.94	2.03
Well Stagnation Temperature -20C	0.99	2.40	2.95	1.86
Well Stagnation Temperature -10C	1.01	2.45	3.01	1.89
Well Stagnation Temperature 0C	0.95	2.22	2.72	0.89
Well Stagnation Temperature 10C	0.96	2.24	2.74	0.85
Well Stagnation Temperature 20C	0.98	2.27	2.78	0.85
Well Stagnation Temperature 30C	1.02	2.35	2.87	0.71
Well Stagnation Temperature 40C	0.90	2.02	2.45	0.71
Well Stagnation Temperature 50C	0.91	2.03	2.47	0.68
Expected H2S 1% (choked flow diameter, rest CH4)	0.23	0.71	0.9	0.58
Expected H2S 3% (choked flow diameter, rest CH4)	0.39	0.94	1.15	0.68
Expected H2S 10% (choked flow diameter, rest CH4)	0.94	2.07	2.51	0.89
Expected H2S 30% (choked flow diameter, rest CH4)	1.43	2.95	3.55	2.07
Expected H2S 1% (choked flow diameter, rest CO2)	0.25	0.69	0.87	2.31

Variable Changed from Example with Example in Bold	IIZ Initial Isolation Zone	PAZ Protective Awareness Zone	EPZ Emergency Planning Zone	ERCBH2S EPZ Emergency Planning Zone
Expected H2S 3% (choked flow diameter, rest CO2)	0.39	1.04	1.31	2.44
Expected H2S 10% (choked flow diameter, rest CO2)	0.63	1.46	1.8	2.49
Expected H2S 30% (choked flow diameter, rest CO2)	0.84	1.88	2.31	2.46

10.4.1 Well Sensitivity Figures

Figures show EPZ vs Sensitivity Parameter as per sensitivity ranges listed in Section 10.1 for gas wells. The red dotted line on each figure is the base case scenario EPZ (km).





10.5 Liquid Pipeline/Well Sensitivity

Variable Changed from Example with Example in Bold	IIZ Initial Isolation Zone	PAZ Protective Awareness Zone	EPZ Emergency Planning Zone	ERCBH2S EPZ Emergency Planning Zone
User Inputs	km	km	km	km
Liquid Pipeline Example	0.03	0.08	0.1	0.11
Pipe Diameter 2"	0.05	0.11	0.14	0.11
Pipe Diameter 3"	0.04	0.10	0.12	0.11
Pipe Diameter 4"	0.03	0.08	0.1	0.11

Variable Changed from Example with Example in Bold	IIZ Initial Isolation Zone	PAZ Protective Awareness Zone	EPZ Emergency Planning Zone	ERCBH2S EPZ Emergency Planning Zone
Pipe Diameter 6"	0.03	0.09	0.11	0.11
Pipe Diameter 8"	0.03	0.09	0.11	0.1
Pipe Diameter 10"	0.02	0.06	0.07	0.1
Pipe Diameter 12"	0.02	0.05	0.07	0.1
Pipe Diameter 14"	0.02	0.06	0.07	0.1
Pipe Diameter 16"	0.02	0.06	0.07	0.1
Expected H2S 0.01%	0.00	0.00	0.01	0.01
Expected H2S 0.03%	0.00	0.00	0.01	0.01
Expected H2S 0.1%	0.00	0.00	0.01	0.01
Expected H2S 0.3%	0.00	0.00	0.01	0.02
Expected H2S 1%	0.00	0.00	0.01	0.03
Expected H2S 3%	0.01	0.02	0.03	0.05
Expected H2S 10%	0.03	0.08	0.1	0.11
Expected H2S 30%	0.10	0.23	0.28	0.2
Liquid Temperature -5C	0.03	0.09	0.12	0.11
Liquid Temperature 5C	0.03	0.08	0.1	0.11
Liquid Temperature 15C	0.02	0.06	0.08	0.11
Liquid Temperature 25C	0.03	0.08	0.09	0.11
Liquid Temperature 35C	0.03	0.10	0.12	0.11
Gas to Liquid Ratio 1	0.00	0.00	0.01	0.01
Gas to Liquid Ratio 3	0.00	0.00	0.01	0.02
Gas to Liquid Ratio 10	0.00	0.01	0.02	0.03
Gas to Liquid Ratio 30	0.01	0.03	0.04	0.06
Gas to Liquid Ratio 100	0.03	0.08	0.1	0.11
Gas to Liquid Ratio 300	0.08	0.20	0.25	0.2
Gas to Liquid Ratio 1000	0.18	0.43	0.52	0.38
Liquid Flow Rate 1 m3/d	0.00	0.00	0.01	0.01
Liquid Flow Rate 3 m3/d	0.00	0.00	0.01	0.02
Liquid Flow Rate 10 m3/d	0.00	0.01	0.01	0.03
Liquid Flow Rate 30 m3/d	0.01	0.03	0.03	0.06
Liquid Flow Rate 100 m3/d	0.03	0.08	0.1	0.11
Liquid Flow Rate 300 m3/d	0.09	0.22	0.26	0.2
Liquid Flow Rate 1000 m3/d	0.24	0.50	0.6	0.38
Liquid Flow Rate 3000 m3/d	0.47	0.96	1.15	0.71
Liquid Flow Rate 10000 m3/d	1.00	2.02	2.44	1.33
Ignition Time 15 minutes	0.01	0.05	0.06	0.09

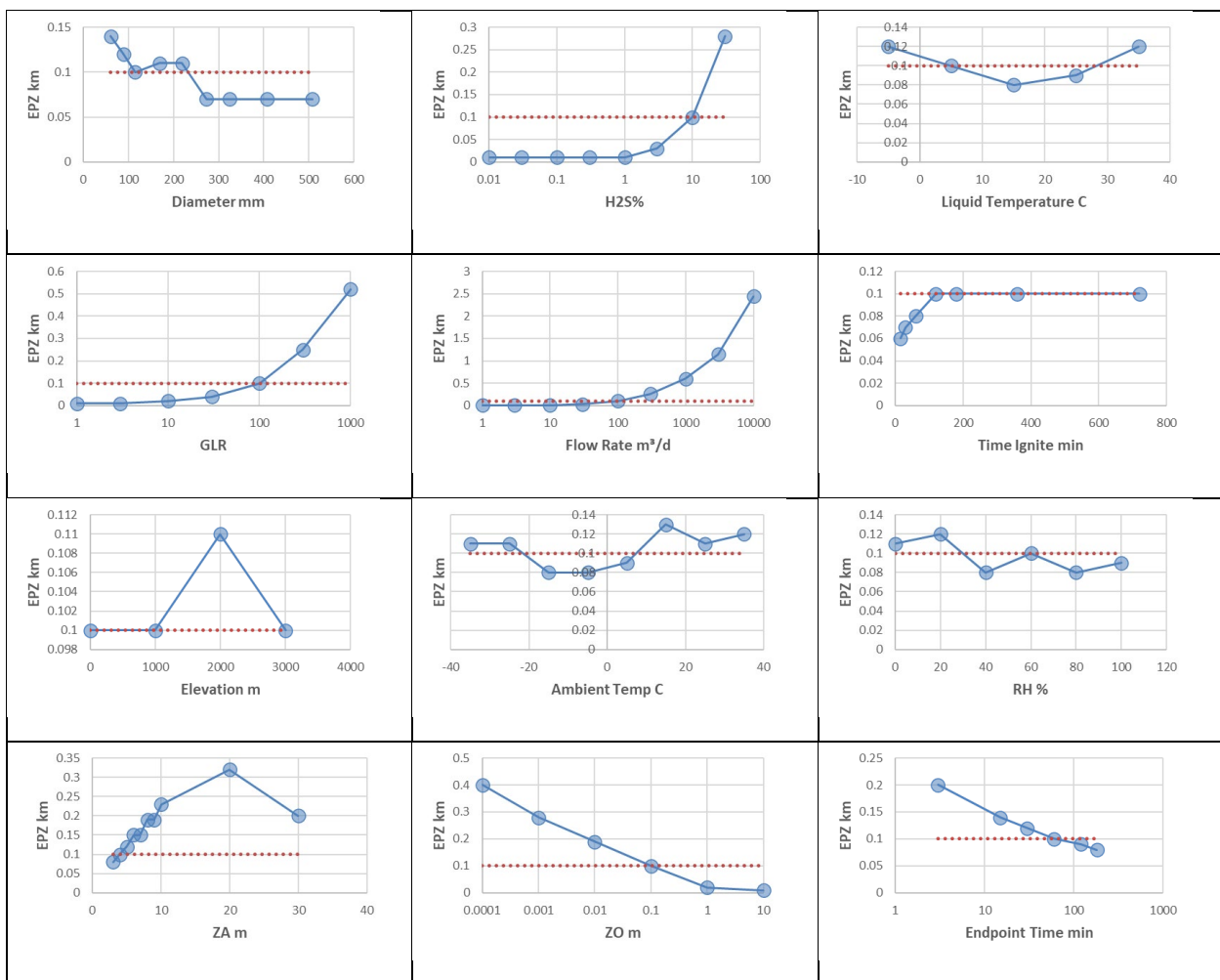
Variable Changed from Example with Example in Bold	IIZ Initial Isolation Zone	PAZ Protective Awareness Zone	EPZ Emergency Planning Zone	ERCBH2S EPZ Emergency Planning Zone
Ignition Time 30 minutes	0.01	0.05	0.07	0.09
Ignition Time 60 minutes	0.02	0.06	0.08	0.09
Ignition Time 120 minutes	0.03	0.08	0.1	0.1
Ignition Time 180 minutes	0.03	0.08	0.1	0.11
Ignition Time 360 minutes	0.03	0.08	0.1	0.11
Ignition Time 720 minutes	0.03	0.08	0.1	0.11
Elevation 0 m	0.03	0.08	0.1	0.1
Elevation 1000 m	0.03	0.08	0.1	0.11
Elevation 2000 m	0.03	0.09	0.11	0.12
Elevation 3000 m	0.03	0.08	0.1	0.12
Ambient Temperature -35C	0.03	0.08	0.11	0.1
Ambient Temperature -25C	0.03	0.08	0.11	0.1
Ambient Temperature -15C	0.02	0.07	0.08	0.1
Ambient Temperature -5C	0.02	0.06	0.08	0.11
Ambient Temperature +5C	0.03	0.07	0.09	0.11
Ambient Temperature +15C	0.04	0.10	0.13	0.11
Ambient Temperature +25C	0.03	0.09	0.11	0.11
Ambient Temperature +35C	0.03	0.10	0.12	0.11
Relative Humidity 0%	0.03	0.08	0.11	0.11
Relative Humidity 20%	0.04	0.10	0.12	0.11
Relative Humidity 40%	0.02	0.06	0.08	0.11
Relative Humidity 60%	0.03	0.08	0.1	0.11
Relative Humidity 80%	0.02	0.06	0.08	0.11
Relative Humidity 100%	0.03	0.07	0.09	0.11
Anemometer Height 3 m	0.02	0.06	0.08	0.1
Anemometer Height 4 m	0.03	0.08	0.1	0.11
Anemometer Height 5 m	0.04	0.10	0.12	0.12
Anemometer Height 6 m	0.05	0.13	0.15	0.12
Anemometer Height 7 m	0.04	0.12	0.15	0.12
Anemometer Height 8 m	0.07	0.16	0.19	0.07
Anemometer Height 9 m	0.06	0.15	0.19	0.07
Anemometer Height 10 m	0.08	0.19	0.23	0.07
Anemometer Height 20 m	0.11	0.27	0.32	0.06
Anemometer Height 30 m	0.06	0.17	0.2	0.05
Surface Roughness 0.0001 m	0.15	0.33	0.4	0.05

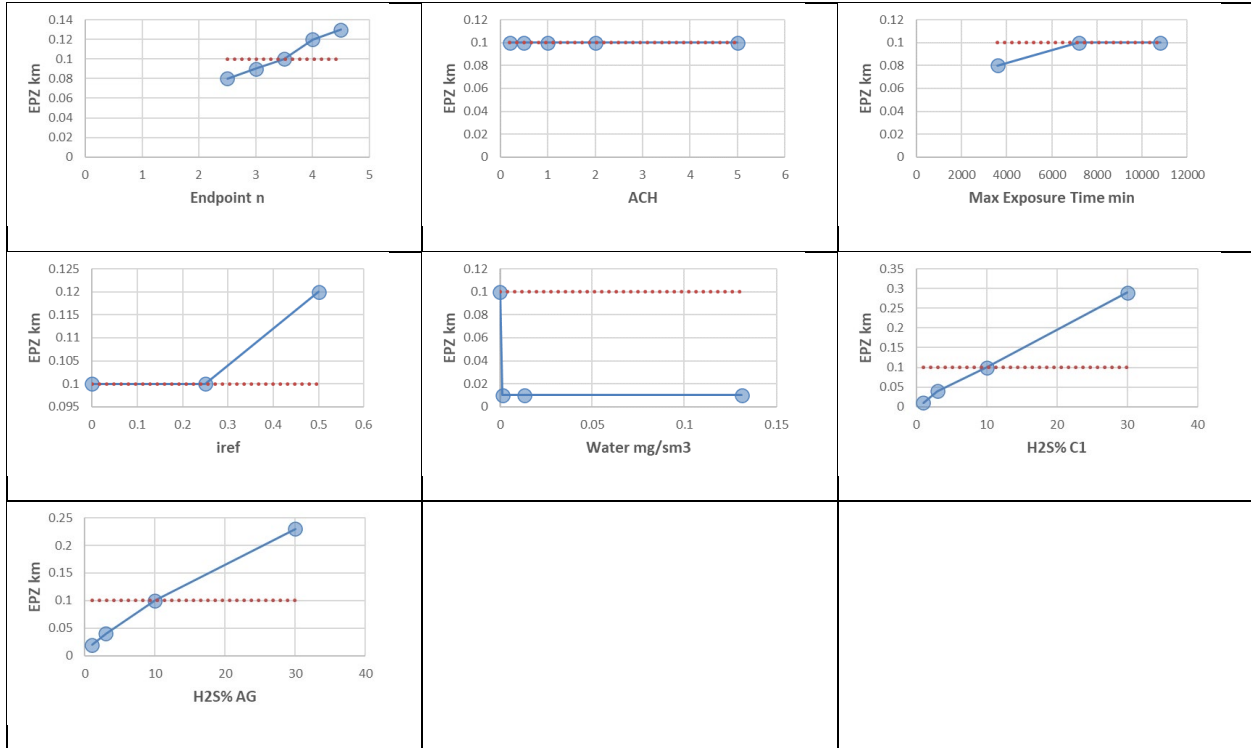
Variable Changed from Example with Example in Bold	IIZ Initial Isolation Zone	PAZ Protective Awareness Zone	EPZ Emergency Planning Zone	ERCBH2S EPZ Emergency Planning Zone
Surface Roughness 0.001 m	0.10	0.23	0.28	0.06
Surface Roughness 0.01 m	0.07	0.16	0.19	0.12
Surface Roughness 0.1 m	0.03	0.08	0.1	0.11
Surface Roughness 1 m	0.00	0.02	0.02	0.08
Surface Roughness 10 m	0.00	0.00	0.01	0.03
Endpoint Duration 3 minutes	0.07	0.20	0.2	0.17
Endpoint Duration 15 minutes	0.05	0.14	0.14	0.14
Endpoint Duration 30 minutes	0.04	0.12	0.12	0.12
Endpoint Duration 60 minutes	0.03	0.10	0.1	0.11
Endpoint Duration 120 minutes	0.02	0.09	0.09	0.1
Endpoint Duration 180 minutes	0.02	0.08	0.08	0.09
Exponent 2.5	0.03	0.06	0.08	0.09
Exponent 3	0.03	0.07	0.09	0.1
Exponent 3.5	0.03	0.08	0.1	0.11
Exponent 4	0.03	0.10	0.12	0.12
Exponent 4.5	0.03	0.11	0.13	0.13
Air Changes per Hour 0.2	0.01	0.08	0.1	0.11
Air Changes per Hour 0.5	0.02	0.08	0.1	0.11
Air Changes per Hour 1	0.03	0.08	0.1	0.11
Air Changes per Hour 2	0.04	0.08	0.1	0.11
Air Changes per Hour 5	0.04	0.08	0.1	0.11
Maximum Exposure Time 3600 s	0.01	0.06	0.08	0.09
Maximum Exposure Time 7200 s	0.02	0.08	0.1	0.1
Maximum Exposure Time 10800 s	0.03	0.08	0.1	0.11
Fluctuation Intensity iref 0	0.03	0.08	0.1	0.1
Fluctuation Intensity iref 0.25	0.03	0.08	0.1	0.11
Fluctuation Intensity iref 0.5	0.03	0.10	0.12	0.12
Water Content 0.0000 (0 mg/m³)	0.03	0.08	0.1	0.11
Water Content 0.0013 (1000 mg/m ³)	0.00	0.00	0.01	0.11
Water Content 0.0131 (10000 mg/m ³)	0.00	0.00	0.01	0.11
Water Content 0.1312 (100000 mg/m ³)	0.00	0.00	0.01	0.11
Expected H2S 1% (rest CH4)	0.00	0.00	0.01	0.03
Expected H2S 3% (rest CH4)	0.01	0.03	0.04	0.05
Expected H2S 10% (rest CH4)	0.03	0.08	0.1	0.1
Expected H2S 30% (rest CH4)	0.11	0.24	0.29	0.2
Expected H2S 1% (rest CO2)	0.01	0.01	0.02	0.03

Variable Changed from Example with Example in Bold	IIZ Initial Isolation Zone	PAZ Protective Awareness Zone	EPZ Emergency Planning Zone	ERCBH2S EPZ Emergency Planning Zone
Expected H2S 3% (rest CO2)	0.01	0.03	0.04	0.06
Expected H2S 10% (rest CO2)	0.04	0.08	0.1	0.12
Expected H2S 30% (rest CO2)	0.09	0.19	0.23	0.22

10.5.1 Liquids Pipelines/Wells Sensitivity Figures

Figures show EPZ vs Sensitivity Parameter as per sensitivity ranges listed in Section 10.1 for Liquids Pipelines and Wells.. The red dotted line on each figure is the base case scenario EPZ (km).





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Appendix 1 AERFLASH Thermodynamics Program

AERFLASH Ver 1.0.0.1
Clearstone Thermodynamics Programs
2005

Updated for AERH2S version 3.07
18 August 2025

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I Introduction

This document describes the program AERFLASH.EXE (version 1.0.0.1) created by Clearstone Engineering Ltd. for the Alberta Energy Regulator (AER), Calgary Alberta. The program allows the users to perform thermodynamic calculations required for the preparation of a portion of the input data going into the AERH2S dispersion modelling spreadsheet developed by the AER. The required properties are based on real fluid behaviour using Clearstone's thermodynamic properties engine.

II System Requirements

- 1) 2024 EXE version, operates Windows 11, Windows 10. AERFLASH.EXE is not limited to OFFICE 32bit because it is run externally to Office.
- 2) 2005 DLL version, requires Microsoft Office 32bit. Operates on Windows XP, Windows 2000 or Windows NT 4.0 service pack 3 or greater (though not tested, it may be possible to run the programs on Windows 95 or 98).

The AERFLASH.EXE is called by the AERH2S_menu.xla application spreadsheet. The THERMOUDB.DLL is called by AERFLASH.EXE for the real fluid properties.

III Updates

All versions of AERFLASH have used the same 1.0.0.1 version number. For practical use, versions of the AERFLASH are identified by release dates.

- 2024:
 - AERFLASH.DLL converted AERFLASH.exe with external AERFLASH.inp and AERFLASH.out file transfers
 - Contemporary updates Peng-Robinson equations of state
 - Solver adjustments to avoid crashes for selected gas composition cases. Systematic testing of gas composition ranges to determine non-solution scenarios.
- 2005
 - Pre-release version AERFLASH.exe with external AERFLASH.inp and AERFLASH.out file transfers converted to AERFLASH.DLL with internal data transfer
 - Version 1.0.0.1 (2005) released as AERFLASH.DLL

IV Description

The AERFLASH program allows users to obtain a part of required input data for the AERH2S.xls spreadsheet in the form of a text file that is automatically pasted into the spreadsheet. The input data for the program is provided using an ascii text file in the format of "AERFLASH.inp" in Table 1 of Attachment 1. The required

results are provided in the format of “AERFLASH.out” along with the echo of input data used for the calculations by the program as shown in Table 2 of Attachment 1.

Attachment 2 is a flowchart of AERFLASH. The program reads the input composition data and trims out the components whose composition is zero. Since some of the pure component data are not available for helium the program considers it as nitrogen for calculation purposes. The input data are the standard gas composition analysis results in mole fraction (see Attachment 3 for the list of available chemicals), the initial temperature in K, the initial pressure in kPa abs, the release source type whether it is a WELL or a PIPELINE, critical mass flux at the exit in kg/m²/s, a guess for exit pressure in kPa abs, a guess for the exit temperature in K, the drag coefficient Cd, the ambient pressure in kPa abs and the ambient temperature in K.

Then it carries out the calculations as specified in Attachment 1 based upon whether the source is WELL or PIPELINE. The output properties for the AERH2S spreadsheet are calculated at the initial condition, initial exit condition upon release, average exit conditions for the release, and, the R-plane condition. Subsequently, an isenthalpic flash is carried out to determine the temperature of the fluid at stagnation conditions after expanding from the initial pressure to the ambient pressure. The properties of the gas at the flash conditions are then determined. The dew temperature of the mixture at the ambient pressure is also determined.

The thermodynamic computations needed for the above procedures are carried out using the thermodynamic engine THERMO99 developed by Clearstone Engineering Ltd. It uses the cubic equation of state of Peng and Robinson (1976) for the computation of vapour and liquid phase properties. This equation is popularly used for computing gas and liquid properties for light hydrocarbon mixtures encountered in gas processing industries. For multi-component mixtures the Peng-Robinson Equation of State requires the binary interaction parameters between various constituent chemical components. The binary interaction parameters, when available, are taken from Oellrich et. al. (1981) and the unavailable binary interaction parameters are estimated using the method of Trebble and Sigmund (1990).

The thermodynamic package has been tested by Clearstone and found to be satisfactory for the typical natural gas mixtures being transported in gas pipelines for a pressure range up to 18,000 kPa and the temperature ranging from 100K to 450K.

The AER, with the assistance of CAPP, also compared the predictions to HYSIS, the industry standard for thermodynamic process simulations, as summarized in

Attachment 4. The results of this program vary slightly from other simulation packages because of the variations in the binary interaction parameters used.

These variations, most of the time, do not affect the results significantly for purely hydrocarbon mixtures. However, the deviations could be large for mixtures containing large amounts of polar compounds like water and hydrogen sulphide that are typically encountered in the upstream gas and oil processing industries. The flash calculations are carried out based on the existence of only two phases: vapour and liquid. Since water and hydrogen sulphide are not completely miscible in hydrocarbon liquid, three-phase equilibrium of vapour-liquid-liquid type are possible. The results from this program are to be used with caution in these cases since the calculations are carried out for two-phase equilibrium only.

V References

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Attachment 1 AERFLASH Technical Specifications

Introduction

The attached Tables 1 and 2 provide the inputs and outputs, respectively, to the AERFLASH program Clearstone Engineering Ltd. developed for the AER. Units, numerical formats and comments are specified.

The AERFLASH program provides the required properties based on real fluid behaviour using Clearstone's THERMO99 thermodynamic properties engine. At the reference conditions of 25 C and 101.325 kPa the enthalpy and entropy are zero. The user will copy the input data columns from a spreadsheet into a text file known as AERFLASH.INP, run the AERFLASH.EXE program, and then copy the text file output, AERFLASH.OUT, back into the spreadsheet. The AER has automated this file transfer process within the spreadsheet.

Referring to Table 1, the gas analysis will be normalized to 1 within the spreadsheet. The calculation type is identified as well or pipeline. The pressures and temperatures are input as absolute values. Pressures are in kPa. The average mass flux at the exit and a drag coefficient are also provided.

Referring to Table 2, the output of the AERFLASH program will be used as input to the source models and the AERSLAB dispersion model. The same output file is produced for wells and pipelines. There are no blank lines between the output lines. For the source model, the density and speed are required at the initial, exit and atmospheric conditions. The calculations depend on whether a pipeline or well release is being modeled, as discussed below.

Well Outputs

For a well release, the mass flux m_e/A_e and the initial temperature T_{of} are specified. The subscripts f and g are used here to indicate a final or guessed value. For a well release the initial exit conditions are the same as the average exit conditions. The initial pressure P_{of} must be solved for by the AERFLASH program. The initial guesses input to the model are based on ideal gas properties. A solution procedure follows:

1. Note if P_{0g} and P_{eig} equal the atmospheric pressure P_a the flow is not choked, then carry out the following calculation steps:
 - a) Determine the initial enthalpy H_0 at pressure P_0 and Temperature T_0 .
 - b) If mass flux m_e/A_e is less than 1.0, set it to 1.0 kg/s/m².
 - c) Determine the temperature T_s such that the mass flux is equal to m_e/A_e and the total energy is equal to H_0
 - d) If m_e/A_e specified is greater than the critical mass flux then set the specified mass flux to the critical mass flux and carry out step c) till the value of m_e/A_e is less than or equal to the critical mass flux. If iteration exceeds maximum limit print error message and exit.
 - e) If m_e/A_e is less than or equal to critical mass flux set the final value of P_{eif} , T_{eif} , ρ_{eif} , C_{eif} , l_{eif} .

f) Determine P_{0s} and ρ_{0s} by carrying out the isentropic compression to a point where the enthalpy is equal to H_0 .

g) Determine the polytropic exponent k_f , for the isentropic expansion from:

$$k_f = \ln(P_{0s}/P_{eif}) / \ln(\rho_{0s}/\rho_{eif})$$

h) Set $P_{0f} = P_{0s}$ and $T_{0f} = T_{0s}$.

i) Set average condition same as initial condition:

$$P_{eaf} = P_{eif}, T_{eaf} = T_{eif}, \rho_{eaf} = \rho_{eif}, c_{eaf} = c_{eif}, l_{eaf} = l_{eif}.$$

2. If P_{0g} and P_{eag} are greater than the atmospheric pressure P_a the flow is choked, then determine initial density ρ_{0g} , entropy S_{0g} and enthalpy H_{0g} at (T_{0f}, P_{0g}) .

3. Determine the exit pressure P_{ei} under isentropic expansion from pressure P_{0g} such that the total energy under critical flow is equal to the enthalpy H_{0g} at pressure P_{0g} and T_{0f} using secant search method for single variable.

4. Check if the critical mass flux at above exit pressure is equal to the specified mass flux m_e/A_e . Update P_{0g} until the critical mass flux equals the specified mass flux.

5. Set the final value of P_{eif} , T_{eif} , ρ_{eif} , c_{eif} , l_{eif} .

6. Determine the polytropic exponent k_f , for the isentropic expansion from:

$$k_f = \ln(P_{0f}/P_{eif}) / \ln(\rho_{0f}/\rho_{eif})$$

7. If P_{eif} is less than the atmospheric pressure carry out the procedure in step 1.

8. If P_{eif} is greater than the atmospheric pressure set $P_{0f} = P_{0g}$.

9. Set average condition same as initial condition:

$$P_{eaf} = P_{eif}, T_{eaf} = T_{eif}, \rho_{eaf} = \rho_{eif}, c_{eaf} = c_{eif}, l_{eaf} = l_{eif}.$$

10. Isenthalpically expand from H_{0f} at (T_{0f}, P_{0f}) to atmospheric pressure to determine flashed properties of temperature T_f , density ρ_f and quality l_f (liquid mass fraction) at P_a .

Pipeline Outputs

For a pipeline release, the initial temperature T_0 and pressure P_0 are specified. Two exit plane conditions are required; the initial critical throat conditions and average throat conditions that yield the specified mass flux. The mass flux is initially estimated from ideal gas properties; AERFLASH is run a second time by the user with refined inputs based on the real gas properties from the first pass. The subscripts g and f are used to indicate a guessed or final value. A solution procedure follows:

1. Note if P_{0g} and P_{eag} equal the atmospheric pressure P_a the flow is not choked, then carry out the following calculation steps:

a) Determine the initial enthalpy H_0 at pressure P_0 and Temperature T_0 .

- b) If mass flux m_e/A_e is less than 1.0, set it to 1.0 kg/s/m².
- c) Determine the temperature T_s such that the mass flux is equal to m_e/A_e and the total energy is equal to H_0
- d) If m_e/A_e specified is greater than the critical mass flux then set the specified mass flux to the critical mass flux and carry out step c) till the value of m_e/A_e is less than or equal to the critical mass flux. If iteration exceeds maximum limit print error message and exit.
- e) If m_e/A_e is less than or equal to critical mass flux set the final value of P_{eif} , T_{eif} , ρ_{eif} , c_{eif} , l_{eif} .
- f) Determine P_{0s} and ρ_{0s} by carrying out the isentropic compression to a point where the enthalpy is equal to H_0 .
- g) Determine the polytropic exponent k_f , for the isentropic expansion from:

$$k_f = \ln(P_{0s}/P_{eif}) / \ln(\rho_{0s}/\rho_{eif})$$

- h) Set $P_{0f} = P_{0s}$ and $T_{0f} = T_{0s}$.
 - i) Set average condition same as initial condition:
 $P_{eaf} = P_{eif}$, $T_{eaf} = T_{eif}$, $\rho_{eaf} = \rho_{eif}$, $c_{eaf} = c_{eif}$, $l_{eaf} = l_{eif}$.
2. Determine initial density ρ_{0f} , entropy S_{0f} and enthalpy H_{0f} at (T_{0f}, P_{0f}) .
 3. If P_{0g} and P_{eag} are greater than the atmospheric pressure P_a the flow is choked, then set $P_0 = P_{0f}$ and $T_0 = T_{0f}$ and determine initial density ρ_{0g} and entropy S_{0g} at (T_{0f}, P_{0f}) .
 4. Determine the exit pressure P_{ei} under isentropic expansion from pressure P_0 such that the total energy under critical flow is equal to the enthalpy H_0 at pressure P_0 and T_0 using secant search method for single variable.
 5. If P_{ei} is less than the ambient pressure P_a the flow is not choked, then carry out the following calculation steps:
 - a) Determine the initial enthalpy H_0 at pressure P_0 and Temperature T_0 .
 - b) If mass flux m_e/A_e is less than 1.0, set it to 1.0 kg/s/m².
 - c) Determine the temperature T_s such that the mass flux is equal to m_e/A_e and the total energy is equal to H_0
 - d) If m_e/A_e specified is greater than the critical mass flux then set the specified mass flux to the critical mass flux and carry out step c) till the value of m_e/A_e is less than or equal to the critical mass flux. If iteration exceeds maximum limit print error message and exit.
 - e) If m_e/A_e is less than or equal to critical mass flux set the final value of P_{eif} , T_{eif} , ρ_{eif} , c_{eif} , l_{eif} .

f) Determine P_{0s} and ρ_{0s} by carrying out the isentropic compression to a point where the enthalpy is equal to H_0 .

g) Determine the polytropic exponent k_f , for the isentropic expansion from:

$$k_f = \ln(P_{0s} / P_{eif}) / \ln(\rho_{0s} / \rho_{eif})$$

h) Set $P_{0f} = P_{0s}$ and $T_{0f} = T_{0s}$.

i) Set average condition same as initial condition:

$$P_{eaf} = P_{eif}, T_{eaf} = T_{eif}, \rho_{eaf} = \rho_{eif}, c_{eaf} = c_{eif}, l_{eaf} = l_{eif}.$$

6. If P_{ei} is greater than or equal to the ambient pressure P_a the flow is choked, then set the final value of $P_{eif} = P_{ei}$, and set the values of T_{eif} , ρ_{eif} , c_{eif} , l_{eif} .

7. Determine the average exit pressure P_{ea} under isentropic expansion from the thermodynamic state with pressure P_{0h} and enthalpy H_0 corresponding to the initial temperature of T_0 and pressure P_0 such that the critical mass flux equals the specified mass flux m_e/A_e using secant search method for single variable. If P_{ea} is less than the ambient pressure P_a the flow is not choked, then carry out the following calculation steps:

a) Determine the initial enthalpy H_0 at pressure P_0 and Temperature T_0 .

b) If mass flux m_e/A_e is less than 1.0, set it to 1.0 kg/s/m².

c) Determine the temperature T_s such that the mass flux is equal to m_e/A_e and the total energy is equal to H_0 .

d) If m_e/A_e specified is greater than the critical mass flux then set the specified critical mass flux to be the critical mass flux and carry out step c) till the value of m_e/A_e is less than or equal to the critical mass flux. If iteration exceeds maximum limit print error message and exit.

e) If m_e/A_e is less than or equal to critical mass flux set the final value of P_{eaf} , T_{eaf} , ρ_{eaf} , c_{eaf} , l_{eaf} .

f) Determine P_{0s} and ρ_{0s} by carrying out the isentropic compression to a point where the enthalpy is equal to H_0 .

g) Determine the polytropic exponent k_f , for the isentropic expansion from:

$$k_f = \ln(P_{0s} / P_{eaf}) / \ln(\rho_{0s} / \rho_{eaf})$$

h) Determine H_{s0} and ρ_{s0} at pressure P_a and specific entropy S_0 (the initial entropy at T_0 and P_0).

i) Determine the kinetic energy KE using the relationship $KE = 0.5 * (m_e/A_e) * (m_e/A_e) / \rho_{s0}$

j) If KE is greater than $H_0 - H_{s0}$ then carryout the following steps:

- i. Set $me/Ae = \rho_{s0} * \text{sqrt}(2.0 * (H_0 - H_{s0}))$.
- ii. Set the final value of P_{eaf} , T_{eaf} , ρ_{eaf} , c_{eaf} , lf_{eaf} .
- iii. Determine P_{0s} and ρ_{0s} by carrying out the isentropic compression to a point where the enthalpy is equal to H_0 .
- iv. Determine the polytropic exponent k_f , for the isentropic expansion from:

$$k_f = \ln(P_{0s} / P_{eaf}) / \ln(\rho_{0s} / \rho_{eaf})$$

9. Isenthalpically expand from H_{0f} at (T_{0f}, P_{0f}) to atmospheric pressure to determine flashed properties of temperature T_f , density ρ_f , and quality lf_f (liquid mass fraction) at P_a .

R-Plane Outputs

The Real gas plane values are input to the AERSLAB model. An isenthalpic flash from the initial conditions yields the stagnation (with zero velocity) temperature T_f , density ρ_f and liquid fraction lf_f . To account for the velocity, kinetic energy is removed from the stagnation enthalpy and the static properties at the R-plane are assigned.

The velocity at the R-plane V_r is based on a momentum balance from the average flow exit plane yielding the velocity at the Q-plane, which is then reduced for drag.

$$\begin{aligned} V_e &= (me/Ae) / \rho_{eaf} \\ V_q &= V_e + (P_{eaf} - P_a) * 1000 / \rho_{eaf} / V_e \\ V_r &= V_q * (4 - C_d) / (4 + C_d) \end{aligned}$$

Note V_q can be supersonic. V_r approaches zero as C_d approaches 4. The isenthalpic flash from initial conditions is then adjusted to determine the static enthalpy H_r :

$$H_r = H_0 - V_r^2 / 2$$

The R-plane temperature T_r , density ρ_r and liquid fraction lf_r are assigned at H_r and P_a .

The dew point temperature T_{dew} at atmospheric pressure P_a is also required.

AERSLAB Dispersion Model Inputs

CPS is the specific heat of the vapour at P_a at the maximum of the ambient temperature T_a and the dew point temperature T_{dew} . If T_a is less than T_{dew} , T_{dew} is used, otherwise T_a is used.

The boiling point, TBP, is the R-plane temperature T_r if there are liquids present. If there are no liquids formed (lf_r liquid mass fraction is zero); then $TBP = T_{dew}$.

hfg is the heat of vapourization of the mixture and is the difference in specific enthalpies between the vapour at (T_{dew}, P_a) and the mixture at (T_r, P_a) , divided by the liquid fraction lf_r . Note T_{dew} is greater than T_r for a multi-component mixture in the phase envelope.

CPSL is the specific heat and RHOSL is the density of the flashed liquid at (T_r , P_a). Note the flashed liquid composition is not the same as the mixture composition.

If there are no liquids formed (the R-plane conditions are such that the enthalpy H_r is outside of the envelope thus $l_f = 0.0$), and there is water present in the composition, the following liquid properties for water are to be provided for input to SLAB:

$$\begin{aligned} \text{hfg} &= 2\,465\,900. & \text{J/kg} \\ \text{CPSL} &= 4186.3. & \text{J/kg/K} \\ \text{RHOSL} &= 999.1 & \text{kg/m}^3 \end{aligned}$$

If there are no liquids formed and there is no water present in the composition, then the condensed liquids at 1 C below the dew point are used to determine hfg, CPSL and RHOSL and the saturation pressure constants SPB and SPC.

If there are no liquids formed ($l_f=0$) and there is no water present in the composition, AERSLAB'S default option is invoked by setting $\text{SPB} = -1.0$ and $\text{SPC} = 0.0$. Otherwise, the Saturation Pressure Constants are derived from a two-point fit of the saturated vapour curve. Two points are adequate as the temperature relationship with pressure follows the Antoine equation. The R-plane temperature T_r if $l_f > 0$ or T_{dew} if $l_f = 0$ and atmospheric pressure P_a define the first point. The second point is at a lower pressure to simulate the partial pressures of the released material in the plume and the resulting decrease in temperature. The dew point temperature T_g is determined at a guessed pressure P_g of 0.9 times the atmospheric pressure. Then, if $T_r < T_{\text{dew}}$:

$$\begin{aligned} \text{slope} \quad \text{SPB} &= \ln(P_a / P_g) / (1/T_r - 1/T_g) \\ \text{intercept} \quad \text{SPA} &= (\text{SPB} / T_r) + \ln(P_a) \\ \text{correction} \quad \text{SPC} &= (\text{SPB} / \text{SPA}) - T_r \end{aligned}$$

If $T_r > T_{\text{dew}}$, replace T_r with T_{dew} in the above equations. SPA is not an input to AERSLAB, it is calculated internally as $\text{SPB} / (\text{TBP} + \text{SPC})$.

Table 1 AERFLASH Inputs
(Shaded area is copied from spreadsheet to create AERFLASH.inp)

AERFLASH MODEL INPUTS			
Input Parameters	Format	Units	Comments
Composition			Order same as lab analysis
hydrogen	n.nnnn	Mole fraction	
helium	n.nnnn	Mole fraction	Defaults to N ₂
nitrogen	n.nnnn	Mole fraction	
carbon dioxide	n.nnnn	Mole fraction	
hydrogen sulphide	n.nnnn	Mole fraction	
methane	n.nnnn	Mole fraction	
ethane	n.nnnn	Mole fraction	
propane	n.nnnn	Mole fraction	
isobutene	n.nnnn	Mole fraction	
n-butane	n.nnnn	Mole fraction	
isopentane	n.nnnn	Mole fraction	
n-pentane	n.nnnn	Mole fraction	
n-hexane	n.nnnn	Mole fraction	
n-heptane	n.nnnn	Mole fraction	
water	n.nnnn	Mole fraction	May contain trace water
Total	1.00000	Mole fraction	Inputs supplied will be normalized
Conditions	WELL or PIPELINE		
Po Initial pressure	nnnnn.nnn	kPa (abs)	Guess for a well, final value for a pipeline
To Initial temperature	nnn.nn	K	Final value for well and pipeline
me/Ae Mass flux at exit	nnnnnn.n	kg/s/m ²	Final value for a well, guess for a pipeline
Pe Exit pressure	nnnnn.nnn	kPa (abs)	Guess based on isentropic expansion to yield mass flux at exit
Te Exit temperature	nnn.nn	K	
Cd Drag coefficient	n.n		Between 0 and 4
Pa Atmospheric pressure	nnnnn.nnn	kPa (abs)	
Ta Ambient temperature	nnn.nn	K	

Table 2a AERFLASH Outputs (1 of 2)
 (Shaded area is copied from AERFLASH.out to spreadsheet)

AERFLASH MODEL OUTPUTS			
Output Parameters	Format	Units	Comments
Initial Conditions			
Po Initial pressure	nnnnn.	kPa (abs)	As input for pipelines, calculated for wells
To Initial temperature	nnn.nn	K	As input
ρ_o Initial density at Po and To	n.nnnn	kg/m ³	
co Initial speed of sound at Po and To	nnn.n	m/s	
Xo Initial liquid fraction at Po and To	n.nnnn		
Exit Conditions			
Pei Initial exit pressure	nnnnn.	kPa (abs)	Isentropic expansion from (To, Po) to critical conditions
Tei Initial exit temperature	nnn.nn	K	
pei Initial exit density at Pei and Tei	n.nnnn	kg/m ³	
cei Initial exit speed of sound at Pei and Tei	nnn.n	m/s	
Xei Initial exit liquid fraction at Pei and Tei	n.nnnn		
Pea Average exit pressure	nnnnn.	kPa (abs)	Same as initial for well, see text for pipeline
Tea Average exit temperature	nnn.nn	K	
ρ_{ea} Average exit density at Pea and Tea	n.nnnn	kg/m ³	
cea Average exit speed of sound at Pea and Tea	nnn.n	m/s	
Xea Average exit liquid fraction at Pea and Tea	n.nnnn		
k Average ratio of Cp/Cv	n.nnn		For average flow

Un-shaded lines are not included in output

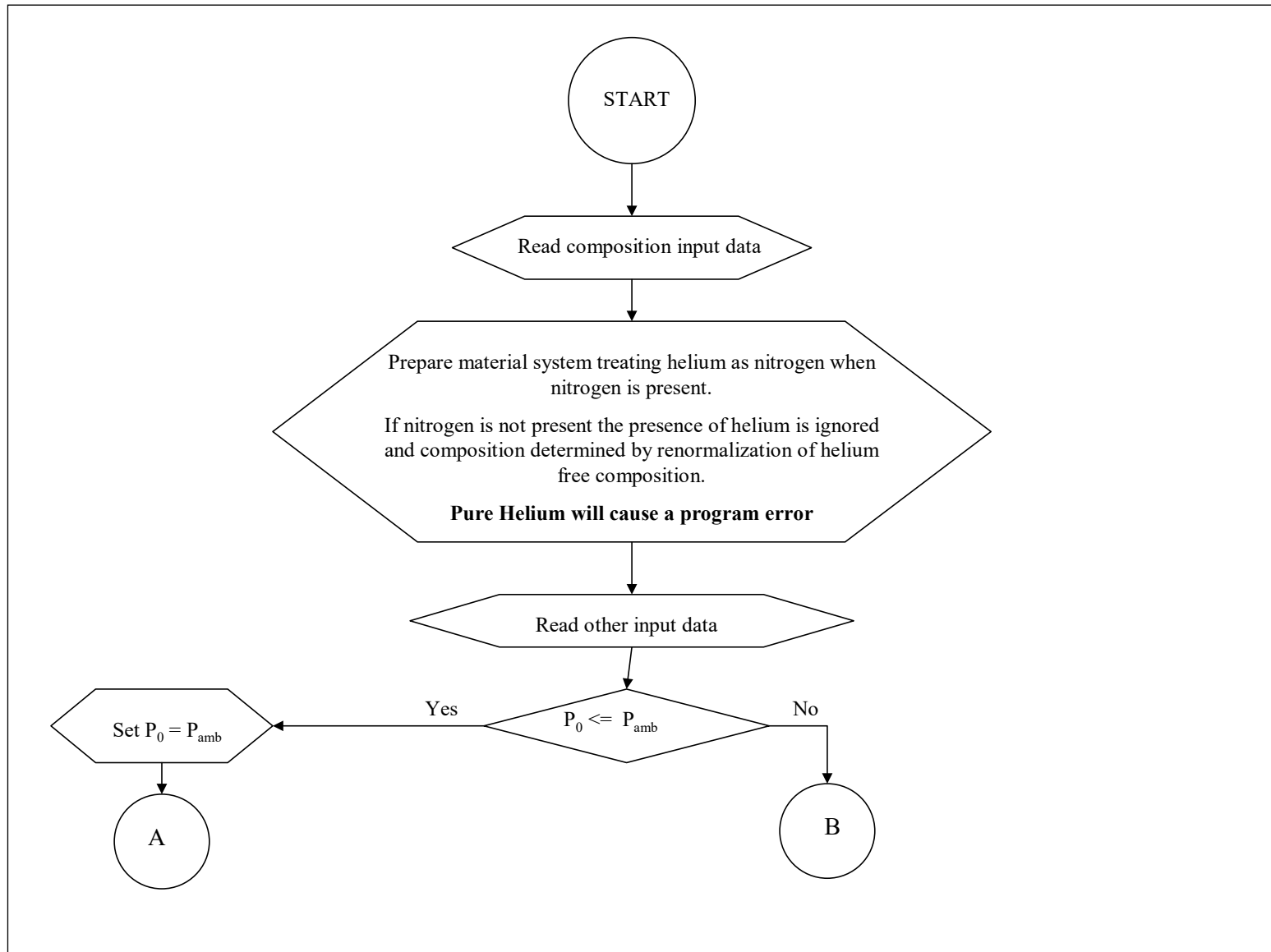
Table 2b AERFLASH Outputs (2 of 2)
(Shaded area is copied from AERFLASH.out to spreadsheet)

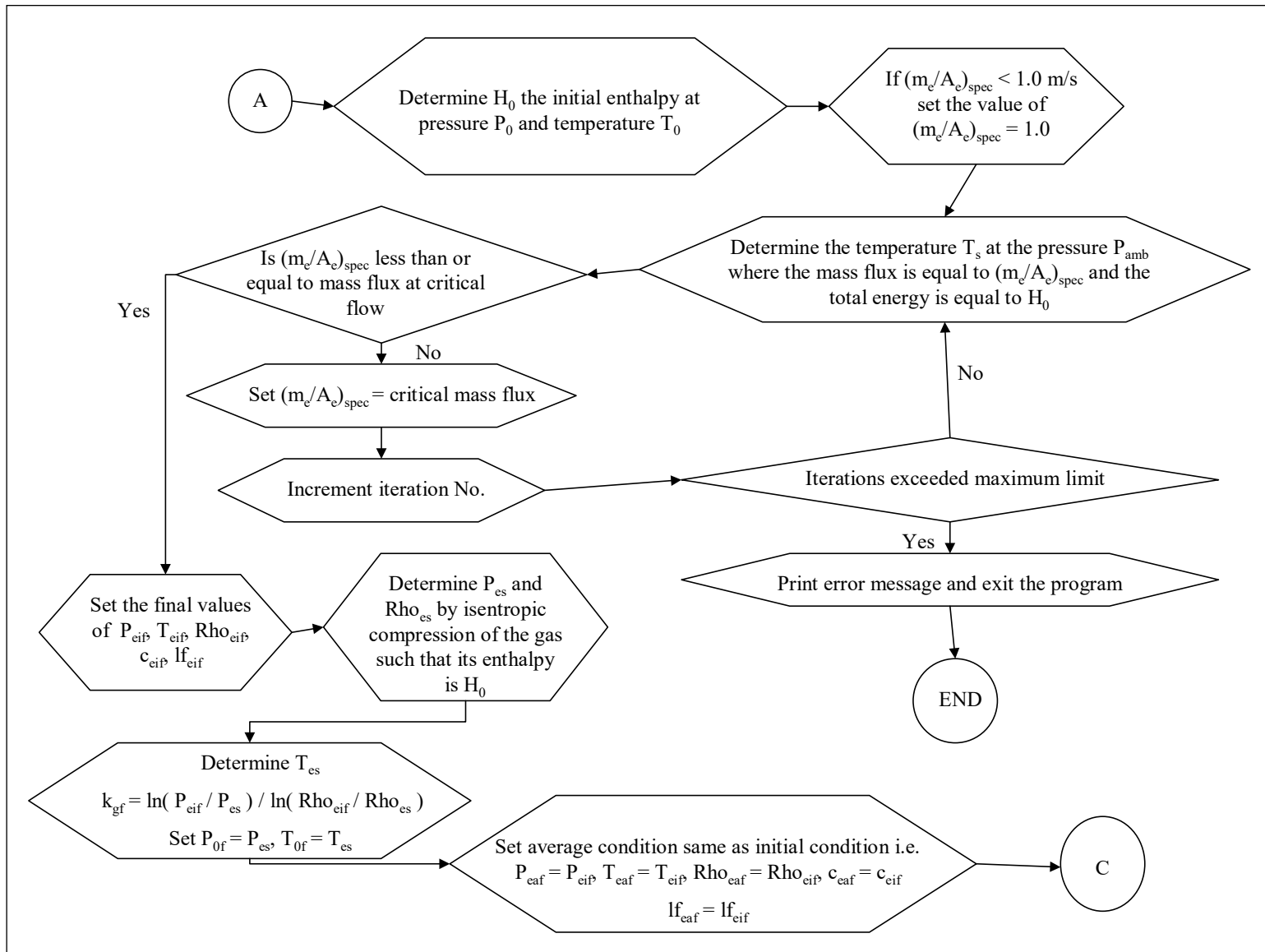
AERFLASH MODEL OUTPUTS			
Output Parameters	Format	Units	Comments
Atmospheric Conditions			
Tf Isenthalpic flash temperature	nnn.nn	K	Isenthalpic flash from (Po, To) to Pa
ρ_f Isenthalpic flash density at Pa and Tf	n.nnnnnn	kg/m ³	Mixture at Tf and Pa
Xf Isenthalpic flash liquid mass fraction	n.nnnn		Mixture at Tf and Pa
Vr R-plane velocity	nnn.n	m/s	Based on exit momentum less drag
Tr R-plane temperature	nnn.nn	K	At Hr, see text
ρ_r R-plane density	n.nnnnnn	kg/m ³	Mixture at Tr and Pa
Xr R-plane liquid mass fraction	n.nnnn		Mixture at Tr and Pa
Tdew Dew point temperature	nnn.nn	K	Mixture at Pa
AERSLAB Dispersion Model Source Properties			
CPS Vapour specific heat capacity	nnnn.n	J/kg/K	At max (Ta, Tdew) at Pa
TBP Boiling point temperature	nnn.nn	K	Tr if Xr > 0, Tdew if Xr = 0
DHE-hfg Liquid heat of vapourization	nnnnnnnn.	J/kg	Liquids at Tr and Pa if X>0 or if X=0.0, see text
CPSL Liquid specific heat capacity	nnnn.n	J/kg/K	
RHOSL Liquid density	nnnn.n	kg/m ³	
SPB Saturation pressure constant	nnnn.nn		From two point curve fit, see text
SPC Saturation pressure constant	nnn.nn		Calculated to yield Tr for SPA and SPB, see text

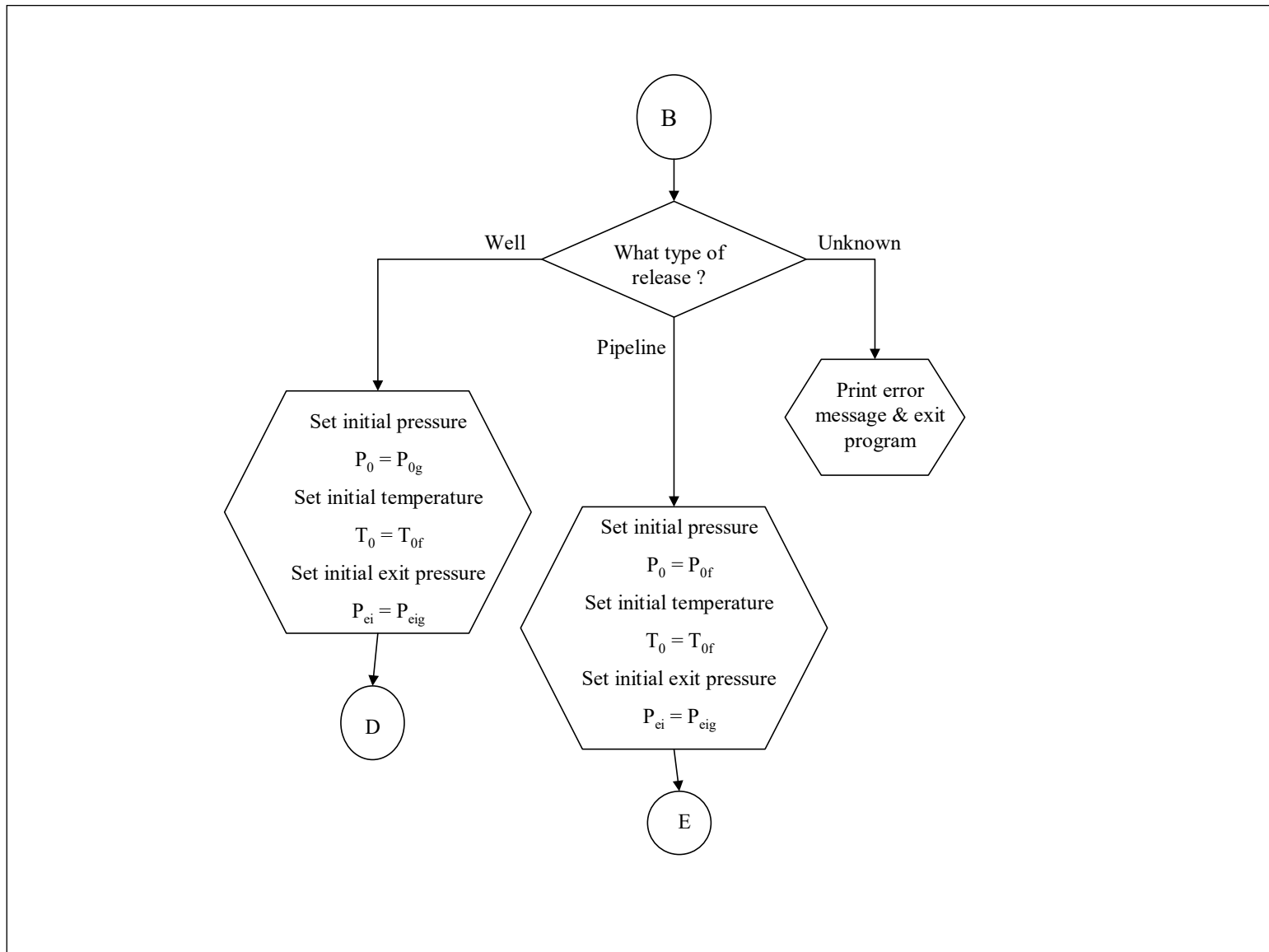
Un-shaded lines are not included in output

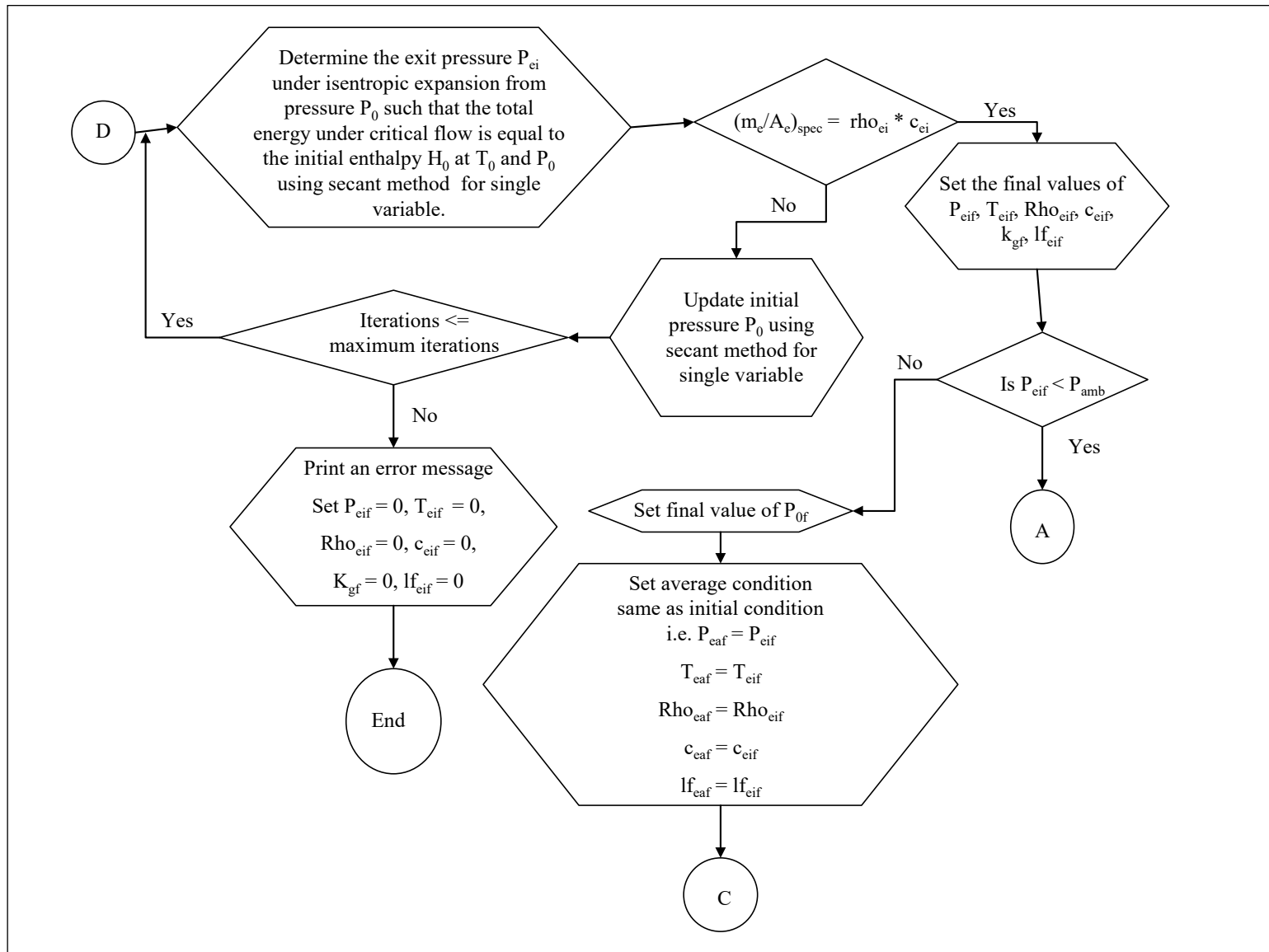
Attachment 2 Flowchart of AERFLASH

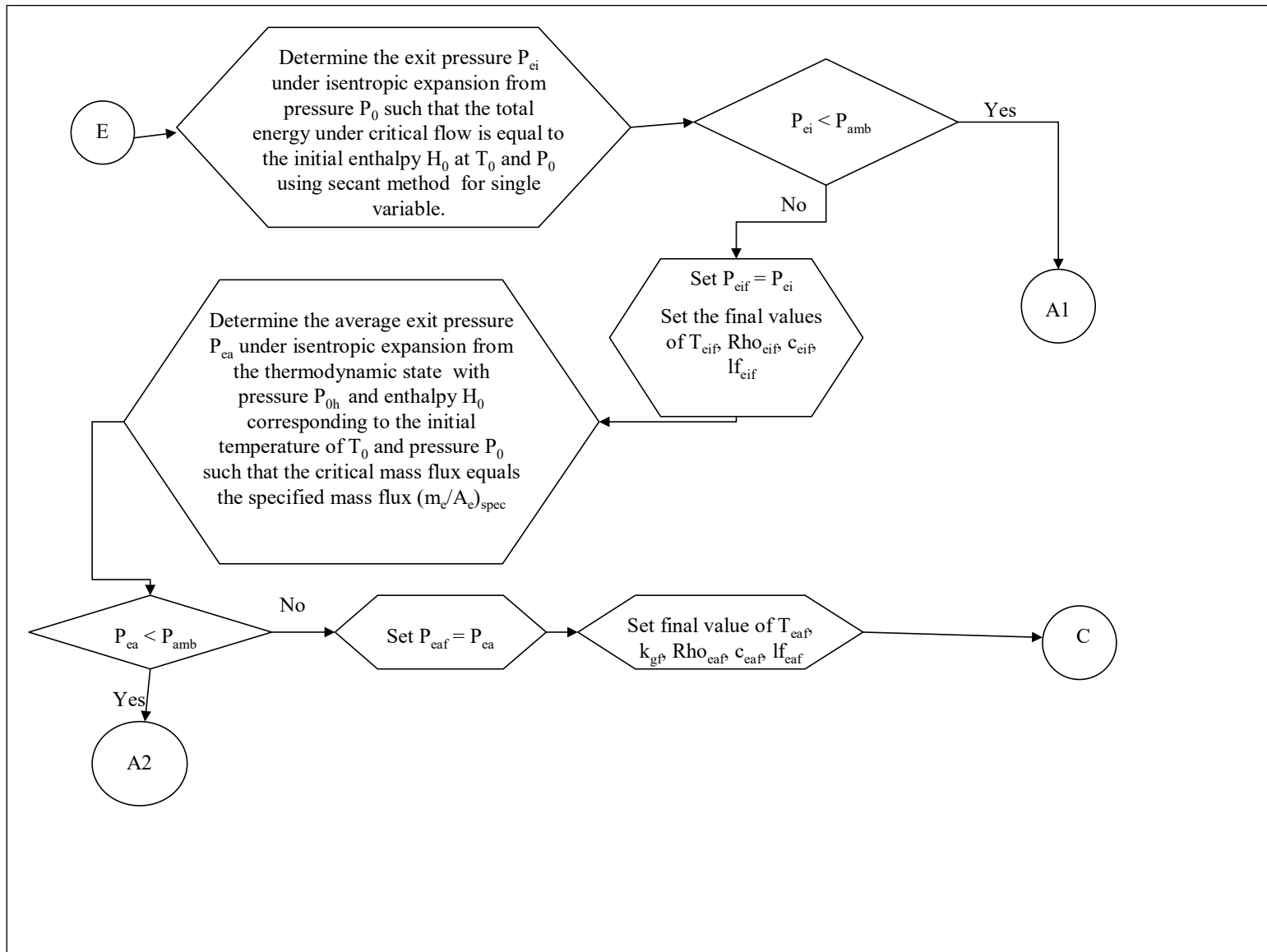
1 of 10

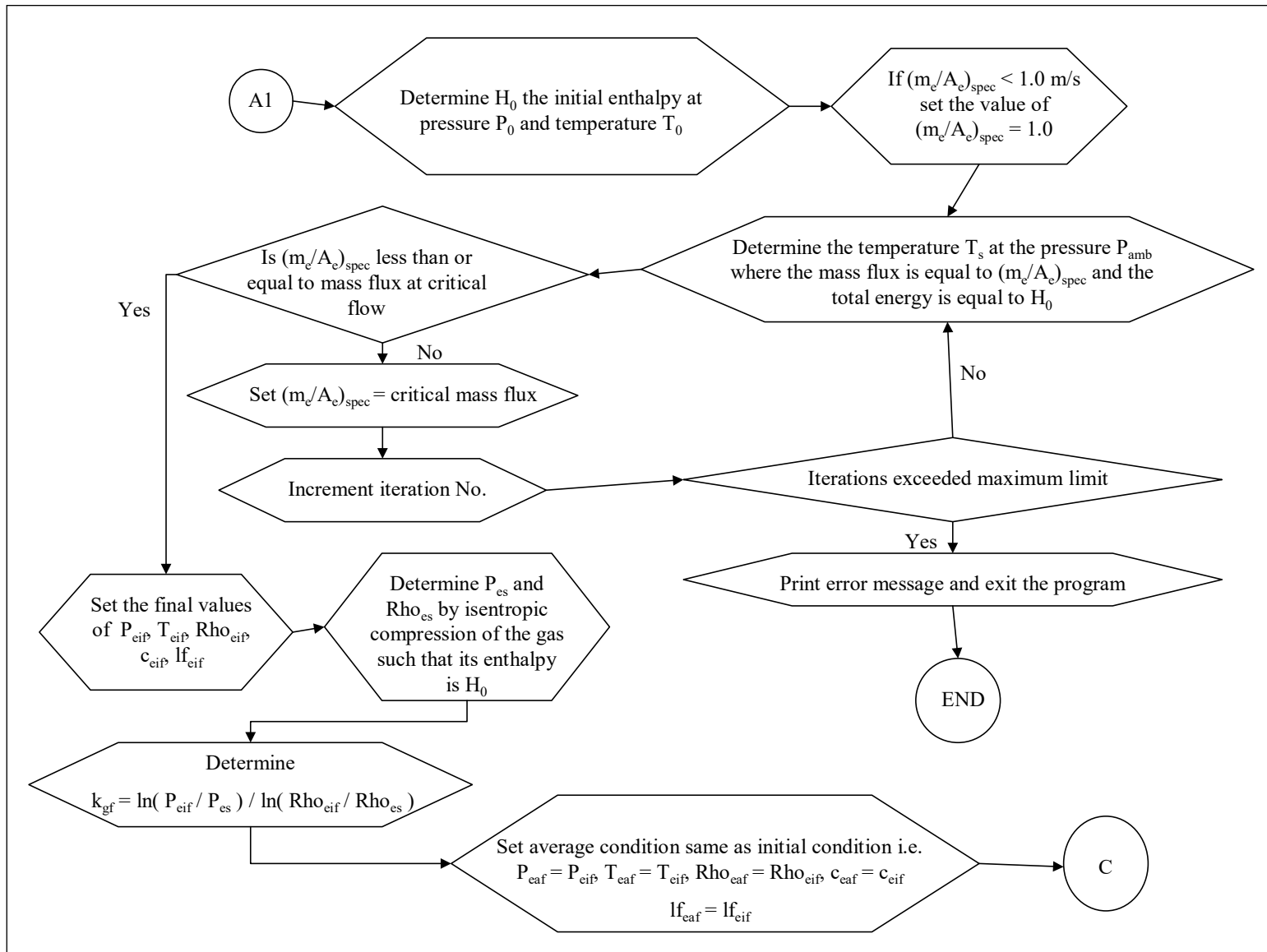


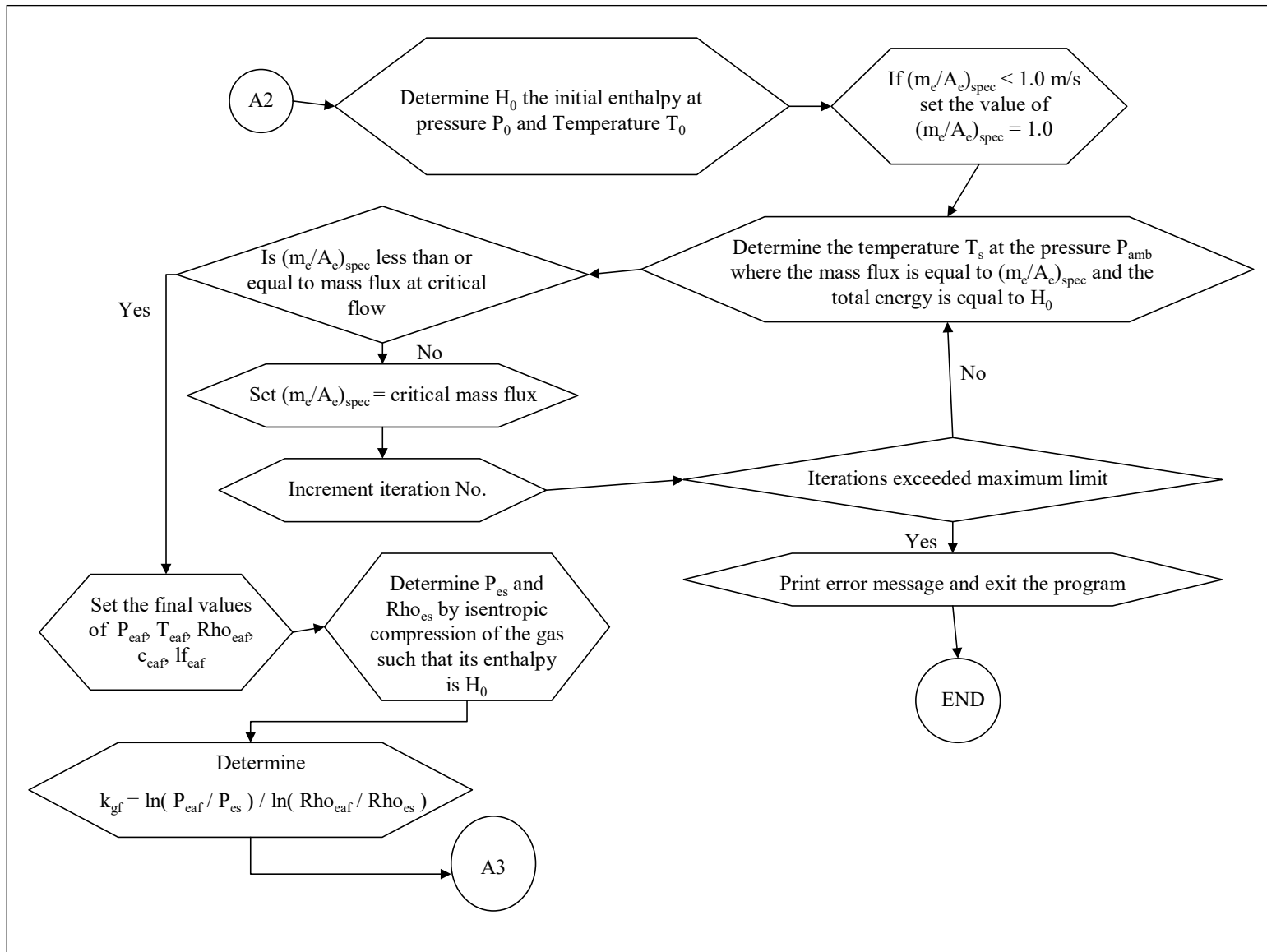


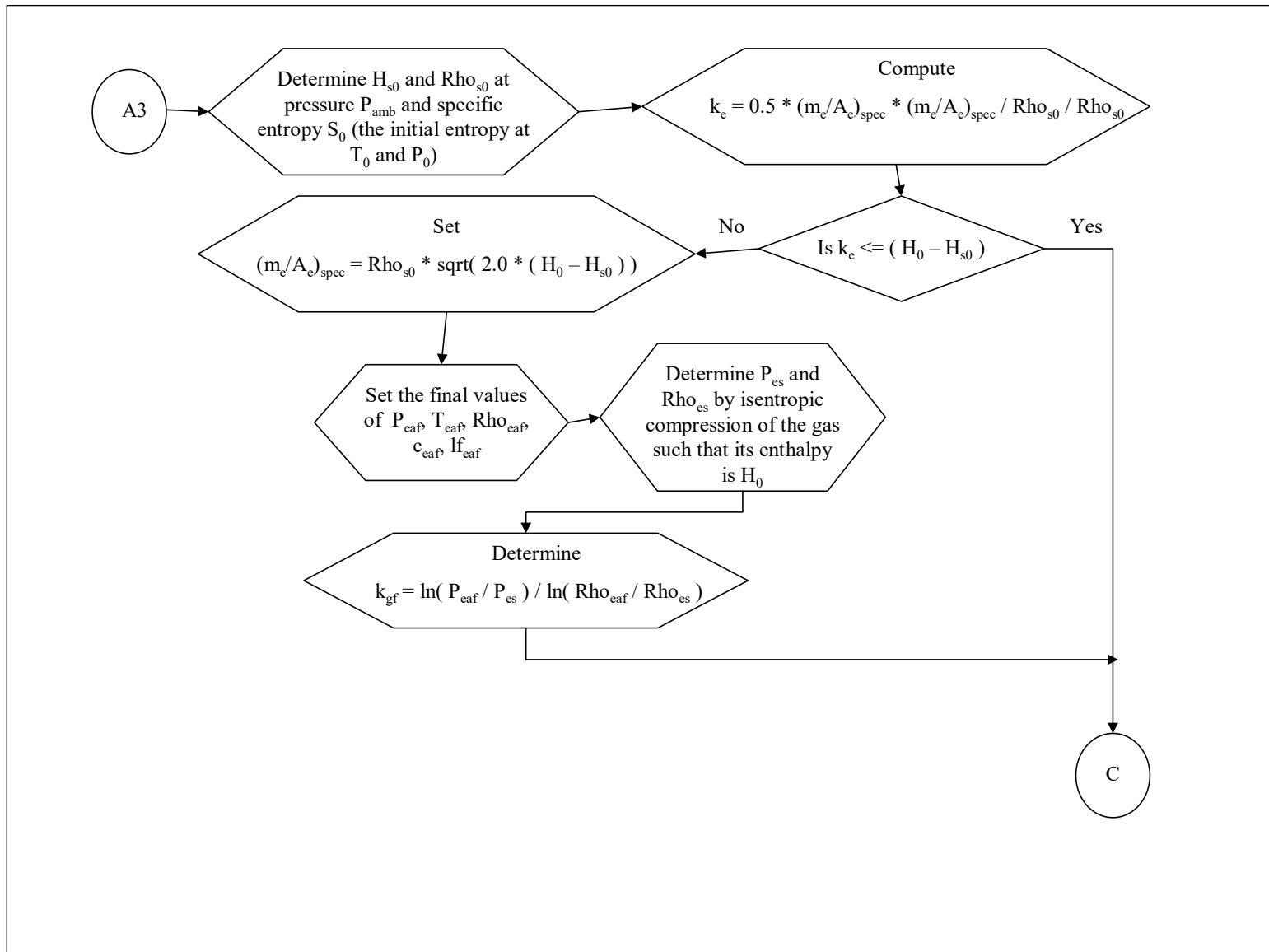


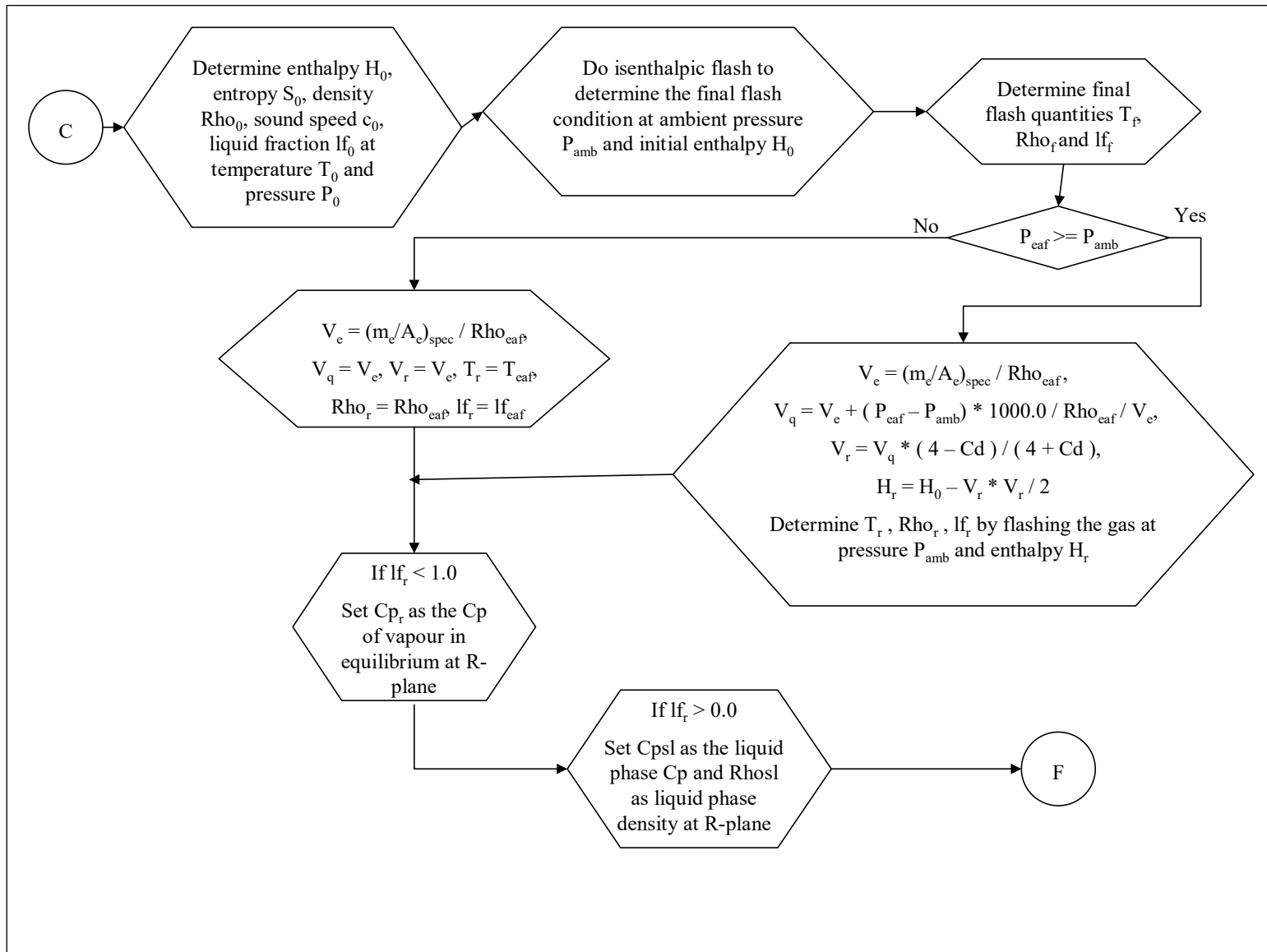


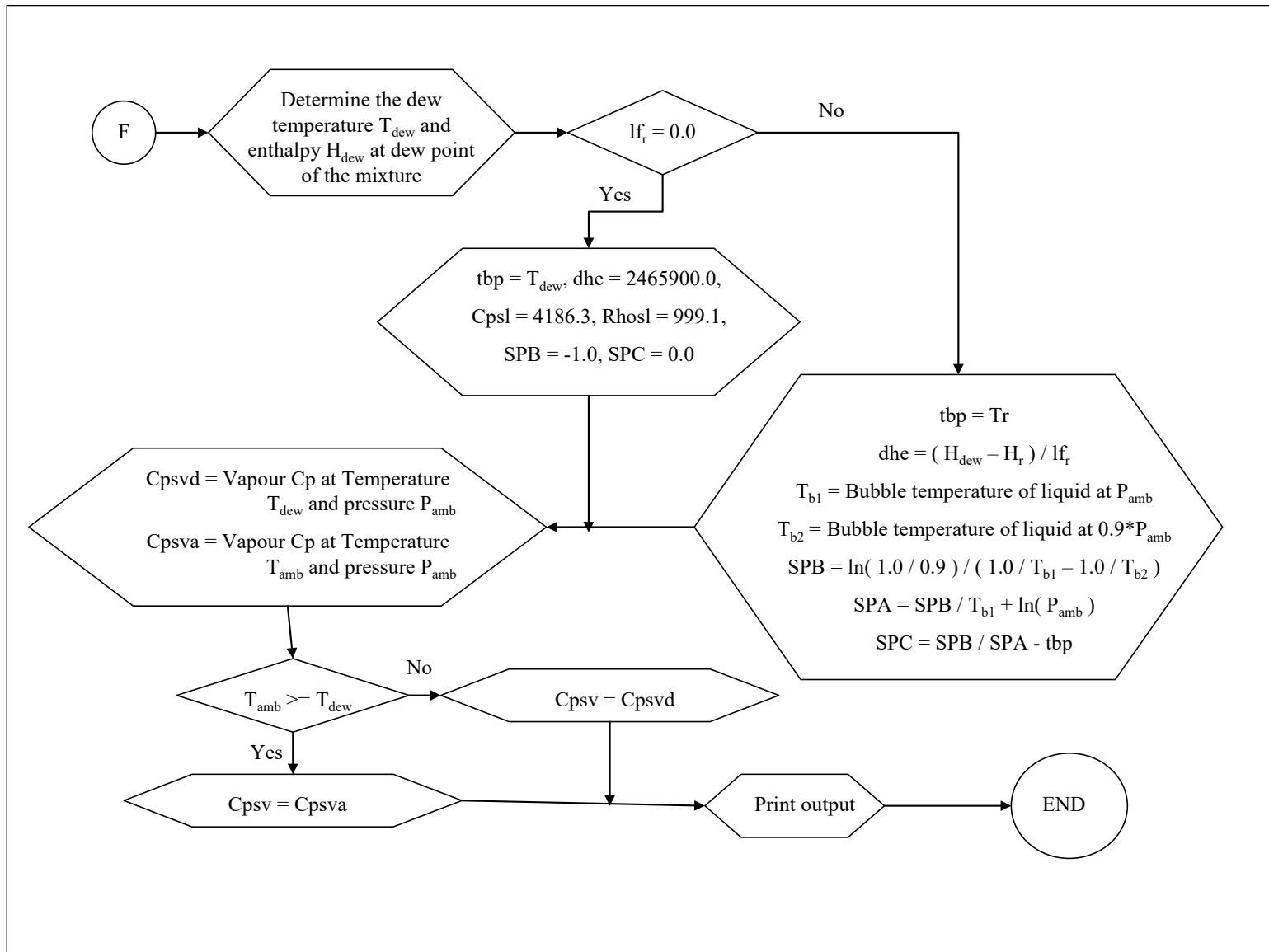












Attachment 3 Available Chemicals

Chemical Name	Formula	CASN
Carbon_dioxide	CO2	00124-38-9
Ethane	C2H6	00074-84-0
Helium	He	07440-59-7
hydrogen_(normal)	H2	01333-74-0
hydrogen_sulfide	H2S	07783-06-4
Isobutane	C4H10	00075-28-5
Isopentane	C5H12	00078-78-4
Methane	CH4	00074-82-8
n-butane	C4H10	00106-97-8
n-heptane	C7H16	00142-82-5
n-hexane	C6H14	00110-54-3
Nitrogen	N2	07727-37-9
n-pentane	C5H12	00109-66-0
Propane	C3H8	00074-98-6
Water	H2O	07732-18-5

Attachment 4 Comparison of AERFLASH to HYSIS Results

This section provides a comparison of AERFLASH and HYSIS thermodynamic simulator predictions. Table 1 provides the composition of 5 typical sour gas streams input to the simulators. CAPP provided the HYSIS results from Shell Canada who has access to the proprietary program.

Tables 2 and 3 compares the predictions for each stream using the base case well and pipeline, respectively. The ratio is the AERFLASH prediction divided by the HYSIS prediction.

The tables are based on the output file from AERFLASH. Input and outputs to the models are identified. The pipeline simulations are for higher pressures than for the well. Many of the AERFLASH outputs require iterative solution. To simplify the study, only parameters that could be easily specified with a pressure and temperature were compared. Thus the R plane values from AERFLASH cannot be compared to HYSIS. Also, HYSIS does not readily provide the speed of sound so it cannot be compared.

Predictions are generally within 1% of each other (a ratio of 0.99 to 1.01). Higher deviations, in the 5-10% range, occur near atmospheric pressure or when only two digit values are compared.

In summary, the AERFLASH program provides comparable results to HYSIS. The differences will have little effect on EPZ predictions when input into the AERSLAB dispersion model.

BASE

Table 1 - Comparison of EUBFLASH to HYSIS for Well		Stream 1			Stream 2			Stream 3			Stream 4			Stream 5		
		EUB Values	HYSIS	Ratio	EUB Values	HYSIS	Ratio	EUB Values	HYSIS	Ratio	EUB Values	HYSIS	Ratio	EUB Values	HYSIS	Ratio
input	P0 Initial Pressure (kPa(abs))	4468	4468		601	601		310	310		184	184		129	129	
input	T0 Initial Temperature (K)	278.15	278.15		278.15	278.15		278.15	278.15		278.15	278.15		278.53	278.53	
output	rho0 Initial Density at T0 and P0 (kg/m3)	45.8201	45.7656	1.0012	5.8235	5.823	1.0001	3.1022	3.1044	0.9993	1.9728	1.9672	1.0028	1.4943	1.4909	1.0023
	c0 Initial Speed of Sound at T0 and P0 (m/s)	347.53	N/A		354.96	N/A		347.74	N/A		345.54	N/A		333.56	N/A	
output	X0 Initial Liquid Fraction at T0 and P0	0.0210	0.0208	1.0096	0.0175	0.0173	1.0116	0.0050	0.0047	1.0638	0.0000	0		0.0000	0	
input	Pei Initial Exit Pressure (kPa(abs))	2516	2516		334	334		172	172		103	103		90	90	
input	Tei Initial Exit Temperature (K)	245.71	245.71		249	249		250.7	250.7		249.44	249.44		257.24	257.24	
output	rhoei Initial Exit Density at Tei and Pei (kg/m3)	28.6333	28.6054	1.0010	3.6187	3.6137	1.0014	1.9243	1.9175	1.0035	1.2319	1.232	0.9999	1.1248	1.126	0.9989
	cei Initial Exit Sound Speed at Tei and Pei (m/s)	326.04	N/A		338.42	N/A		332.81	N/A		320.89	N/A		312.44	N/A	
output	Xei Initial Exit Liquid Fraction at Tei and Pei	0.0534	0.0538	0.9926	0.0396	0.0398	0.9950	0.0338	0.0336	1.0060	0.0220	0.0215	1.0233	0.0029	0.0026	1.1154
	Pea Average Exit Pressure (kPa(abs))	2516			334			172			103			90		
	Tea Average Exit Temperature (K)	245.71			249			250.7			249.44			257.24		
	rhoea Average Exit Density at Tea and Pea (kg/m3)	28.6333			3.6187			1.9243			1.2319			1.1248		
	cea Average Exit Sound Speed at Tea and Pea (m/s)	326.04			338.42			332.81			320.89			312.44		
	Xea Average Exit Liquid Fraction at Tea and Pea	0.0534			0.0396			0.0338			0.022			0.0029		
	k Average ratio of Cp/Cv	1.222			1.2317			1.2246			1.2384			1.2794		
output	Tf Isenthalpic Flash Temperature (K, from P0 and T0 to Pa)	244.09	244.05	1.0002	270.83	270.88	0.9998	275.34	275.43	0.9997	277.33	277.34	1.0000	278.15	278.16	1.0000
output	rhof Isenthalpic Flash Density at Pa and Tf (kg/m3)	0.8899	0.8894	1.0006	0.8729	0.8722	1.0008	0.9000	0.8992	1.0009	0.9596	0.9592	1.0004	1.0382	1.0379	1.0003
output	Xf Isenthalpic Flash Liquid Mass Fraction at Pa and Tf	0.0035	0.0032	1.0938	0.0000	0.0000		0.0000	0.0000		0.0000	0.0000		0.0000	0.0000	
	Vr R Plane Velocity (m/s)	351.5			322.8			277.1			212.4			147.4		
input	Tr R Plane Temperature (K)	215.15			245.86			255.23			262.76			270.38		
	rhorr R Plane Density (kg/m3)	1.0171			0.9674			0.9746			1.0136			1.0685		
	Xr R Plane Liquid Mass Fraction	0.0261			0.0213			0.0123			0			0		
output	Tdew Dew Point Temperature (K at Pa)	246.93	246.69	1.0010	257.8	257.64	1.0006	260.49	260.29	1.0008	259.68	259.47	1.0008	258.69	258.52	1.0007
output	CPS Vapour Specific Heat Capacity (J/kg/K, at Pa)	1893.0	1888.4	1.0024	1788.5	1784.8	1.0021	1694.8	1691.9	1.0017	1556.3	1555.4	1.0006	1405.4	1406.5	0.9992
	TBP Boiling Point Temperature (K)	215.15			245.86			255.23			259.68			258.69		
	HFG Heat of Vaporization (J/kg)	2623511			1362664			1091796			2465900			2465900		
	CPSL Liquid Specific Heat (J/kg/K)	1826.1			1941.7			1978.6			4186.3			4186.3		
	RHOSL Liquid Density (kg/m3)	712.5			700.6			696.4			999.1			999.1		
	SPB saturation pressure constant	861.05			873.58			905.37			-1			-1		
	SPC saturation pressure constant	-113.86			-137.36			-142.7			0			0		
			MAX	1.0938		MAX	1.0116		MAX	1.0638		MAX	1.0233		MAX	1.1154
			MIN	0.9926		MIN	0.9950		MIN	0.9993		MIN	0.9999		MIN	0.9989

BASE

Table 2 - Comparison of EUBFLASH to HYSIS for Pipeline		Stream 1			Stream 2			Stream 3			Stream 4			Stream 5		
		EUB Values	HYSIS	Ratio	EUB Values	HYSIS	Ratio	EUB Values	HYSIS	Ratio	EUB Values	HYSIS	Ratio	EUB Values	HYSIS	Ratio
input	P0 Initial Pressure (kPa(abs))	10020	10020		10020	10020		10020	10020		10020	10020		10020	10020	
input	T0 Initial Temperature (K)	278.15	278.15		278.15	278.15		278.15	278.15		278.15	278.15		278.15	278.15	
output	rho0 Initial Density at T0 and P0 (kg/m3)	125.1640	125.1521	1.0001	148.6753	148.2659	1.0028	166.6872	165.4149	1.0077	210.2084	206.1579	1.0196	284.1193	275.2849	1.0321
	c0 Initial Speed of Sound at T0 and P0 (m/s)	363.21	N/A		297.17	N/A		273.44	N/A		223.83	N/A		176.17	N/A	
output	X0 Initial Liquid Fraction at T0 and P0	0.0000	0.0000		0.0567	0.0599	0.9466	0.0982	0.1059	0.9273	0.2272	0.2282	0.9956	0.5269	0.5039	1.0456
input	Pei Initial Exit Pressure (kPa(abs))	5718	5718		5881	5881		5998	5998		6179	6179		6302	6302	
input	Tei Initial Exit Temperature (K)	245.27	245.27		250.23	250.23		253.28	253.28		258.47	258.47		262.41	262.41	
output	rhoei Initial Exit Density at Tei and Pei (kg/m3)	81.0279	80.8821	1.0018	94.7731	94.4389	1.0035	105.408	104.6705	1.0070	128.4523	126.6443	1.0143	168.2998	164.4428	1.0235
	cei Initial Exit Sound Speed at Tei and Pei (m/s)	289.5	N/A		261.7	N/A		244.19	N/A		214.84	N/A		183.71	N/A	
output	Xei Initial Exit Liquid Fraction at Tei and Pei	0.0779	0.0791	0.9848	0.1706	0.1725	0.9890	0.2289	0.2281	1.0035	0.3502	0.3409	1.0273	0.5225	0.509	1.0265
input	Pea Average Exit Pressure (kPa(abs))	386	386		1086	1086		1567	1567		2094	2094		2587	2587	
input	Tea Average Exit Temperature (K)	197.21	197.21		211.56	211.56		220.61	220.61		232.17	232.17		241.85	241.85	
output	rhoea Average Exit Density at Tea and Pea (kg/m3)	5.0108	5.0094	1.0003	15.8896	15.8785	1.0007	24.8891	24.8086	1.0032	38.6668	38.2802	1.0101	60.5746	59.5811	1.0167
	cea Average Exit Sound Speed at Tea and Pea (m/s)	307.18	N/A		281.37	N/A		264.98	N/A		239.86	N/A		207.79	N/A	
output	Xea Average Exit Liquid Fraction at Tea and Pea	0.0817	0.0817	1.0000	0.1701	0.1706	0.9971	0.2277	0.2259	1.0080	0.3326	0.3232	1.0291	0.4743	0.4625	1.0255
	k Average ratio of Cp/Cv	1.2251			1.1571			1.1093			1.0475			0.9892		
output	Tf Isenthalpic Flash Temperature (K, from P0 and T0 to Pa)	208.47	208.41	1.0003	201.44	201.52	0.9996	193.86	194.20	0.9982	181.15	183.19	0.9889	186.65	186.40	1.0013
output	rhof Isenthalpic Flash Density at Pa and Tf (kg/m3)	1.0521	1.0518	1.0003	1.2045	1.2037	1.0007	1.3239	1.3214	1.0019	1.5863	1.5225	1.0419	1.9164	1.8885	1.0148
output	Xf Isenthalpic Flash Liquid Mass Fraction at Pa and Tf	0.0318	0.0322	0.9876	0.0722	0.0729	0.9904	0.089	0.0899	0.9900	0.1374	0.1363	1.0081	0.2739	0.2569	1.0662
	Vr R Plane Velocity (m/s)	299.7			302.5			293.4			273.6			243.7		
input	Tr R Plane Temperature (K)	189.32			183.79			178.42			179.39			184.87		
	rhorr R Plane Density (kg/m3)	1.1712			1.3455			1.4756			1.6912			2.0318		
	Xr R Plane Liquid Mass Fraction	0.0565			0.1084			0.1296			0.2076			0.3245		
output	Tdew Dew Point Temperature (K at Pa)	246.93	246.69	1.0010	257.8	257.64	1.0006	260.49	260.29	1.0008	259.68	259.47	1.0008	258.69	258.52	1.0007
output	CPS Vapour Specific Heat Capacity (J/kg/K, at Pa)	1893.0	1888.4	1.0024	1788.5	1784.8	1.0021	1694.8	1691.9	1.0017	1554.1	1580.6	0.9832	1398.8	1469.4	0.9520
	TBP Boiling Point Temperature (K)	189.32			183.79			178.42			179.39			184.87		
	HFG Heat of Vaporization (J/kg)	2260486			1584452			1450191			1030906			803921		
	CPSL Liquid Specific Heat (J/kg/K)	1752.8			1748.4			1728			1725.7			1740.6		
	RHOSL Liquid Density (kg/m3)	716.3			722.5			748			862.6			968.5		
	SPB saturation pressure constant	904.57			974.9			1036.89			1073.4			1031.25		
	SPC saturation pressure constant	-91.81			-84.34			-77.85			-76.99			-82.53		
			MAX 1.0024			MAX 1.0035			MAX 1.0080			MAX 1.0419			MAX 1.0662	
			MIN 0.9848			MIN 0.9466			MIN 0.9273			MIN 0.9832			MIN 0.9520	

**Appendix 2 Dispersion, Toxic Load and Odour Calculations for Transient Releases
from Pipeline Ruptures and Gas Well Blowouts**

**DISPERSION, TOXIC LOAD AND ODOUR CALCULATIONS
FOR TRANSIENT RELEASES FROM PIPELINE RUPTURES
AND STEADY RELEASES FROM GAS WELL BLOWOUTS**

DAVID J. WILSON

**TECHNICAL REPORT
djw-eub-2003-2**

ALBERTA ENERGY AND UTILITIES BOARD

DECEMBER 2006

**WITH FORMATTING AND CORRECTIONS TO CHAPTERS 3 AND 4 BY AER
AUGUST 2025**

EXECUTIVE SUMMARY

The primary objective of this study was to develop some new techniques for spreadsheet based hazard assessment modelling of toxic gas and odour releases. A spreadsheet is an attractive user-friendly alternative to executable computer models each with their own idiosyncratic form of data input files. Making hazard assessment dispersion calculations using spreadsheet programs on a platform such as Microsoft Excel has the advantage of allowing the user to insert and change inputs in a widely used and well-understood format. The disadvantage is that spreadsheets are not computationally efficient, and long run times can result if the spreadsheet program invokes an iterative and step-by-step solution of the equations for mass release, dispersion, and toxic load on a downwind receptor. In many cases, dispersion models that solve differential equations cannot be programmed at all for spreadsheet use.

Only the ensemble mean concentration from a steady release rate is predicted by existing atmospheric dispersion models that are suitable for spreadsheet use. In contrast, state-of-the-art dispersion modelling requires calculation of second-by-second ground level concentrations from a source with time-varying flow rate, such as a sour gas pipeline rupture that releases hydrogen sulphide to the atmosphere. As a further complication, the high-pressure gas mixture in a pipeline often emerges at a low temperature with a gas density heavier than atmospheric air. These dense gas jets inhibit mixing of atmospheric air with the pipeline gas, and change the shape and surface area of the plumes. The net effect can increase (less mixing) or decrease (more surface area for mixing) the concentration. A dispersion model must be able to account for these dense gas effects for the time-varying release from a pipeline rupture. Finally, because brief peak concentrations are the most dangerous factor in exposure to most toxic gases, knowledge of the concentration fluctuations is essential for calculating the non-linear toxic load on an exposed individual. To deal with this, toxic exposure and odour models require an estimate for the concentration fluctuations caused by plume meandering during a release event, and by variations between events in a large ensemble of hypothetical release events that make up the ensemble mean concentration.

This report addresses six factors that make it difficult to build a state-of-the-art spreadsheet hazard assessment model for a sour gas pipeline rupture or sour gas well blowout:

- Estimating the mass release rate from a pipeline rupture to account for compressible gas effects on release rates from holes smaller than the entire pipe diameter, and for deviations from ideal gas behavior in estimating mass and velocity.
- Calculating the extra mass that will bypass an emergency shut-down (ESD) valve in a pipeline due to the pressure setting at which the ESD is activated.
- Correcting the release buoyancy flux for non-ideal gas behavior, evaporation of liquid droplets, and conversion of kinetic energy in the high speed release jet to thermal energy in the slow-moving air-gas mixture after air is entrained.
- Transforming steady-release rate models to account for the time-varying blowdown rate from a pipeline rupture.
- Adapting steady release-rate dense gas dispersion models to account for the time-varying release rate in a pipeline rupture.

- Accounting for concentration fluctuations and event-to-event variability on the non-linear toxic load. These short duration peak concentrations are more harmful than long duration low concentration exposure. Peak concentrations can create odour annoyance even when the mean concentration is well below the annoyance threshold.

In six separate chapters explicit equations are developed to deal with these complex situations in a format suitable for efficient programming in a spreadsheet format. Simplifications are suggested to avoid iterative calculations, and to keep the input data requirements manageable. These simplifying assumptions still allow the dispersion models to have the necessary degree of realism and accuracy.

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The errors and omissions that remain are my own.

NOTICE

The equations and analysis in this report are part of on-going research into atmospheric dispersion. Some of the assumptions and approximations have not yet been validated by measurements.

ERRATA

June 2024

- Chapter 3:
 - Figure 3.2, the placement of the V_s vector was moved to below the X-axis to avoid confusion if V_s represented an axis
 - Below Equation 3.22, the character in the font used in the original word document for ‘infinity’ was subsequently replaced with ‘N’. ‘infinity’ was re-inserted.
 - Paragraph below Section ‘Downstream Evolution of Buoyancy Flux with Air Entrainment’, $x=$ ‘infinity’ character re-inserted as ‘infinity’
 - Paragraph below Section ‘Buoyancy Flux Far Downwind’, characters re-inserted for ‘arrow’ and ‘infinity’
 - Typo: Figure 3.3, typo ‘pseudo[]state’
 - Typo: Description of equation 4.43, ‘To eliminate x form [from] the left...’
- Chapter 4:
 - Tables 4.1 and Tables 4.2 were corrected. These tables were inconsistent with other publications by D.J.Wilson.

August 2025

- Document formatting

NOMENCLATURE

A_e	$C_D A_{EXIT}$, effective rupture area, including the jet exit discharge coefficient C_D , m^2
A_{EXIT}	actual flow exit area of rupture, $A_{EXIT} = A_P$ for complete rupture of a pipe, m^2
A_P	$\frac{\pi D^2}{4}$, pipeline x-section area for pipe inside diameter D , m^2
a	exponent in the empirical relation between conditional intensity and total intensity
b_z	plume vertical thickness at distance x in dense-gas box model, m
b_y	plume crosswind half-width measured from plume centerline, m
B_A	extra length parameter, m^{-1} , see Equation (3.21)
B_S	ground level concentration per unit volume source flow rate in a plume with no rise, $(kg/m^3 \text{ of air})/(m^3/s \text{ source gas mixture})$, see Equation (4.6)
B^*	constant in the equation for top entrainment velocity, u_e
B_i	wind-shear constant in the equation for conditional fluctuation intensity
c	$(k Z R T)^{\frac{1}{2}}$, speed of sound in a quasi-ideal gas at temperature T and compressibility factor Z , where $Z = Z(P, T)$, m/s
c_e	$(k Z_e R T_e)^{\frac{1}{2}}$, speed of sound at the adiabatic sonic ($\mathfrak{M} = 1.0$) exit velocity, m/s
c_{ei}	$(k Z_{ei} R T_{ei})^{\frac{1}{2}}$, initial speed of sound at adiabatic exit temperature and $t=0$, m/s
c_{oi}	$(k Z_{oi} R T_{oi})^{\frac{1}{2}}$, speed of sound in the pipeline gas at stagnation conditions, m/s
C_D	A_e/A_{EXIT} , jet exit discharge coefficient to account for flow contraction and exit velocity profile.
C_o	$\frac{\chi_o}{\rho_s}$, ground level volume concentration of contaminant in air, $\frac{m^3 H_2S}{m^3 mixture}$
C_p	specific heat, Joules / (kg K)
C_{pa}	specific heat of atmospheric air, Joules / (kg K)
C_{ps}	specific heat of source gas, including droplets, Joules / (kg K)
C_{pss}	specific heat of source gas, with droplets evaporated, Joules / (kg K)
C_s	$\frac{\chi_s}{\rho_s}$, source volume concentration of contaminant, $\frac{m^3 H_2S}{m^3 source gas}$
D	pipe inside diameter, m
F_b	$g \left(\frac{\rho_a - \rho(x)}{\rho_a} \right) \frac{\dot{Q}(x)}{\pi}$, buoyancy flux of the jet or plume at distance x from the source
$F(\phi)$	effect of density on $2b_y b_z$
F_N	$F(\phi)/F(\phi=0)$, density function normalized by its value for no density difference.
f	friction factor in pipeline isothermal quasi-steady flow
f_s	$m_s/m(x)$, mass fraction of source gas in the jet or plume at distance x from the source

g	acceleration of gravity, 9.81 m/s ²
g_s'	$g \left(\frac{\rho_s - \rho_a}{\rho_a} \right)$, effective acceleration of gravity of the source gas mixture
G	effect of turbulence scale L_a , surface roughness z_o and friction velocity u_* on $2b_y b_z$
h	plume rise above ground, m
$h(x)$	enthalpy at local temperature T in the jet or plume at distance x from source, Joules / kg
h_a	$C_{pa}T_a$, static enthalpy of atmospheric air, Joules / kg
h_f	enthalpy of the vapour phase, Joules / kg
h_{fg}	enthalpy of vaporization, Joules / kg
$h_{fg,s}$	enthalpy of vaporization at source temperature T_s , Joules / kg
h_g	enthalpy of a gas or vapour, Joules / kg
h_i	plume rise above ground for the initial mass release rate at $t=0$, m
h_o	$h(x) + \frac{V^2(x)}{2}$, stagnation enthalpy at temperature T_o of gas at velocity V at distance x from the source, Joules / kg
h_s	$C_{ps}T_s$ enthalpy of source mixture, Joules / kg
h_{ss}	$C_{ps}T_{ss}$ enthalpy of a virtual source vapour after all liquid is adiabatically evaporated, Joules / kg
H	dense gas dispersion similarity function, see Equation (5.20)
i	$\chi_{rms} / \bar{\chi}$, concentration fluctuation intensity about mean, including periods of zero concentration, and for fluctuations during any one release event AND the fluctuations caused by event-to-event variability in a large ensemble.
i_p	$\chi_{p,rms} / \bar{\chi}_p$ in-plume fluctuation intensity conditional on concentration being greater than zero, so excluding intermittent periods of zero concentration for both the mean and the fluctuations $\chi_{p,rms}$, and for fluctuations during any one release event AND the fluctuations caused by event-to-event variability in a large ensemble.
$i_{p\infty}$	constant in-plume fluctuation intensity in the highly intermittent fringes of a plume where $\gamma \rightarrow 0$ and $i \rightarrow \infty$, and for fluctuations during any one release event AND the fluctuations caused by event-to-event variability in a large ensemble.
k	$\frac{C_p}{C_v}$, specific heat ratio for pipeline gas mixture, assumed constant
$K_{fluctuation}$	Adjustment factor to multiply by the mean concentration $\bar{\chi}$ to include concentration fluctuations in the mean toxic load \bar{L}
$K_{inertia}$	$\dot{m}_{ei} / \dot{m}_{ei,isentropic}$ empirical constant used to adjust inertialess quasi-steady initial release rate to account for pipeline gas inertia at the moment of rupture $t=0$.
\bar{L}	$\int_0^\infty \chi^n dt$, mean toxic load for an exposure to time-varying instantaneous concentrations
L_{eff}	$L_{ESD} + L_{extra}$, effective pipeline length including mass leakage past ESD valve, m
L_{ESD}	length of pipe from rupture to ESD valve, m

L_{extra}	extra length added to L_{ESD} that contains the mass M_{extra} that flows past the ESD valve before it closes, m
\dot{m}	mass flow rate, kg/s
\dot{m}_a	mass flow rate of air entrained into the jet or plume from the source to distance x, kg/s
\dot{m}_e	mass flow rate from the pipe exit, kg/s
\dot{m}_{ei}	inertia-adjusted initial mass release rate from the pipe exit, kg/s
\dot{m}_s	$\rho_s \dot{q}_s$, time varying total source gas mass release rate, (kg mixture)/s
\dot{m}_{si}	initial source gas mass release rate, (kg mixture)/s
M	molecular mass of pipeline gas mixture, kg/kmol
M	molecular mass of jet or plume mixture at distance x from the source, kg/kmol
M_a	molecular mass of atmospheric air, kg/kmol
M_s	molecular mass of source mixture of vapour and liquid, kg/kmol
\mathfrak{M}	V/c, local Mach number in the flow
\mathfrak{M}_e	sonic Mach number at exit temperature and pressure conditions
M_i	$\int_0^{\infty} \dot{m}_e dt$, total mass released from the rupture, equal to initial mass in the pipeline
	effective length L_{eff} , kg of gas mixture
m_{extra}	extra mass that leaks past the ESD valve, calculated at the initial pipeline density ρ_i , kg of gas mixture.
n	exponent in toxic load exposure model \bar{L}
N	number of kilomoles of a substance
P	$\rho Z_{oi} RT$, pressure along the pipeline at position x and time t, Pa absolute
P_a	atmospheric pressure, Pa absolute
P_{atm}	atmospheric pressure, Pa absolute
P_o	$P + (\rho V^2 / 2)$, stagnation pressure of gas with velocity V, Pa absolute
P_{oi}	pressure before pipeline rupture, Pa absolute
P_{ei}	pressure at the pipe rupture exit area A_e after isentropic expansion from (P_{oi}, T_{oi}) , Pa absolute
P_{ESD}	pressure set point for ESD valve closure, Pa absolute
\dot{q}_s	$\frac{\dot{m}_s}{\rho_s}$, volume release rate of source gas mixture, (m ³ source gas)/s
\dot{Q}	$\frac{\dot{m}(x)}{\rho(x)}$, jet or plume volume flow rate at distance x from the source, m ³ /s
Q_s	mass release rate of contaminant gas component, (kg H ₂ S)/s
r_s	effective source radius at (P_a, T_s) , m
R	\bar{R} / M , ideal gas constant, Joules/(kg K)
R	$\frac{\chi_{oi, no rise}}{\chi_{oi, with rise}}$, ratio of concentration at ground level with and without plume rise

\bar{R}	8314.5, universal gas constant, Joules/(kg-kmol K)
Re_D	Reynolds number in the pipeline
Ri^*	Richardson number based on friction velocity u_*
S_a	Length scale of atmospheric turbulence at z_{ref} , m
t_a	time after rupture or time after arrival of the “frozen” release, s
t_{eq}	equivalent steady averaging time for calculation of plume spreading, s
t_{ESD}	ESD valve activation time delay, s
$t_{exposure}$	equivalent exposure time to a steady concentration, s
t_{avg}	averaging time over which a mean concentration or plume spread is calculated, s
t_{MAX}	time after arrival of a release that the maximum ground-level concentration occurs, s
T	temperature in the moving gas stream inside or outside the pipe, K
T_a	atmospheric temperature, K
T_{ei}	temperature in the moving gas at sonic velocity in the exit plane area A_e , K
T_o	stagnation temperature after a moving stream is brought to rest adiabatically, K
T_{oe}	stagnation temperature in the moving gas at sonic velocity in the exit plane area A_e , K
T_{oi}	initial gas stagnation temperature in the pipeline before rupture, K
T_{os}	stagnation temperature of the source gas at atmospheric pressure, including real-gas effects in the adiabatic expansion from (P_{oi}, T_{oi}) to atmospheric pressure P_a , K
T_{oss}	$T_{SS} + \frac{V_s^2}{2C_{pSS}}$ effective stagnation temperature at source velocity V_s of a virtual source gas after adiabatic droplet evaporation, K
T_s	source gas temperature, with liquid droplets, K
T_{SS}	source gas temperature, for of a virtual source gas after adiabatic droplet evaporation, K
$u_{e,top}$	turbulent air entrainment velocity into top of a dense plume, m/s
$u_{e,side}$	turbulent air entrainment velocity into the side edges of a dense plume, m/s
u_*	friction velocity in log-law velocity profile, m/s
U	wind speed in the atmosphere, varying with height above ground, m/s
U_a	wind speed in the atmosphere, varying with height above ground, m/s
U_c	effective wind speed, the mass convection velocity of a plume passing a position x , m/s
U_{ref}	wind speed at a fixed reference height z_{ref} above ground, m/s
V	$\dot{m}/\rho A_p$, local pipe velocity or jet velocity, m/s
V_s	source mixture velocity, after expansion to atmospheric pressure, m/s
V_x	horizontal component of jet or plume velocity at distance x from the source, m/s
V_z	vertical component of jet or plume velocity at distance x from the source, m/s
W_s	source gas mixture velocity at non-ideal gas stagnation temperature T_{os} and P_a , m/s
x	downwind distance from source, m
x_{wave}	position of the moving density wave in the pipeline at time t after rupture, m
z_c	reference height above ground where local wind speed U is the same as the plume mass convection velocity U_c , m

z_{ref}	reference height above ground where the windspeed U_{ref} is measured, m
Z	gas compressibility factor including mass of any droplets at (P, T)
Z_a	atmospheric air compressibility factor at (P_a, T_a)
Z_e	gas compressibility factor at exit plane conditions (P_e, T_e)
Z_{ei}	gas compressibility factor at the exit plane (P_{ei}, T_{ei}) at the moment of rupture $t=0$
Z_{oi}	gas compressibility factor inside the pipe at stagnation conditions before rupture, (P_{oi}, T_{oi})
Z_r	gas compressibility factor of source gas component in diluted jet or plume at distance x from the source, evaluated at the partial pressure $p_a(x)$ of the source gas component and the mixture temperature $T(x)$

Greek Symbols

α	initial time constant adjustment factor
α_e	entrainment constant in $u_e = \alpha_e u^*$ for a passive plume with no density difference
β	final isothermal inertialess pipeline release time constant, s
χ	instantaneous contaminant mass concentration, $(\text{kg H}_2\text{S})/\text{m}^3$
$\overline{\chi}$	mean contaminant mass concentration, $(\text{kg H}_2\text{S})/\text{m}^3$
$\overline{\chi}^n$	n^{th} power of mean concentration
$\overline{\chi}^n$	mean of n^{th} moment of concentration for mean toxic load \overline{L} , $(\text{kg H}_2\text{S} / \text{m}^3)^n$
χ'	$(\chi - \overline{\chi})^2$, instantaneous concentration fluctuation about the mean $\overline{\chi}$, $(\text{kg H}_2\text{S})/\text{m}^3$
$\overline{\chi'^2}$	(χ'^2) , mean-square of mass concentration fluctuations about the mean, $(\text{kg H}_2\text{S})/\text{m}^3$
$\chi_{effective}$	effective mass concentration for calculating the mean toxic load \overline{L} , $(\text{kg H}_2\text{S})/\text{m}^3$
χ_o	plume centerline mass concentration, $(\text{kg H}_2\text{S})/\text{m}^3$
χ_p	in-plume mean of non-zero mass concentrations, $(\text{kg H}_2\text{S})/\text{m}^3$
χ_{rms}	$(\overline{\chi'^2})^{\frac{1}{2}}$, root-mean-square (standard deviation) of concentration fluctuations about the mean, $(\text{kg H}_2\text{S})/\text{m}^3$
$\chi_{p,rms}$	standard deviation of in-plume, non-zero concentrations, $(\text{kg H}_2\text{S})/\text{m}^3$
χ_s	mass concentration of contaminant (H_2S) in the source gas, $(\text{kg H}_2\text{S})/\text{m}^3$
ϕ	$\left(\frac{g_s'^2 \dot{q}_s}{U_{ref}^5} \right)^{\frac{1}{5}}$, dimensionless variable for continuous steady release of a dense gas
γ	intermittency factor, fraction of time concentration is non-zero, $\chi > 0$
ρ	gas density at x and time t , kg/m^3

ρ_a	air density in the atmosphere, kg/m ³
ρ_e	source gas mixture density in the moving flow at rupture exit plane (P_e, T_e), kg/m ³
ρ_{ei}	density of the moving gas at sonic velocity and (P_e, T_e) in the exit plane, kg/m ³
ρ_o	stagnation density after a moving stream is brought to rest adiabatically, kg/m ³
ρ_{oi}	mixture density at stagnation conditions (P_{oi}, T_{oi}), kg/m ³
ρ_s	effective density of the source gas required to produce the same fully-mixed buoyancy flux $F_b(\infty)$ for the high speed non-ideal gas release, kg/m ³
σ_y	vertical spread of a gaussian plume, m
σ_z	crosswind spread of a gaussian plume, m
τ	time constant, s

Commonly Used Subscripts

a	atmospheric air
e	at the rupture exit plane, before expansion of the source jet to atmospheric pressure
i	initial conditions at time $t = 0$, the moment of rupture
o	stagnation conditions with gas brought adiabatically to rest
p	in-plume conditions excluding zero concentrations in intermittent periods
s	source conditions including any droplets in their liquid phase and with real-gas effects; after the release expands to atmospheric pressure, but before any air entrainment
ss	virtual source conditions with droplets evaporated adiabatically, and with real-gas effects; after release expands to atmospheric pressure, but before any air entrainment.

1 Double Exponential for Mass Release Rate

For a sour gas release that is confined to a fixed length of pipeline L_{eff} the mass release rate of sour gas \dot{m}_e can be approximated by the double exponential function developed by Wilson (1979), and refined by Wilson (1981) to include an inertial delay constant K_i to correct the inertialess initial release rate equation. For an effective pipeline length, L_{eff} , from the rupture,

$$L_{eff} = L_{ESD} + L_{extra} \quad (1.1)$$

with extra length L_{extra} to account for mass that flows past the ESD (Emergency Shut-Down) valve before it starts to close. The mass flow rate from the rupture exit area A_e is approximated by a double exponential equation

$$\dot{m}_e = \left(\frac{1}{1 + \alpha} \right) \left[\dot{m}_{ei} \exp\left(-\frac{t}{\alpha^2 \beta} \right) + \frac{M_i}{\beta} \exp\left(-\frac{t}{\beta} \right) \right] \quad (1.2)$$

where the total initial mass M_i , kg, in the pipeline at the moment of rupture is $M_i = \rho_{oi} A_p L_{eff}$, and ρ_{oi} is the constant density in the pipeline before rupture. The density ρ_{oi} is calculated from the stagnation (zero flow) pressure and temperature in the pipeline before rupture, P_{oi} and T_{oi} , which are values averaged over the pipe length L_{eff} . These averages can be very accurately approximated by P and T half-way along the pipe, at $x = L_{eff}/2$.

The mass release rate in (1.2) is for only **one** side of a pipeline rupture. **In all pipe ruptures, flow from the rupture area A_e comes from the pipe segments on both sides of the rupture, and (1.2) must be written for both segments and summed, with the rupture area shared by the two flows.** In practice, the worst-case situation of a complete rupture produces independent flows each with an exit area equal to the pipe cross-sectional area $\pi D^2/4$, and a coefficient of discharge $C_D = 1.0$.

By mass conservation, we know that M_i is also equal to the total mass released from the rupture,

$$M_i = \int_0^{\infty} \dot{m}_e dt \quad (1.3)$$

Integrating Equation (1.2) and equating it to M_i yields the value of the initial time constant adjustment factor α

$$\alpha = \frac{M_i}{\beta \dot{m}_{ei}} \quad (1.4)$$

Using Equation (1.4) the initial blowdown time constant $\alpha^2 \beta$ in (1.2) is

$$\alpha^2 \beta = \frac{M_i^2}{\beta \dot{m}_{ei}^2} \quad (1.5)$$

Wilson (April 1989, unpublished notes for GASCON2) revised the double exponential model to allow rupture area A_e to be less than the entire pipe area A_p and then corrected it (May 1989, unpublished notes to allow for stagnation pressure). Zelensky, based on Wilson's derivation of the extra mass re-derives the time constant in the next chapter to be the same as the corrected version (May 1989, unpublished notes to allow for stagnation pressure).

$$\beta = \frac{2}{3} \frac{\rho_{oi} A_p}{B_A \dot{m}_{ei}} \left(\left(1 + B_A L_{eff} \right)^{\frac{3}{2}} - 1 \right) \quad (1.6)$$

with constant B_A defined from gas properties or calculated real gas flow rate and density

$$\begin{aligned} B_A &= \left(\frac{2}{k+1} \right)^{\frac{k+1}{k-1}} \left(\frac{K_{inertia} A_e}{A_p} \right)^2 \left(\frac{Z_e}{Z_{oi}} \right) \frac{k f}{D} \\ &= \frac{\dot{m}_{ei}^2 f}{\rho_{oi} D P_{oi} A_p^2} \end{aligned} \quad (1.7)$$

where

$\rho_{oi} = (P_{oi}/Z_{oi} RT_{oi})$, the density in the pipe at pre-rupture conditions (kg/m^3)

P_{oi} = the initial pressure in the pipe at stagnation conditions (Pa)

T_{oi} = the initial temperature in the pipe at stagnation conditions (K)

Z_{oi} = compressibility factor at initial stagnation conditions, (P_{oi}, T_{oi})

Z_e = compressibility factor at throat conditions, (P_e, T_e)

$k = c_p/c_v$, specific heat ratio for pipeline gas mixture, assumed constant

$A_p = \pi D^2/4$, pipeline x-section area (m^2) for pipe inside diameter D (m)

$A_e = C_D \pi D^2/4$, effective hole area, **including the jet exit discharge coefficient C_D** (m^2)

- f = friction factor in pipeline isothermal quasi-steady flow
 R = \bar{R}/M gas constant, where $\bar{R} = 8314.5$ J/(kg-kmol K) is the universal gas constant
 M = molecular mass of pipeline gas mixture, (kg/kmol)
 L_{eff} = effective length of the pipeline, including extra length L_{extra} to contain mass that leaks past the ESD valve (m), as defined in next chapter
 $K_{inertia}$ = inertial delay factor as discussed later
 \dot{m}_{ei} = initial mass release rate including inertial delay (kg/s), defined later

By defining $A_e = C_D \pi D^2 / 4$ including the jet exit discharge coefficient, the choice of an appropriate discharge coefficient is left to the user. For flow out of pipes, including leaks from broken-off branch lines, the emerging flow is straight and parallel and $C_D \sim 1.0$ is a reasonable assumption. For flow through a sharp-edged rip or puncture in a pipe wall, $C_D \sim 0.6$ is the smallest value expected for a contracting jet flowing through a thin sharp-edged orifice.

Equation (1.6) and the second exponential in (1.2) is the **exact** solution for the inertialess flow rate from an isothermal pipe at constant temperature T_{oi} along its length, filled with a quasi-ideal gas. Here, “quasi-ideal” refers to a gas that has a constant compressibility factor Z , independent of the varying pressure along the pipeline and with time. The assumption of isothermal flow requires heat from the pipe walls to be added to the moving gas to keep its temperature from dropping as its pressure decreases as it moves along the pipe toward the rupture point. Except for the last few hundred meters before the rupture, this isothermal assumption is generally valid.

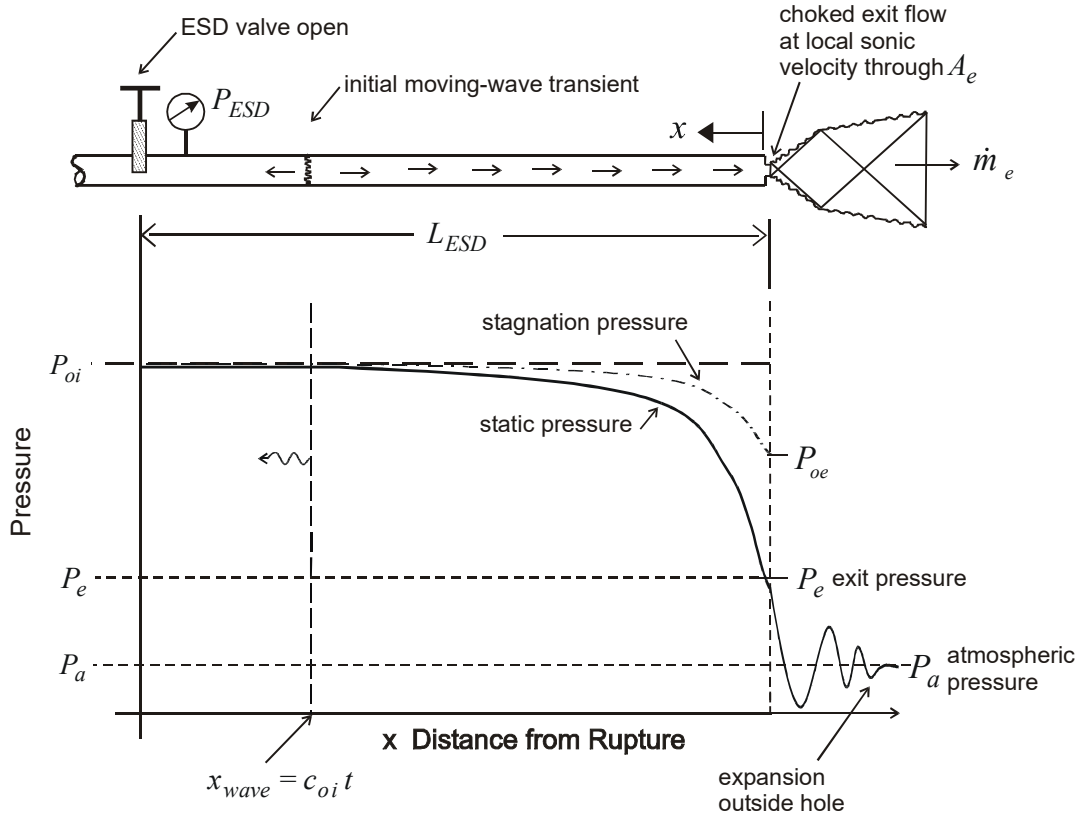


Figure 1-1 Pipeline pressure distribution along a short time t after rupture, before the moving-wave rupture transient reaches the ESD valve

Because the first exponential in (1.2) is only an approximation for the initial blowdown transient in \dot{m}_e , it comes as no surprise that (1.5) for $\alpha^2\beta$ has a minor physical flaw. The flaw is that the initial time constant $\alpha^2\beta$ in (1.5) is expressed in terms of the final decay constant β . This can't be correct, because the final time constant β in (1.6) contains the effective pipe length L_{eff} . In reality, the initial blowdown time constant $\alpha^2\beta$ can't "know" anything about the pipeline length L_{eff} before the density wave traveling at the speed of sound reaches the end of the pipe.

For adiabatic flow out of the exit hole, neglecting inertia, and including the discharge coefficient C_D with the physical exit area A_{EXIT} so the effective exit area is $A_e = C_D A_{EXIT}$

$$\dot{m}_e = \rho_e A_e c_e \quad (1.8)$$

$$c_e = (k Z_e R T_e)^{\frac{1}{2}} \quad (1.9)$$

where c_e is the speed of sound at choked exit where $T = T_e$. For flow with gas initially at rest, at the adiabatic stagnation temperature T_{oi}

$$\frac{T_{oi}}{T_e} = 1 + \left(\frac{k-1}{2} \right) \mathfrak{M}_e^2 = \frac{k+1}{2} \quad (1.10)$$

where $\mathfrak{M}_e = 1.0$ is the sonic Mach number at exit conditions, denoted by the subscript “e”. As shown in Figure 1.1, the Mach number \mathfrak{M} is low enough along most of the pipe to allow us to approximate the stagnation pressure P_o by the static pressure P . Near the adiabatic choked flow exit this is not true. It is not obvious why the compressibility factor Z does not appear in (1.10). For a quasi-ideal gas, it is easy to show from the definition of enthalpy $C_p T = C_v T + P/\rho$ that $C_p - C_v = ZR$, so that $1 - 1/k = ZR/C_p$, and the R in this relation will cancel the R in (1.9) when deriving (1.10) for a constant Z .

1.1 Isentropic Initial Mass Release Rate $\dot{m}_{ei, isentropic}$

At $t = 0$ there is no frictional loss and we have an adiabatic, frictionless (isentropic) expansion. We make the further assumption that the inertia of the gas can be neglected so that at any time the flow is the same as a steady flow at that temperature and pressure. This is referred to as “quasi-steady” or “inertialess”. Denoting this entire oversimplified approximation by the subscript “isentropic”, and using the isentropic process equation for a non-ideal gas with compressibility factor Z ,

$$\frac{P_{ei, isentropic}}{\rho_{ei, isentropic}^k} = \frac{P_{oi}}{\rho_{oi}^k} \quad (1.11)$$

where P_{oi} and ρ_{oi} are the initial (subscript i) stagnation (zero flow) pressure and density in the pipeline before the rupture occurs. Note that in the general derivation of (1.11) for non-ideal gases with constant specific heat (and thus constant k), Z cancels out and does not appear in (1.11), even though it is in the equation of state for the non-ideal pipeline gas,

$$P = \rho Z R T \quad (1.12)$$

Replacing the pressures in (1.11) with (1.12) yields

$$\frac{\rho_{ei, isentropic} Z_{ei, isentropic} R T_{ei}}{\rho_{ei, isentropic}^k} = \frac{\rho_{oi} Z_{oi} R T_{oi}}{\rho_{oi}^k} \quad (1.13)$$

Note that the temperature of the gas at the exit, T_{ei} , requires only that the flow is adiabatic and allows pipe friction to cause temperature changes, see (1.10). The temperature of the isentropic (frictionless, adiabatic) flow is the same as the adiabatic flow with friction, and the isentropic subscript is not required because temperature $T_{ei, isentropic} = T_{ei}$. Solving (1.13) for the density ratio at the instant of rupture,

$$\frac{\rho_{ei, isentropic}}{\rho_{oi}} = \left(\frac{Z_{ei, isentropic} T_{ei}}{Z_{oi} T_{oi}} \right)^{\frac{1}{k-1}} \quad (1.14)$$

The isentropic, inertialess initial mass flow $\dot{m}_{ei, isentropic}$ is from (1.11)

$$\dot{m}_{ei, isentropic} = \rho_{ei, isentropic} A_e c_{ei} \quad (1.15)$$

where as usual the subscript “i” indicates time $t = 0$, the moment of rupture. With (1.14) and $\rho_{oi} = P_{oi} / (Z_{oi} R T_{oi})$ the mass flow in (1.15) becomes

$$\dot{m}_{ei, isentropic} = \left(\frac{P_{oi} A_e}{Z_{oi} R T_{oi}} \right) \left(\frac{Z_{ei, isentropic} T_{ei}}{Z_{oi} T_{oi}} \right)^{\frac{1}{k-1}} \left(k Z_{ei, isentropic} R T_{ei} \right)^{\frac{1}{2}} \quad (1.16)$$

Using (1.10) to eliminate the temperature ratio, this can be rearranged to yield,

$$\dot{m}_{ei, isentropic} = \left(\frac{Z_{ei, isentropic}}{Z_{oi}} \left(\frac{2}{k+1} \right) \right)^{\frac{k+1}{2(k-1)}} \left(\frac{k}{Z_{oi} R T_{oi}} \right)^{\frac{1}{2}} P_{oi} A_e \quad (1.17)$$

Then, a correction factor $K_{inertia}$ is introduced to reduce the isentropic inertialess release rate in (1.17) to account for the inertia of the gas as it starts from rest at the moment of rupture,

$$\dot{m}_{ei} = K_{inertia} \dot{m}_{ei, isentropic} \quad (1.18)$$

where $K_{inertia}$ is assumed here to be a true constant, independent of the thermodynamic states $(P_{ei, isentropic}, T_{ei})$ and (P_{oi}, T_{oi}) and the compressibility factors $Z_{ei, isentropic}$ and Z_{oi} .

The actual exit pressure P_e produced by the inertia-adjusted initial release rate \dot{m}_e is calculated from (1.11), using (1.12) for ρ_e and (1.9) for the speed of sound c_e to get

$$\dot{m}_e = \frac{P_e A_e}{Z_e R T_e} (k Z_e R T_e)^{\frac{1}{2}} \tag{1.19}$$

which yields

$$P_e = \frac{\dot{m}_e}{A_e} \left(\frac{Z_e R T_e}{k} \right)^{\frac{1}{2}} \tag{1.20}$$

with Z_e evaluated at P_e, T_e , and T_e calculated from T_o and (1.10). The density ρ_e at the inertia-adjusted mass flow rate \dot{m}_e is, from(1.12),

$$\rho_e = \frac{P_e}{Z_e R T_e} \tag{1.21}$$

This completes the set of equations required to calculate the release rate \dot{m}_e .

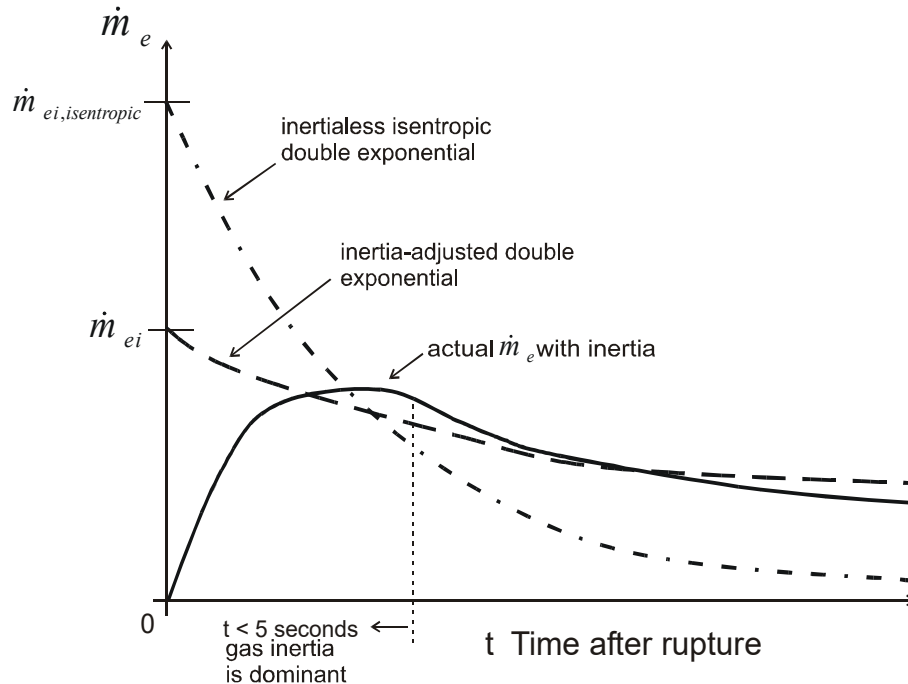


Figure 1-2 *Approximating the actual mass release rate with inertia by an inertialess flow*

1.2 Equivalent Steady Release Duration for a Transient Release

Using Wilson (1995) p11, the equivalent release time for evaluating the effect of averaging time on crosswind plume meandering is

$$t_{eq} = \frac{\left[\int_0^{\infty} \frac{\dot{m}_s(t)}{\dot{m}_{si}} dt \right]^2}{\int_0^{\infty} \left(\frac{\dot{m}_s(t)}{\dot{m}_{si}} \right)^2 dt} \quad (1.22)$$

1.2.1 Case 1: Exponential Decay of a Transient Release

For example, for a single exponential transient release decaying with time constant τ

$$\frac{\dot{m}_s}{\dot{m}_{si}} = e^{-\frac{t}{\tau}} \quad (1.23)$$

With this exponential decay in the definition for t_{eq}

$$t_{eq} = \frac{\left[\int_0^{\infty} e^{-\frac{t}{\tau}} dt \right]^2}{\int_0^{\infty} e^{-\frac{2t}{\tau}} dt} = \frac{\tau^2}{\left(\frac{\tau}{2} \right)} = 2\tau \quad (1.24)$$

1.2.2 Case 2: Double Exponential Decay of a Transient Release

For pipeline releases, a more realistic model for the release rate is a double exponential that conserves the total mass M_i being released, while providing for a short initial time constant $\alpha^2\beta$ as the pressure wave from the rupture travels down the pipeline, and a second time constant β for the final blowdown phase after the pressure wave reaches the end of the pipeline (or the emergency shutdown valve),

$$\dot{m}_e = \left(\frac{1}{1+\alpha} \right) \left[\dot{m}_{ei} \exp\left(-\frac{t}{\alpha^2\beta} \right) + \frac{M_i}{\beta} \exp\left(-\frac{t}{\beta} \right) \right] \quad (1.25)$$

where M_i is the initial mass is the pipeline effective length L_{eff} , and the dimensionless factor α is related to the other parameters by

$$\alpha = \frac{M_i}{\beta \dot{m}_{ei}} \quad (1.26)$$

Then, performing the integrations in (1.22) yields the surprisingly simple result that the equivalent release time is just the sum of the two time constants,

$$t_{eq} = \beta + \alpha^2 \beta \quad (1.27)$$

for double exponential release

1.3 References

- Wilson, D.J. 1979. Release and Dispersion of Toxic Gas from Pipeline Ruptures, Alberta Environment Pollution Control Division Technical Report, 91 pages.
- Wilson, D.J. 1981. Expansion and Plume Rise of Gas Jets from High Pressure Pipeline Ruptures, Alberta Environment Pollution Control Division Technical Report, contract #790686, April 1981, 61 pages.
- Wilson, D.J. 1995. Concentration Fluctuations and Averaging Time in Vapor Clouds, Center for Chemical Process Safety, American Institute of Chemical Engineers, New York, 181 pages.

2 Extra Mass Released due to Delayed ESD Valve Closure

2.1 Assumptions for Pipe Blowdown Analysis

1. Flow in pipe is isothermal at T_{oi} except near the pipe exit where the flow velocity is very high, the heat transfer through the pipe walls is too slow to keep the flow isothermal, and the exit flow adiabatic, with stagnation temperature $T_{oe} = T_{oi}$.
2. The gas in the line is approximated as an ideal gas with $P = \rho Z_{oi} RT$, where Z_{oi} is the compressibility factor of the gas at the initial conditions (P_{oi}, T_{oi}) before the pipeline rupture.
3. As the density and pressure change along the pipe, the friction factor decreases and the compressibility factor Z and stagnation density ratio ρ_o/ρ increase as the flow approaches the exit. We assume that the term $(f\rho_o)/(Z\rho)$ remains constant with distance x .
4. Flow acceleration (caused by changing density with distance x) produces only small pressure gradients that are negligible compared to the pressure gradient caused by wall friction. With this assumption the flow can be treated as quasi-steady with the same mass flow rate $\dot{m} = \dot{m}_e$ at each x position.

Assumption # 4, of inertialess quasi-steady flow, is the key to finding the explicit analytical equations, rather than having to resort to case-by-case numerical solutions of the differential equations of motion. Solution of the non-linear flow equation $\Delta P \propto \rho f V^2 \Delta x$, (where V^2 is the non-linear contribution of velocity $V = \dot{m}/\rho A_p$) is difficult. One previous study, see Botros et. al. (1989), used numerical solutions of an approximate linearized equation. The reader is referred to Shaprio (1953) for a comprehensive review of the thermodynamics of compressible flow.

In the first few seconds after rupture, the gas accelerates from rest, after the density wave sweeps by each x location at the speed of sound. During these first few seconds our assumptions of inertialess flow will over-predict the maximum start-up release rate at $t = 0$ by about a factor of two. However, this error is rapidly reduced by a compensating error from our assumption of quasi-steady flow. The quasi-steady assumption forces the mass flow \dot{m} at every x position to accelerate instantly to the value \dot{m}_e at the pipe exit. This overestimate of \dot{m} produces frictional pressure losses along the entire length from $x = 0$ to $x = x_{wave}$ (where x_{wave} is the position of the moving density wave that sets the stationary pipeline gas into motion.) The pressure drop will be over-predicted by the quasi-steady assumption, and this pressure drop over-prediction will produce a lower exit density ρ_e , resulting in an under-prediction of the exit mass flow \dot{m}_e . The net effect, hopefully, is that the \dot{m}_e error from the quasi-steady assumption will cancel the \dot{m}_e error from the inertialess assumption.

The double exponential model, summarized in Chapter 1, makes no attempt to model realistically the release rate \dot{m}_e for the first few seconds, but instead fits a smooth, rapidly-decaying initial exponential function as an empirical curve from $\dot{m}_e = \dot{m}_{ei}$ at $t = 0$ to the final isothermal quasi-steady inertialess blowdown that is correctly represented by an exponential decay.

$$\dot{m}_e = \frac{M_i}{\beta} \exp\left(-\frac{t}{\beta}\right) \quad (2.1)$$

final isothermal decay

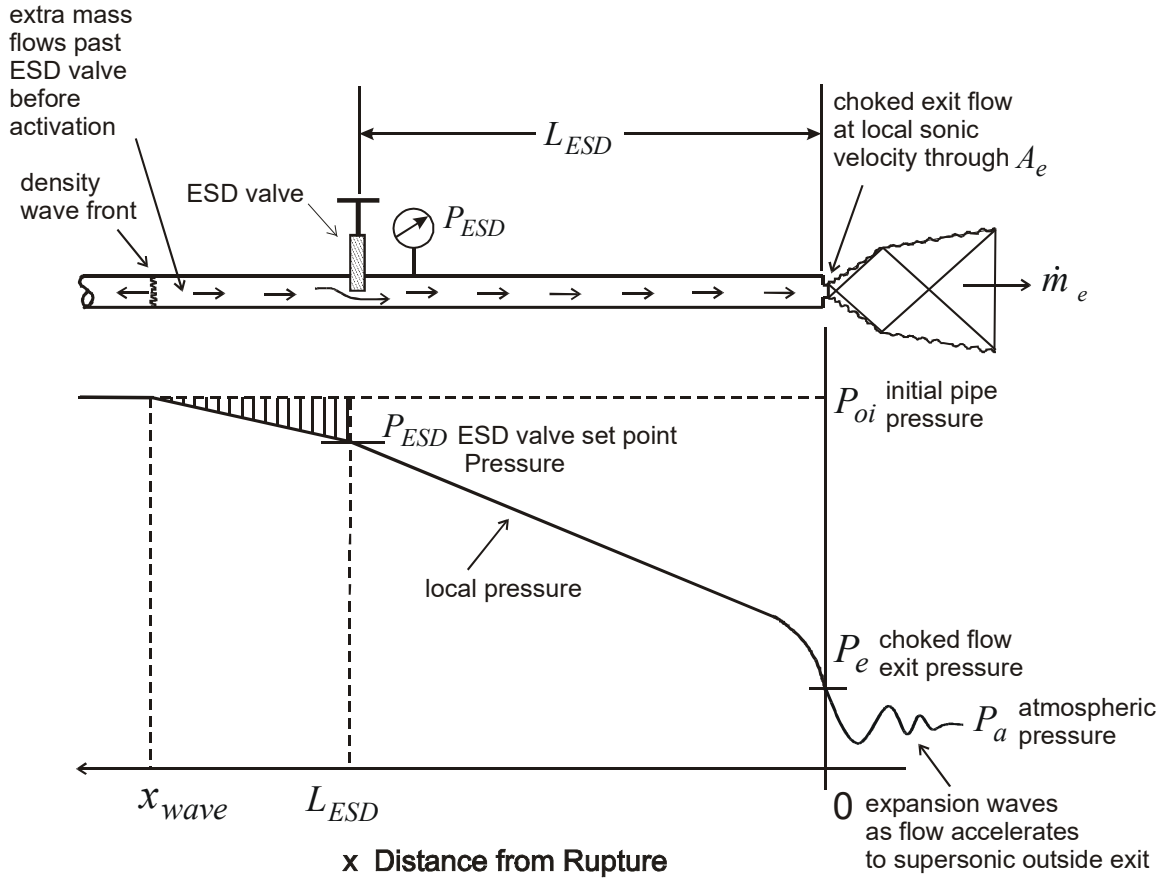


Figure 2-1 *Pressure variation along the pipe at the instant when the ESD valve is activated and begins to close.*

Because we assume the gas is stationary (zero flow rate) in the pipeline before it ruptures, $P_{oi} = P_i$ and $T_{oi} = T_i$, where the subscript “o” indicates isentropic (frictionless) stagnation conditions.

2.2 Pressure and Density Variation along the Pipeline

A density profile method will be used to calculate the amount of mass that leaks past the ESD valve before it reaches its closure activation pressure set-point P_{ESD} . In order to calculate the density ρ at each x position we first relate the density variation to the pressure variation along the pipe. For isothermal flow at $T = T_{oi}$, the initial temperature of the gas at rest in the pipe,

$$\rho = \frac{P}{Z R T_{oi}} \quad (2.2)$$

where

ρ	=	gas density at x and time t (kg/m ³)
P	=	absolute pressure at x and time t (Pa abs)
Z	=	gas compressibility factor at (P, T_{oi})
R	=	ideal gas constant, \bar{R} / M (Joules / kg K)
M	=	molecular mass of gas mixture (kg/kmol)
\bar{R}	=	8314.5, universal gas constant (Joules / kmol K)

The relevant variables for a non-ideal-gas analysis are:

T_{oi}	=	initial gas temperature in the pipeline (K)
P_{oi}	=	initial pipeline pressure before rupture (Pa abs)
Z_{oi}	=	compressibility factor at (T_{oi}, P_{oi})
\dot{m}_e	=	mass flow rate from the pipe exit (kg / s)
A_p	=	pipe cross-sectional flow area (m ²)
A_e	=	effective exit plane flow area (m ²)

For adiabatic inertialess flow, the stagnation temperature $T = T_{oi}$ remains constant with the distance x , and the isentropic (frictionless) stagnation pressure P_o is reduced below the initial stagnation pressure P_{oi} by frictional losses, see Shapiro (1953).

$$\frac{\partial P_o}{\partial x} = \rho \frac{f V^2}{D} \quad (2.3)$$

where $P_o = P + (\rho V^2 / 2)$, stagnation pressure (Pa abs)
 $V =$ local velocity of the quasi-steady flow (m/s)
 $D =$ pipe inside diameter (m)
 $f =$ friction factor

The friction factor is a function of local Reynolds number Re_D , and pipe roughness:

$$Re_D = \frac{\rho V D}{\mu} \quad (2.4)$$

Our assumption of quasi-steady flow requires the mass flow \dot{m} to be constant at each position x for a given time t , so $\dot{m} = \dot{m}_e$ and by definition,

$$V = \frac{\dot{m}_e}{\rho A_p} = \frac{4\dot{m}_e}{\pi \rho D^2} \quad (2.5)$$

Using (2.5) in (2.4)

$$Re_D = \frac{4\dot{m}_e}{\pi \mu D} \quad (2.6)$$

so for quasi-steady flow, Re_D is constant with x , and f will also be constant with x , varying only in time. Then, taking the x derivative of (2.2) to find the relations between stagnation pressure gradient and stagnation density gradient

$$\frac{\partial P_o}{\partial x} = Z_o R T_o \frac{\partial \rho_o}{\partial x} \quad (2.7)$$

where Z_o is the compressibility factor at (P_o, T_o) at each x , and ρ_o is the stagnation density at P_o, T_o . Equating (2.3) to (2.7), with (2.5) for V :

$$Z_o R T_o \frac{\partial \rho_o}{\partial x} = \frac{\rho f \dot{m}_e^2}{2D \rho^2 A_p^2} \quad (2.8)$$

At a given time t , (2.8) gives the variation of ρ_o with the x as:

$$\rho_o d\rho_o = \frac{\dot{m}_e^2 f}{2D Z_o R T_o A_p^2} \frac{\rho_o}{\rho} dx \quad (2.9)$$

Equation (2.9) is difficult to integrate because several of the variables on the right hand side are functions of pressure and velocity, which both change along the pipe with x . The density ratio ρ_o / ρ is a function of the local Mach number $\mathfrak{M} = V / c$, where c is the local speed of sound,

$$\frac{\rho_o}{\rho} = \left(1 + \left(\frac{k-1}{2} \right) \mathfrak{M}^2 \right)^{\frac{1}{k-1}} \quad (2.10)$$

Note that the compressibility factor ratio is 1 with the quasi-ideal gas assumption and does not appear in functions for ρ_o / ρ or for T_o / T or P_o / P . Typically $k = 1.4$ so that $\rho_o / \rho < 1.05$ for Mach Number $\mathfrak{M} < 0.3$, which is true over most of the pipe length, except for the last few hundred diameters where the flow accelerates rapidly and adiabatically to exit sonically at $\mathfrak{M} = 1$ from the rupture. Plotting the variation of f , Z and ρ_o / ρ along the pipe,

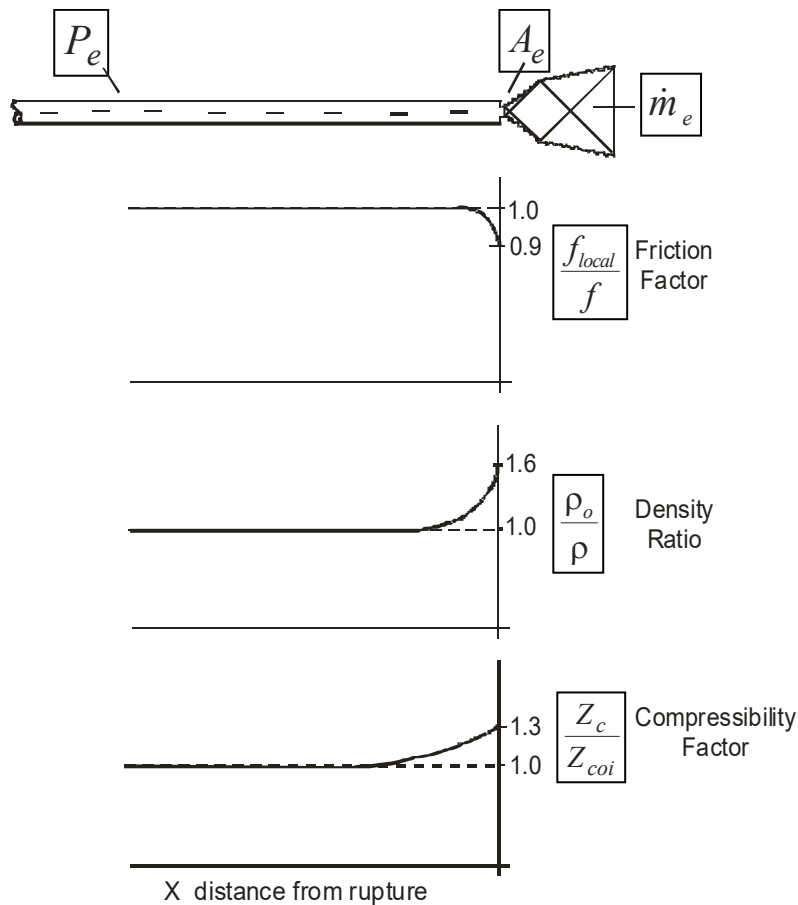


Figure 2.2 *Variation of Friction Factor, Density Ratio and Compressibility Factor Near the Rupture*

The compressibility factor Z increases as the pressure drops to the exit pressure, and outside the rupture exit, Z jumps to $Z = 1.00$ at atmospheric pressure. The friction factor f stays almost constant with distance x , because $\dot{m} = \dot{m}_e$ is constant with x . However, f does drop somewhat near the pipe exit as the flow accelerates from $\mathfrak{M} < 0.3$ to $\mathfrak{M} = 1.0$ at the exit. The flow

acceleration suppresses turbulence production in the flow and so lowers mixing and drag near the pipe wall.

These effects tend to cancel each other in the right side of (2.9), and we will assume that the right side of (2.9) is constant with x , so that in (2.9) we can make the approximation,

$$\int_0^x \frac{f_{local}}{Z} \left(\frac{\rho_o}{\rho} \right) dx = \frac{f x}{Z_{oi}} \quad (2.11)$$

so that (2.9) integrates from the exit stagnation density $\rho_o = \rho_{oe}$ at $x = 0$ to ρ_o at x .

$$\rho_o^2 - \rho_{oe}^2 = \frac{\dot{m}_e^2 f x}{D Z_{oi} R T_{oi} A_p^2} \quad (2.12)$$

At the pipe exit the flow is choked at sonic velocity, and the mass flow rate is,

$$\dot{m}_e = K_{inertia} \rho_e c_e A_e \quad (2.13)$$

where the constant $K_{inertia}$ in (2.13) is an empirical value (typically 0.5) to correct for initial flow rate errors caused by gas inertia and c_e is the speed of sound at the adiabatic sonic ($\mathfrak{M} = 1.0$) exit velocity,

$$c_e = (k Z_e R T_e)^{\frac{1}{2}} \quad (2.14)$$

The temperature decreases as the flow accelerates adiabatically from its stagnation temperature T_o at rest to temperature T at Mach number \mathfrak{M} is

$$\frac{T_o}{T} = 1 + \left(\frac{k-1}{2} \right) \mathfrak{M}^2 \quad (2.15)$$

and for sonic velocity $\mathfrak{M} = 1.0$ at the rupture exit, denoted by subscript “e”, and

$$\frac{T_{oi}}{T_e} = \left(\frac{k+1}{2} \right) \quad (2.16)$$

Keep in mind that $T_{oi} = T_i$ because the gas is initially at rest. Also, from (2.10)

$$\frac{\rho_{oe}}{\rho_e} = \left(\frac{k+1}{2} \right)^{\frac{1}{k-1}} \quad (2.17)$$

Combining (2.13), (2.14), (2.16) and (2.17),

$$\rho_{oe}^2 = \left(\frac{k+1}{2} \right)^{\frac{k+1}{k-1}} \frac{\dot{m}_e^2}{k Z_e R T_{oi} K_{inertia}^2 A_e^2} \quad (2.18)$$

Then use (2.18) to define an initial isentropic mass release rate at $t = 0$, where $\rho_{oe} = \rho_{oi}$ the initial density of the stationary gas in the pipeline

$$\begin{aligned}\dot{m}_{ei} &= K_{inertia} \left(\frac{2}{k+1} \right)^{\frac{k+1}{2(k-1)}} \rho_{oi} A_e (k Z_e R T_{oi})^{\frac{1}{2}}, \text{ or} \\ \dot{m}_{ei} &= K_{inertia} \rho_{oi} \left(\frac{Z_{ei}}{Z_{oi}} \frac{2}{k+1} \right)^{\frac{k+1}{2(k-1)}} \cdot A_e \cdot (k Z_{oi} R T_{oi})^{\frac{1}{2}}\end{aligned}\quad (2.19)$$

Combining (2.12) with (2.18) and normalizing with (2.19) yields the stagnation density variation along the pipe at any time t as,

$$\frac{\rho_o}{\rho_{oi}} = \frac{\dot{m}_e}{\dot{m}_{ei}} [1 + B_A x]^{\frac{1}{2}} \quad (2.20)$$

with the constant B_A defined from properties of calculated from gas properties or from the real gas mass flow rate and density,

$$\begin{aligned}B_A &= \left(\frac{2}{k+1} \right)^{\frac{k+1}{k-1}} \left(\frac{K_{inertia} A_e}{A_p} \right)^2 \left(\frac{Z_e}{Z_{oi}} \right) \frac{k f}{D} \\ &= \frac{\dot{m}_{ei}^2 f}{\rho_{oi} D P_{oi} A_p^2}\end{aligned}\quad (2.21)$$

Equations (2.20) and (2.21) apply to inertialess, quasi-steady, isothermal flow.

To further simplify this equation, it will be assumed in the following analysis that

$Z_e / Z_{oi} = \text{CONSTANT}$ so that B_A remains constant with time. Note that the empirical inertial lag correction constant $K_{inertia}$ appears as part of the normalization by the initial mass flow rate \dot{m}_{ei} .

2.3 Integration of Density Profile for ESD Leakage

The extra mass that leaks past the ESD valve before the pressure at the valve drops to the set-point pressure P_{ESD} is found by integrating the density profile $\rho(x)$ along the pipe from $x = L_{ESD}$ to $x = x_{\text{wave}}$, where $\rho(x)$ has just started to change from its initial constant density ρ_i in the stationary gas, as shown in Figure 2.1. The first step is to determine the position x_{wave} at the time t_{ESD} when the ESD is activated. For quasi-ideal (Z ratio=1), isothermal flow, the pressure ratio is equal to the density ratio, so (2.20) becomes:

$$\frac{P_o}{P_{oi}} = \frac{\rho_o}{\rho_{oi}} = \frac{\dot{m}_e}{\dot{m}_{ei}} [1 + B_A x]^{\frac{1}{2}} \quad (2.22)$$

In the slow subsonic flow far from the rupture, stagnation and static pressure are almost equal, so $P_o = P$ is a good approximation. At the instant the ESD valve is activated, (2.22) becomes:

$$\frac{P_{ESD}}{P_{oi}} = \frac{\dot{m}_{e,ESD}}{\dot{m}_{ei}} [1 + B_A L_{ESD}]^{\frac{1}{2}} \quad (2.23)$$

solving (2.23) for the mass flow rate at $t = t_{ESD}$,

$$\frac{\dot{m}_{e,ESD}}{\dot{m}_{ei}} = \frac{P_{ESD}}{P_{oi}} \left[\frac{1}{[1 + B_A L_{ESD}]^{\frac{1}{2}}} \right] \quad (2.24)$$

The stagnation density profile along the pipe at $t = t_{ESD}$ is determined by putting (2.24) into (2.22) at $t = t_{ESD}$ to obtain,

$$\left. \frac{\rho_o}{\rho_{oi}} \right|_{t=t_{ESD}} = \left(\frac{P_{ESD}}{P_{oi}} \right) \left[\frac{1 + B_A x}{1 + B_A L_{ESD}} \right]^{\frac{1}{2}} \quad (2.25)$$

All the terms on the right hand side of (2.25) are independent of time, so (2.25) gives the remarkable result that the density profile $\rho_o(x)$ along the pipeline at the moment of ESD closure is independent of the delay time t_{ESD} before closure. This time-independence of $\rho_o(x)$ will produce an extra mass M_{extra} that leaks past the ESD that is independent of any explicit dependence on activation time delay t_{ESD} . In (2.25) note that the empirical inertia lag constant $K_{inertia}$ has cancelled, making the extra mass M_{extra} independent of pipeline gas inertia in the initial rupture transient.

The position x_{wave} of the density wave can be determined from (2.25) by setting $\rho_o = \rho_{oi}$ at $x = x_{wave}$ to obtain:

$$1 + B_A x_{wave} = \left(\frac{P_{oi}}{P_{ESD}} \right)^2 [1 + B_A L_{ESD}] \quad (2.26)$$

The extra mass that escapes past the ESD valve during the activation delay time t_{ESD} is found by integrating the density change along the pipeline from $x = L_{ESD}$ to $x = x_{wave}$, see Figure 2.1.

$$M_{extra} = \int_{L_{ESD}}^{x_{wave}} (\rho_i - \rho) A_p dx \quad (2.27)$$

For constant initial density ρ_i in the gas at rest before rupture,

$$M_{extra} = \rho_i A_p \int_{L_{ESD}}^{x_{wave}} \left(1 - \frac{\rho}{\rho_i} \right) dx \quad (2.28)$$

with $\rho = \rho_o$ for all $x \geq L_{ESD}$, equation (2.25) can be used in equation (2.28) to obtain,

$$M_{extra} = \underbrace{\left\{ \rho_{oi} A_p [x_{wave} - L_{ESD}] \right\}}_{TERM 1} - \underbrace{\left\{ \frac{\rho_{oi} A_p (P_{ESD}/P_{oi})}{[1 + B_A L_{ESD}]^{\frac{1}{2}}} \int_{L_{ESD}}^{x_{wave}} [1 + B_A x]^{\frac{1}{2}} dx \right\}}_{TERM 2} \quad (2.29)$$

$$M_{extra} = (TERM 1) - (TERM 2)$$

We can express TERM 1 in equation (2.29) as:

$$TERM 1 = \frac{\rho_{oi} A_p}{B_A} \left([1 + B_A x_{wave}] - [1 + B_A L_{ESD}] \right) \quad (2.30)$$

Then, using (2.26) for x_{wave} , (2.30) becomes

$$TERM 1 = \frac{\rho_{oi} A_p}{B_A} [1 + B_A L_{ESD}] \left(\left(\frac{P_{oi}}{P_{ESD}} \right)^2 - 1 \right) \quad (2.31)$$

The integration from the ESD valve to the density wave in TERM 2 can be carried out by defining the integrand as $\psi^{\frac{1}{2}}$, where $\psi = (1 + B_A x)$ and $d\psi = B_A dx$. With this transformation TERM 2 integrates to:

$$TERM 2 = \frac{2}{3} \frac{\rho_{oi} A_p}{B_A} \left(\frac{P_{ESD}}{P_{oi}} \right) [1 + B_A L_{ESD}]^{-\frac{1}{2}} \left((1 + B_A x_{wave})^{\frac{3}{2}} - (1 + B_A L_{ESD})^{\frac{3}{2}} \right) \quad (2.32)$$

Then with (2.26) to define x_{wave} in (2.32),

$$TERM 2 = \frac{\rho_{oi} A_p}{B_A} [1 + B_A L_{ESD}] \left(\frac{2}{3} \left(\frac{P_{oi}}{P_{ESD}} \right)^2 - \frac{2}{3} \left(\frac{P_{ESD}}{P_{oi}} \right) \right) \quad (2.33)$$

Subtracting (2.33) from (2.31) yields the final expression for the extra mass:

$$M_{extra} = \frac{\rho_{oi} A_p}{B_A} [1 + B_A L_{ESD}] \left(\frac{1}{3} \left(\frac{P_{oi}}{P_{ESD}} \right)^2 + \frac{2}{3} \left(\frac{P_{ESD}}{P_{oi}} \right) - 1 \right) \quad (2.34)$$

where B_A is defined by (2.21) and contains the ratio A_e/A_p of the effective exit area A_e of the rupture to the pipe area A_p . The extra mass flow is best expressed as an extra length L_{extra} that contains m_{extra} at the initial pipeline density $\rho_i = \rho_{oi}$,

$$m_{extra} = \rho_i A_p L_{extra} \quad (2.35)$$

Equating (2.34) to (2.35), and using (2.21) to define B_A ,

$$\frac{L_{extra}}{L_{ESD}} = \left[1 + \left(\frac{Z_{oi}}{Z_e} \right) \left(\frac{A_p}{A_e} \right)^2 \left(\frac{k+1}{2} \right)^{\frac{k+1}{k-1}} \left(\frac{D}{k f L_{ESD}} \right) \right] \left[\frac{1}{3} \left(\frac{P_{oi}}{P_{ESD}} \right)^2 + \frac{2}{3} \left(\frac{P_{ESD}}{P_{oi}} \right) - 1 \right] \quad (2.36)$$

2.4 Numerical Example for Extra Length Due to Valve Closure Pressure Setting

Assume:

$Z_e / Z_{oi} = 1.0$	No change in compressibility during expansion
$k = 1.4$	Ratio of specific heats for the quasi-ideal gas
$f = 0.015$	Friction factor in the pipe
$D = 0.305$ m	Inside diameter of the pipe
$L_{ESD} = 2000$ m	Length of pipe from rupture to ESD valve

Then in (2.36)

$$\frac{L_{extra}}{L_{ESD}} = \left[1 + 0.0217 \left(\frac{A_p}{A_e} \right)^2 \right] \left[\frac{1}{3} \left(\frac{P_{oi}}{P_{ESD}} \right)^2 + \frac{2}{3} \left(\frac{P_{ESD}}{P_{oi}} \right) - 1 \right]$$

$$TERM A = \left[1 + 0.0217 \left(\frac{A_p}{A_e} \right)^2 \right]$$

Case 1 Full Area Rupture $A_e = A_p$, TERM A = 1.02

Case 2 10% Area Large Leak $A_e = 0.1A_p$, TERM A = 3.17

Table 2-1: Effect of ESD valve set point on extra length of mass release

Set Point for ESD Valve Closure P_{ESD}/P_{oi}	L_{extra}/L_{ESD}	
	Case 1 Full Area Rupture	Case 2 10% Area Leak
0.9	0.018	0.037
0.75	0.095	0.294
0.67	0.193	0.600
0.50	0.681	2.113
0.33	2.33	7.23
0.25	4.6	14.3

2.5 Activation Time Delay for an ESD Valve

The extra length L_{extra} and extra mass M_{extra} is independent of the functional form for the mass release rate. This is reassuring because the double exponential model for release rate \dot{m}_e is an empirical approximation to the initial rate of decrease combined with an exact expression for the final blowdown after the ESD valve closes. Next, we need an estimate for the delay time t_{ESD} before the ESD valve closes. This time delay is of interest to operators in developing improved ESD valve control strategies that will reduce the activation delay.

The obvious method for estimating the time at which the ESD valve actuates is to substitute the double exponential mass release rate from Chapter 2 directly in (2.23). This approach produces large errors in estimating t_{ESD} , because (2.23) defines the rate of release $\dot{m}_{e,ESD}$ rather than the total extra mass released M_{extra} . This error occurs because the double exponential function for \dot{m}_e is only an empirical approximation for times before the ESD valve closes. A more accurate method for estimating t_{ESD} is to use the total extra mass released, M_{extra} , (the integral of \dot{m}_e) than from the rate \dot{m}_e itself. By using M_{extra} the integral of the exact solution for the final isothermal decay (the second term in (2.37) below) is being used, rather than the initial blowdown approximation (the first term in (2.37)). See Figure 1.2 in Chapter 1 for an illustration of the errors that occur at

short release times, before the sound wave from the rupture reaches the effective “end” of the pipe at time $t = (L_{ESD} + L_{extra})/c_o$.

The first step in estimating t_{ESD} is to allow a travel time L_{ESD}/c_o for a sound wave to travel from the rupture along the pipe to the ESD valve position at $x = L_{ESD}$. Then, starting with the double exponential release rate from Chapter 1, Equation (1.2) with (1.4),

$$\frac{\dot{m}_e}{\dot{m}_{ei}} = \left(\frac{1}{1 + \alpha} \right) \left(\exp\left(-\frac{t}{\alpha^2 \beta} \right) + \alpha \exp\left(-\frac{t}{\beta} \right) \right) \quad (2.37)$$

Integrating this from $t = L_{ESD}/C_o$ to $t = t_{ESD}$ yields the extra mass,

$$M_{extra} = \frac{\dot{m}_{ei}}{1 + \alpha} \int_{\frac{L_{ESD}}{c_o}}^{t_{ESD}} \left(\exp\left(-\frac{t}{\alpha^2 \beta} \right) + \alpha \exp\left(-\frac{t}{\beta} \right) \right) dt \quad (2.38)$$

where

$$c_o = (k Z_{oi} R T_{oi})^{1/2} \quad (2.39)$$

is the speed of sound at the initial pipe stagnation temperature T_{oi} . Integration yields,

$$M_{extra} = \frac{\dot{m}_{ei}}{1 + \alpha} \left[-\alpha^2 \beta \exp\left(-\frac{t}{\alpha^2 \beta} \right) - \alpha \beta \exp\left(-\frac{t}{\beta} \right) \right]_{\frac{L_{ESD}}{c_o}}^{t_{ESD}} \quad (2.40)$$

Evaluating the integral at its limits,

$$\begin{aligned} M_{extra} &= \frac{\dot{m}_{ei}}{1 + \alpha} \left(\alpha^2 \beta \exp\left(-\frac{L_{ESD}}{c_o \alpha^2 \beta} \right) - \alpha \beta \exp\left(-\frac{L_{ESD}}{c_o \beta} \right) \right) \\ &\quad - \frac{\dot{m}_{ei}}{1 + \alpha} \left(\alpha^2 \beta \exp\left(-\frac{t_{ESD}}{\alpha^2 \beta} \right) - \alpha \beta \exp\left(-\frac{t_{ESD}}{\beta} \right) \right) \end{aligned} \quad (2.41)$$

The constant α can be eliminated by using Equations (1.3) and (1.4) from Chapter 1 to obtain,

$$\begin{aligned} M_{extra} &= \frac{1}{1 + \frac{M_i}{\dot{m}_{ei} \beta}} \left(\frac{M_i^2}{\dot{m}_{ei} \beta} \exp\left(-\frac{\dot{m}_{ei}^2 \beta L_{ESD}}{c_o M_i^2} \right) + M_i \exp\left(-\frac{L_{ESD}}{c_o \beta} \right) \right) \\ &\quad - \frac{1}{1 + \frac{M_i}{\dot{m}_{ei} \beta}} \left(\frac{M_i^2}{\dot{m}_{ei} \beta} \exp\left(-\frac{\dot{m}_{ei}^2 \beta t_{ESD}}{M_i^2} \right) - M_i \exp\left(-\frac{t_{ESD}}{\beta} \right) \right) \end{aligned} \quad (2.42)$$

The activation time delay for the ESD valve is found by first calculating L_{extra} from (2.35) and (2.36), with the known pressure set-point P_{ESD} , and then equating this to (2.42) and solving for t_{ESD} by a recursive numerical method.

2.5.1 Time Constant Derivation for Pipe Blowdown

Based on the previous derivations and Wilson's unpublished papers, Zelensky provided the following derivation of the pipeline blowdown time constant. The mass that escapes from the segment during the activation delay time t_{ESD} includes the extra mass that flowed by the ESD valve and the mass that left the segment before the ESD valve closes. It is found by integrating the density change along the pipeline from $x = 0$ to $x = L_{eff}$,

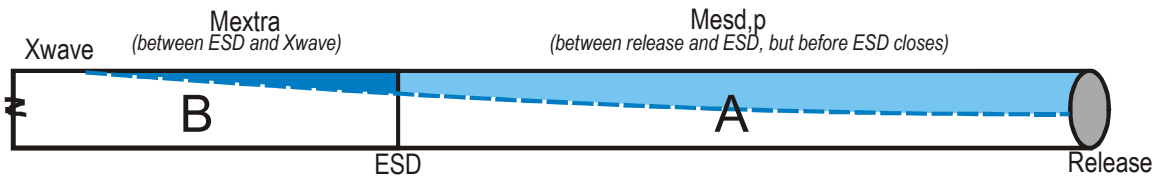


Figure 2.2 Pressure Variation along pipeline from point of release ($x=0$) to ESD Valve and beyond ($x=L_{eff}$)

$$\begin{aligned}
 M_i &= M_{remaining} + M_{exited} = \rho_{oi} A_p L_{eff} \\
 M_{exited} &= (\rho_{oi} - \rho_A) A_p L_{eff} - \int_0^{L_{eff}} (\rho - \rho_A) A_p dx \\
 M_{remaining} &= \int_0^{L_{eff}} (\rho - \rho_A) A_p dx + \rho_A A_p L_{eff}
 \end{aligned} \tag{2.43}$$

where define terms and watch the o and L_{eff} . Note the adjustment for ρ_A to give the correct mass when $\rho = \rho_i$ and when $\rho = \rho_A$. For constant initial density ρ_{oi} in the gas at rest before rupture,

$$M_{remaining} = \rho_{oi} A_p \int_0^{L_{eff}} \left(\frac{\rho}{\rho_{oi}} - \frac{\rho_A}{\rho_{oi}} \right) dx + \rho_A A_p L_{eff} \tag{2.44}$$

From (2.22),

$$\frac{P_o}{P_{oi}} = \frac{\rho_o}{\rho_{oi}} = \frac{\dot{m}_e}{\dot{m}_{ei}} [1 + B_A x]^{\frac{1}{2}} \tag{2.45}$$

so

$$M_{remaining} = \rho_{oi} A_p \left\{ -\frac{\rho_A L_{effective}}{\rho_{oi}} + \frac{\dot{m}_e}{\dot{m}_{ei}} \int_0^{L_{eff}} [1 + B_A x]^{\frac{1}{2}} dx \right\} + \rho_A A_p L_{eff} \quad (2.46)$$

The first term is an adjustment for the mass of gas left in the pipe at atmospheric conditions, which cancels with the third term which is a constant. As done in the previous derivation by Wilson, the second term integration from the rupture to L_{eff} can be carried out by defining the integrand as $\psi^{\frac{1}{2}}$, where $\psi = (1 + B_A x)$ and $d\psi = B_A dx$. With this transformation it integrates to:

$$M_{remaining} = \frac{2}{3} \frac{\rho_{oi} A_p}{B_A} \frac{\dot{m}_e}{\dot{m}_{ei}} \left((1 + B_A L_{eff})^{\frac{3}{2}} - 1 \right) + \rho_{oi} A_p L_{effective} - \frac{2}{3} \frac{\rho_{oi} A_p}{B_A} \left((1 + B_A L_{eff})^{\frac{3}{2}} - 1 \right) \quad (2.47)$$

Note initially the first term is zero and then it is less than the third term, thus there is a minimum L_{eff} that gives a positive $M_{remaining}$ for each mass flow rate in time. Then with (2.19),

$$\dot{m}_{ei} = K_{inertia} \left(\frac{2}{k+1} \right)^{\frac{k+1}{2(k-1)}} \rho_{oi} A_e (k Z_e R T_{oi})^{\frac{1}{2}} \quad (2.48)$$

and B_A as defined in (2.21)

$$B_A = \left(\frac{2}{k+1} \right)^{\frac{k+1}{k-1}} \left(\frac{K_{inertia} A_e}{A_p} \right)^2 \left(\frac{Z_e}{Z_{oi}} \right) \frac{k f}{D} = \frac{\dot{m}_{ei}^2 f}{\rho_{oi} D P_{oi} A_p^2} \quad (2.49)$$

so

$$M_{remaining} = \left\{ \left[\frac{2}{3 C_o} \left(\frac{A_p}{K_{inertia} A_e} \right)^3 \frac{D}{k f} \left(\frac{k+1}{2} \right)^{\frac{3(k+1)}{2(k-1)}} \left(\frac{Z_{oi}}{Z_e} \right)^{\frac{3}{2}} \right] \left[\left(1 + \left(\frac{2}{k+1} \right)^{\frac{k+1}{k-1}} \left(\frac{K_{inertia} A_e}{A_p} \right)^2 \left(\frac{Z_e}{Z_{oi}} \right) \frac{k f}{D} L_{eff} \right)^{\frac{3}{2}} - 1 \right] \right\} \dot{m}_e + \rho_{oi} A_p L_{eff} - \frac{2}{3} \frac{\rho_{oi} A_p}{B_A} \left((1 + B_A L_{eff})^{\frac{3}{2}} - 1 \right) \quad (2.50)$$

define C_o or

$$\begin{aligned}
M_{remaining} &= \frac{2}{3} \rho_{oi}^2 P_{oi} \frac{A_p^3}{\dot{m}_{ei}^3} \frac{D}{f} \left(\left(1 + \frac{\dot{m}_{ei}^2 f}{\rho_{oi} D P_{oi} A_p^2} L_{eff} \right)^{\frac{3}{2}} - 1 \right) \dot{m}_e \\
&\quad - \rho_{oi} A_p L_{eff} + \frac{2}{3} \frac{\rho_{oi} A_p}{B_A} \left((1 + B_A L_{eff})^{\frac{3}{2}} - 1 \right)
\end{aligned} \tag{2.51}$$

The second and third terms above can be shown to be equal with a Taylor expansion $((1+a)^{3/2} \sim 3/2a+1)$ so that when \dot{m}_e is zero, $M_{remaining}$ is zero.

For a simple exponential blowdown the mass flow rate in time is,

$$\begin{aligned}
\dot{m}_e &= \dot{m}_{ei} \exp\left(\frac{-t}{\beta}\right) \\
&\text{with} \\
\beta &= \frac{M_i}{\dot{m}_{ei}}
\end{aligned} \tag{2.52}$$

and the mass is

$$\begin{aligned}
M_{exited} &= \int_0^t \dot{m}_e dt \\
&= \beta \dot{m}_{ei} \left[1 - \exp\left(\frac{-t}{\beta}\right) \right] + C \\
M_{remaining} &= M_i - M_{exited} \\
&= M_i - M_{initial} \left[1 - \exp\left(\frac{-t}{\beta}\right) \right] + C \\
&= M_i \exp\left(\frac{-t}{\beta}\right) + C \\
&= \beta \dot{m}_e + C
\end{aligned} \tag{2.53}$$

and, with the constant C in the above equal to the last two terms of (2.51), then:

$$\begin{aligned}
\beta &= \left\{ \frac{2}{3 C_o} \left(\frac{A_p}{K_{inertia} A_e} \right)^3 \frac{D}{k f} \left(\frac{k+1}{2} \right)^{\frac{3(k+1)}{2(k-1)}} \left(\frac{Z_{oi}}{Z_e} \right)^{\frac{3}{2}} \right. \\
&\quad \left. \left(\left(1 + \left(\frac{2}{k+1} \right)^{\frac{k+1}{k-1}} \left(\frac{K_{inertia} A_e}{A_p} \right)^2 \left(\frac{Z_e}{Z_{oi}} \right) \frac{k f}{D} L_{eff} \right)^{\frac{3}{2}} - 1 \right) \right\} \\
&= \frac{2 D \rho_{oi}^2 P_{oi} A_p^3}{3 f \dot{m}_{ei}^3} \left(\left(1 + \frac{\dot{m}_{ei}^2 f}{\rho_{oi} D P_{oi} A_p^2} L_{eff} \right)^{\frac{3}{2}} - 1 \right) \\
&= \frac{2 \rho_{oi} A_p}{3 B_A \dot{m}_{ei}} \left((1 + B_A L_{eff})^{\frac{3}{2}} - 1 \right)
\end{aligned} \tag{2.54}$$

In the limit, B_A can be very small or L_{eff} can be very large. As B_A approaches zero due to small hole sizes A_e , the above equations become indeterminant. The bracketed term can be expanded as a Taylor series in the form

$$(1+a)^{\frac{3}{2}} - 1 \approx \frac{3}{2} a \tag{2.55}$$

As A_e approaches zero:

$$\begin{aligned}
\beta &= \frac{L_{eff}}{C_o} \left(\frac{A_p}{K_{inertia} A_e} \right) \left(\frac{k+1}{2} \right)^{\frac{1(k+1)}{2(k-1)}} \left(\frac{Z_{oi}}{Z_e} \right)^{\frac{1}{2}} \\
&= \frac{\rho_{oi} A_p}{\dot{m}_{ei}} L_{eff} \\
&= \frac{M_i}{\dot{m}_{ei}}
\end{aligned} \tag{2.56}$$

This is the solution for the isothermal blowdown of a long storage tank that produces the simple exponential blowdown. For the other extreme, where L_{eff} and thus a is very large, the bracketed term can be approximated by

$$(1+a)^{\frac{3}{2}} - 1 \approx a^{\frac{3}{2}} \tag{2.57}$$

If L_{eff} is very large

$$\beta \approx \frac{2 L_{eff}}{3 C_o} \left(\frac{k f L_{eff}}{D} \right)^{\frac{1}{2}} \tag{2.58}$$

which is independent of the hole size fraction and the form given in Wilson (1981).

Recall that

$$\frac{L_{extra}}{L_{ESD}} = \left[1 + \frac{1}{B_A L_{ESD}} \right] \left(\frac{1}{3} \left(\frac{P_{oi}}{P_{ESD}} \right)^2 + \frac{2}{3} \left(\frac{P_{ESD}}{P_{oi}} \right) - 1 \right) \quad (2.59)$$

so that the total mass of gas that escapes is proportional to:

$$L_{eff} = L_{ESD} \cdot \left(1 + \frac{L_{extra}}{L_{ESD}} \right) \quad (2.60)$$

2.6 References

- Botros, K.K., Jungowski, W.M. and Weiss, M.H. 1989. Models and Methods of Simulating Gas Pipeline Blowdown. Canadian Journal of Chemical Engineering 67, 529-539.
- Shapiro, A.H. 1953. The Dynamics and Thermodynamics of Compressible Fluid Flow. Volume 1, Ronald Press, p164

3 Variation of Buoyancy Flux in a High Velocity Jet with Air Entrainment and Droplet Evaporation

Most industrial hazard assessment dispersion models, and SLAB in particular, do not account for the conversion of kinetic energy in a high velocity jet into thermal energy as the jet entrains air and slows down. This kinetic energy to thermal energy conversion increases the temperature of the jet, and can cause the jet to change from cold heavier-than-air to warm lighter-than-air. For jets of ideal gas, the kinetic energy conversion in the source jet can be accounted-for by using the stagnation temperature of the ideal gas in the pipeline or storage vessel. Non-ideal gases and mixtures of vapour and liquid droplets require a more sophisticated approach. In this chapter, an analysis of the evolution of jet buoyancy flux as air is entrained will lead to a simple model for non-ideal gases with specific heats that are constant, or at most functions only of temperature. With this limitation, non-ideal gas effects that can be accounted for by a compressibility factor “Z” correction to the ideal gas law.

3.1 Energy Conversion in a High Velocity Jet: Horizontal Jet Pointed Downwind

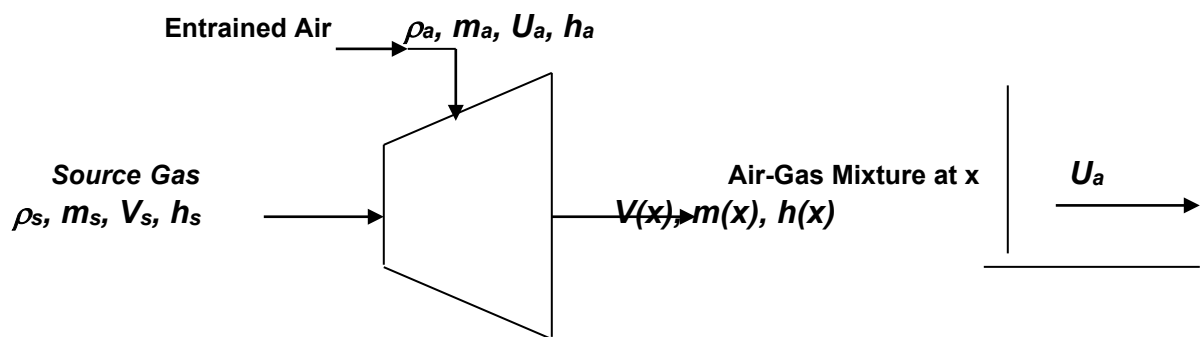


Figure 3-1 Jet entrainment mass balance from source to distance x

By a mass balance, the exit mass flux is

$$\dot{m}_s + \dot{m}_a = \dot{m}(x) \quad (3.1)$$

The mass fraction of the source gas-liquid mixture (not just the H₂S) in the plume is defined as

$$f_s(x) \equiv \frac{\dot{m}_s}{\dot{m}(x)} \quad (3.2)$$

Then, the momentum balance of the jet at constant pressure (no x -forces) is

$$\dot{m}_s V_s + \dot{m}_a U_a - \dot{m}(x) V(x) = 0$$

So

$$V(x) = \frac{\dot{m}_s}{\dot{m}(x)} V_s + \frac{\dot{m}_a}{\dot{m}(x)} U_a \quad (3.3)$$

Using (3.1)

$$\dot{m}_a = \dot{m}(x) - \dot{m}_s \quad (3.4)$$

So that using (3.4) in (3.3)

$$V(x) = \frac{\dot{m}_s}{\dot{m}(x)} V_s + \frac{\dot{m}(x) - \dot{m}_s}{\dot{m}(x)} U_a$$

Or, with the definition in (3.2) the horizontal x -momentum equation is for jet velocity $V(x)$,

$$V(x) = f_s V_s + (1 - f_s) U_a \quad (3.5)$$

3.2 Energy Conservation for Adiabatic Mixing

$$\dot{m}(x) \left(h(x) + \frac{V^2(x)}{2} \right) = \dot{m}_s \left(h_s + \frac{V_s^2}{2} \right) + \dot{m}_a \left(h_a + \frac{U_a^2}{2} \right) \quad (3.6)$$

Divide by $m(x)$ and use (3.4) to reduce (3.6) to

$$h(x) + \frac{V^2(x)}{2} = f_s \left(h_s + \frac{V_s^2}{2} \right) + (1 - f_s) \left(h_a + \frac{U_a^2}{2} \right) \quad (3.7)$$

The term on the left side of (3.7) is the stagnation enthalpy $h_o(x)$. Equation (3.7) is written in terms of the static enthalpy $h(x)$ because we want to calculate the static density $\rho(x)$ for the buoyancy flux $F_b(x)$. To do this we must use $h(x)$ to define $T(x)$, and then calculate $\rho(x)$ for the constant pressure jet with $P(x) = P_a$. Squaring (3.5),

$$\begin{aligned} V^2(x) &= f_s^2 V_s^2 + 2f_s(1-f_s)V_s U_a + (1-f_s)^2 U_a^2 \\ &= f_s^2 V_s^2 + 2f_s(1-f_s)V_s U_a + (1-2f_s+f_s^2)U_a^2 \\ &= f_s^2 V_s^2 + 2f_s(1-f_s)V_s U_a + U_a^2 - 2f_s U_a^2 + f_s^2 U_a^2 \end{aligned} \quad (3.8)$$

Then put (3.8) into (3.7)

$$\begin{aligned} h(x) + f_s^2 \frac{V_s^2}{2} + 2f_s(1-f_s) \frac{V_s U_a}{2} + \cancel{\frac{U_a^2}{2}} - \cancel{2f_s} \frac{U_a^2}{2} + f_s^2 \frac{U_a^2}{2} = \\ f_s h_s + f_s \frac{V_s^2}{2} + h_a + \cancel{\frac{U_a^2}{2}} - f_s h_a - f_s \cancel{\frac{U_a^2}{2}} \end{aligned} \quad (3.9)$$

Removing the cancelled terms in (3.9)

$$h(x) = f_s h_s + (1-f_s)h_a + \frac{f_s(1-f_s)}{2} [V_s^2 - 2V_s U_a + U_a^2]$$

Grouping terms

$$h(x) = f_s h_s + (1-f_s)h_a + f_s(1-f_s) \frac{(V_s - U_a)^2}{2} \quad (3.10)$$

horizontal, adiabatic, real fluid jet

3.3 Energy Conversion in a High Velocity Jet: Vertical Jet in a Crosswind

For a vertical jet both the x (horizontal) and z (vertical) momentum equations are required. Only the source velocity V_s contributes to the vertical component of the jet velocity $V_z(x)$ measured at

horizontal distance x . The wind velocity U_a is the only contributor to the horizontal component of jet velocity $V_x(x)$

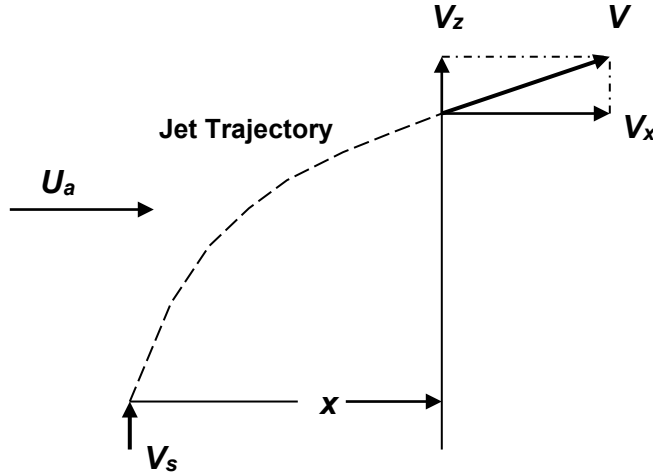


Figure 3-2 Vertical and horizontal jet trajectory velocity components

In a constant pressure jet dilution process the horizontal x momentum equation is developed in the same way as (3.5) to yield

$$V_x(x) = (1 - f_s)U_a \quad (3.11)$$

and the vertical z momentum equation is, like (3.5),

$$V_z(x) = f_s V_s \quad (3.12)$$

The magnitude of the jet velocity is just

$$V^2(x) = V_x^2(x) + V_z^2(x) \quad (3.13)$$

Squaring (3.11) and (3.12), (3.13) becomes for a vertical jet

$$V^2(x) = f_s V_s^2 + (1 - f_s)^2 U_a^2 \quad (3.14)$$

Then, put (3.14) in the energy balance equation (3.7)

$$h(x) + f_s^2 \frac{V_s^2}{2} + (1 - f_s)^2 \frac{U_a^2}{2} = f_s \left(h_s + \frac{V_s^2}{2} \right) + (1 - f_s) \left(h_a + \frac{U_a^2}{2} \right) \quad (3.15)$$

Expanding the terms on the right side of (3.15) and transposing the velocity terms from the left side yields

$$h(x) = f_s h_s + (1 - f_s) h_a + f_s (1 - f_s) \frac{(V_s^2 + U_a^2)}{2} \quad (3.16)$$

vertical, adiabatic, real fluid jet

Comparing (3.16) for the vertical jet to (3.10) for the horizontal jet, the only difference is how V_s and U_a combine in the last term. In the next section it will be shown that for high velocity source jets (3.10) and (3.16) are identical, greatly simplifying the buoyancy flux analysis.

3.4 High Velocity Gas Jets with Constant Specific Heat

Assume the specific heats of source gas and air are constant with temperature at P_a .

$$h(x) = C_p(x)T(x)$$

$$h_s = C_{ps}T_s$$

$$h_a = C_{pa}T_a$$

In addition, assume $V_s \gg U_a$ so that in (3.10) for the horizontal jet, $(V_s - U_a)^2 = V_s^2$ and in (3.16) for the vertical jet $V_s^2 + U_a^2 = V_s^2$ too, so that the energy equation for both horizontal and vertical source jet orientations can be approximated by

$$C_p(x)T(x) = f_s C_{ps}T_s + (1 - f_s)C_{pa}T_a + f_s(1 - f_s)\frac{V_s^2}{2} \quad (3.17)$$

Solving (3.11) for the temperature ratio $T(x)/T_a$, divide both sides by $C_p(x) T_a$

$$\frac{T(x)}{T_a} = (1 - f_s) \frac{C_{pa}}{C_p(x)} + f_s \frac{C_{ps}}{C_p(x)} \frac{T_s}{T_a} + f_s(1 - f_s) \frac{V_s^2}{2C_p(x)T_a} \quad (3.18)$$

non-ideal gas with constant C_p , and $V_s \gg U_a$

3.5 Buoyancy Flux

The general definition for buoyancy flux as a function of x in a jet is

$$F_b(x) \equiv g \left(\frac{\rho_a - \rho(x)}{\rho_a} \right) \frac{\dot{Q}(x)}{\pi} \quad (3.19)$$

where $Q(x)$ is the volume flow in the jet at x

$$\dot{Q}(x) = \frac{\dot{m}(x)}{\rho(x)} \quad (3.20)$$

Use (3.1) for the $f_s = m_s / m(x)$ and (3.20) to write the buoyancy flux in (3.19) as

$$F_b(x) = \frac{g}{\pi} \left(\frac{\rho_a - \rho(x)}{\rho_a} \right) \frac{\dot{m}_s}{\rho(x) f_s} \quad (3.21)$$

Then, move the $\rho(x)$ into the brackets and move ρ_a out to obtain

$$F_b(x) = \frac{g}{\pi} \left(\frac{\rho_a}{\rho(x)} - 1 \right) \frac{\dot{m}_s}{\rho_a f_s} \quad (3.22)$$

for all fluids

Note that far downstream when $x = \infty$, $(m_s / f_s) = \infty$ and $(\rho_a / \rho(x) - 1) = 0$ so in (3.22) $F_b(\infty)$ yields an indeterminate value of $(0) \cdot (\infty)$. In order to find the far-downstream value of F_b further analysis is needed.

3.6 Buoyancy Flux for Gas with Compressibility Factor Z

For a non-ideal gas $P = \rho ZRT / M$, where R is the universal gas constant and M is the molecular mass, the density ratio at x is

$$\frac{\rho_a}{\rho(x)} = \frac{T(x)}{T_a} \frac{Z(x)}{Z_a} \frac{M_a}{M(x)} \quad (3.23)$$

and the buoyancy flux (3.22) becomes

$$F_b(x) = \frac{g \dot{m}_s}{\pi \rho_a f_s} \left(\frac{T(x)}{T_a} \frac{Z(x)}{Z_a} \frac{M_a}{M(x)} - 1 \right) \quad (3.24)$$

Use (3.18) for the temperature in a non-ideal gas mixture with constant specific heats, making mixture specific heat $C_p(x)$ a function only of the mass fraction f_s of source gas (or gas-liquids),

$$F_b(x) = \frac{g \dot{m}_s}{\pi \rho_a f_s} \left(\frac{Z(x)}{Z_a} \frac{M_a}{M(x)} \frac{C_{pa}}{C_p(x)} \left(\frac{1}{f_s} - 1 + \frac{C_{ps}}{C_{pa}} \frac{T_s}{T_a} + \frac{(1-f_s)V_s^2}{2C_{pa}T_a} \right) - \frac{1}{f_s} \right) \quad (3.25)$$

3.7 Buoyancy Flux at the Source

At the source, no air has been entrained, and $x = 0$, $f_s = 1.0$, $M(x) = M_s$ and $C_p(x) = C_{ps}$ so (3.25) becomes

$$F_b(x=0) = \frac{g \dot{m}_s}{\pi \rho_s} \left(\frac{\rho_s}{\rho_a} \right) \left(\frac{Z_s}{Z_a} \frac{M_a}{M_s} \frac{T_s}{T_a} - 1 \right) \quad (3.26)$$

for a non-ideal gas with compressibility factor Z

$$\frac{\rho_s}{\rho_a} = \frac{Z_a}{Z_s} \frac{M_s}{M_a} \frac{T_a}{T_s} \quad (3.27)$$

so, for a non-ideal gas, (3.26) becomes

$$F_b(0) = g \left(\frac{T_s - \frac{Z_a}{Z_s} \frac{M_s}{M_a} T_a}{T_s} \right) \frac{\dot{m}_s}{\pi \rho_s} \quad (3.28)$$

Because we know ρ_a , but not ρ_s , rearrange (3.28) in terms of ρ_a to get the final result,

$$F_b(0) = g \left(\frac{\frac{Z_s}{Z_a} \frac{M_a}{M_s} T_s - T_a}{T_a} \right) \frac{\dot{m}_s}{\pi \rho_a} \quad (3.29)$$

Note that (3.28) and (3.29) are equivalent to (3.22) with $f_s = 1.0$. Because non-ideal fluid software gives ρ not Z as an output, (3.22) is often the best equation for spreadsheet calculations.

3.8 Downstream Evolution of Buoyancy Flux with Air Entrainment

Far downwind $x = \infty$, $M(x) = M_a$ and $C_p(x) = C_{pa}$. Both $M(x)$ and $C_p(x)$ depend on the mass fraction, f_s . The non-ideal behavior embodied in the compressibility factor Z acts to change the gas density $\rho = (P M)/(Z R T)$. The effective molecular mass of a non-reacting mixture of any two substances can be calculated from the molar sum $N = (N_s + N_a)$, where N is the number of moles of mixture, N_s is the number of moles of source gas-liquid and N_a is the number of moles of entrained air. Expressing the molar balance in terms of mass flow rates through the boundaries of the control volume, $N = \dot{m} / M$, and $N_a = \dot{m}_a / M_a$ and $N_s = \dot{m}_s / M_s$. Using the definition of the source gas mass fraction $f_s = \dot{m}_s / \dot{m}$,

$$\frac{1}{M(x)} = \frac{f_s}{M_s} + \frac{(1-f_s)}{M_a} \quad (3.30)$$

$$M(x) = \frac{M_s M_a}{M_a f_s + M_s (1-f_s)} \quad (3.31)$$

The specific heat $C_p(x)$ is found from the mass fraction of source gas f_s

$$C_p(x) = f_s C_{ps} + (1-f_s) C_{pa} \quad (3.32)$$

Transposing M_a in (3.30)

$$\frac{M_a}{M(x)} = \frac{M_a}{M_s} f_s + 1 - f_s \quad (3.33)$$

Equations (3.33), and (3.32) can be combined to yield

$$\frac{M_a}{M(x)} \frac{C_{pa}}{C_p(x)} = \frac{\frac{M_a}{M_s} f_s + 1 - f_s}{\frac{C_{ps}}{C_{pa}} f_s + 1 - f_s} \quad (3.34)$$

Using (3.34) in (3.25),

$$F_b(x) = \frac{g \dot{m}_s}{\pi \rho_a} \left(\frac{Z(x)}{Z_a} \right) \left[\left(\frac{\frac{M_a}{M_s} f_s + 1 - f_s}{\frac{C_{ps}}{C_{pa}} f_s + 1 - f_s} \right) \left(\frac{1}{f_s} - 1 + \frac{C_{ps}}{C_{pa}} \frac{T_s}{T_a} + \frac{(1-f_s)V_s^2}{2C_{pa}T_a} \right) - \frac{1}{f_s} \right] \quad (3.35)$$

Then, factor out the specific heat term to obtain

$$F_b(x) = \frac{g \dot{m}_s}{\pi \rho_a} \left(\frac{C_{ps}}{C_{pa}} f_s + 1 - f_s \right) \left(\frac{Z(x)}{Z_a} \right) \left[\left(\frac{M_a}{M_s} f_s + 1 - f_s \right) \left(-1 + \frac{C_{ps}}{C_{pa}} \frac{T_s}{T_a} + \frac{(1-f_s)V_s^2}{2C_{pa}T_a} \right) + \frac{M_a}{M_s} + \frac{1}{f_s} - \lambda - \frac{C_{ps}}{C_{pa}} - \frac{1}{f_s} + \lambda \right] \quad (3.36)$$

for a non-ideal gas with $C_p = C_p(f_s)$ only, and $f_s = f_s(x)$,

Note that at the source where $f_s = 1.0$ at $x = 0$ the general equation (3.36) reduces to (3.29) to give the buoyancy flux $F_b(0)$ in the high-speed source jet.

3.9 Buoyancy Flux Far Downwind

Because the two $1/f_s$ terms cancel out of the buoyancy flux evolution equation (3.30), the limit as $x \rightarrow \infty$ and $f_s \rightarrow 0$ can be found simply by setting $f_s = 0$. Far downstream the source gas is completely diluted, and the pressure is atmospheric, so, $Z(x) = Z_a$ as $f_s \rightarrow 0$ and (3.36) is

$$F_b(\infty) = \frac{g \dot{m}_s}{\pi \rho_a} \left(\frac{C_{ps}}{C_{pa}} \left(\frac{T_s}{T_a} + \frac{V_s^2}{2C_{ps}T_a} \right) + \frac{M_a}{M_s} - \frac{C_{ps}}{C_{pa}} - 1 \right) \quad (3.37)$$

The source gas (vapour + liquid droplets) has a specific heat of C_{ps} and a stagnation temperature

$$T_{os} = T_s + \frac{V_s^2}{2C_{ps}} \quad (3.38)$$

With (3.38) in (3.37),

$$F_b(\infty) = \frac{g \dot{m}_s}{\pi \rho_a} \left(\frac{C_{ps} T_{os}}{C_{pa} T_a} + \frac{M_a}{M_s} - \frac{C_{ps}}{C_{pa}} - 1 \right) \quad (3.39)$$

for a non-ideal gas with $C_p = C_p(f_s)$ only, and $f_s = f_s(x)$,

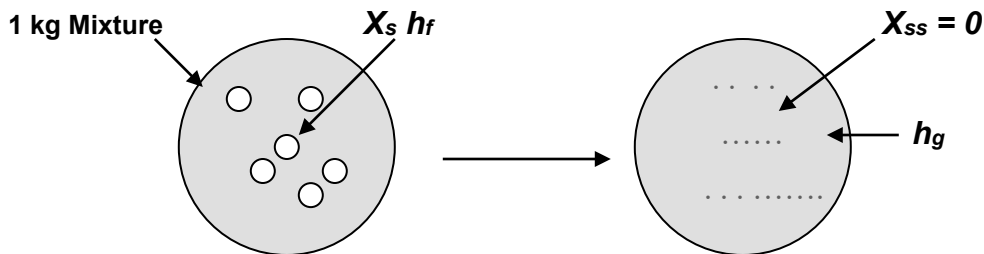
From (3.39) we see that the fully-mixed buoyancy flux $F_b(\infty)$ is reduced when the source gas has a higher specific heat than air, and increased when the source gas has a lower molecular mass than air.

Finally, we define an effective source gas density ρ_s as the density of slowly moving source gas that will produce the correct buoyancy flux $F_b(\infty)$ of the actual high velocity source gas after it is fully mixed with ambient air. This effective source density is found by setting $x = \infty$ in (3.22) and equating this to (3.39) so that from $\rho_s = \rho(\infty)$,

$$\rho_s = \frac{\rho_a}{\left(\frac{C_{ps}}{C_{pa}} \left(\frac{T_s}{T_a} + \frac{V_s^2}{2C_{ps}T_a} \right) + \frac{M_a}{M_s} - \frac{C_{ps}}{C_{pa}} \right)} \quad (3.40)$$

3.10 Effect of Evaporating Liquid Droplets on Buoyancy Flux

Most liquid droplets in the source jet evaporate very rapidly, and are usually gone by the time the source gas fraction $f_s < 0.2$, that is, a factor of five mass dilution. In order to account for the cooling effect of the evaporating droplets, we will define a virtual source gas condition where all the droplets evaporate in the source gas before it mixes with atmospheric air. This evaporation process occurs with no heat net heat transfer, as shown in Figure 3.3.



“s” with droplets

“ss” vapor only

X_s = mass fraction of liquid in source gas

T_s = actual temperature of source gas

Figure 3-3 *Evaporation of liquid droplets with no air entrainment produces the virtual evaporated droplet “ss” pseudo state*

The adiabatic energy balance gives an effective source temperature T_{ss} , defined by the isenthalpic process from “s” with droplets to “ss” with droplets evaporated. Then, T_{ss} is used to calculate the effective stagnation temperature T_{oss} with droplet evaporation. The buoyancy flux with droplet evaporation is found from (3.38) by replacing T_{os} with T_{oss} . Equating enthalpies $h_s = h_{ss}$, for 1 kg of mixture

$$X_s h_f(T_s) + (1 - X_s) h_g(T_s) = h_g(T_{ss}) \quad (3.41)$$

Then, use the definition of the enthalpy of vaporization h_{fg} in the form

$$h_g(T_s) = h_f(T_s) + h_{fg}(T_s) \quad (3.42)$$

To eliminate $h_f(T_s)$ from the left hand side of (3.41) to get

$$X_s (h_g(T_s) - h_{fg}(T_s)) + (1 - X_s) h_g(T_s) = h_g(T_{ss}) \quad (3.43)$$

which reduces to

$$h_g(T_s) - X_s h_{fg}(T_s) = h_g(T_{ss}) \quad (3.44)$$

Then use the assumption of constant (temperature-independent) specific heat to write $C_{ps} = C_{ps}$ of the vapour fraction. With this in (3.44) we have $h_g(T_s) = C_{ps} T_s$ and $h_g(T_{ss}) = C_{ps} T_{ss}$ so that

$$T_{ss} = T_s - \frac{X_s}{C_{ps}} h_{fg,s} \quad (3.45)$$

Where $h_{fg,s}$ is the enthalpy of evaporation at T_s , and X_s is the mass fraction of liquid droplets in the release mixture at the source.

By definition, the stagnation temperature with all droplets evaporated is

$$T_{oss} = T_{ss} + \frac{V_s^2}{2C_{pss}} \quad (3.46)$$

So, for a non-ideal gas with $C_{pss} = \text{constant}$ with varying temperature T , and $Z(\infty) = Z_a$ when the source gas is diluted by air far downstream, the buoyancy flux F_b at “infinity”, with droplets evaporated, is calculated using (3.46) and (3.38) in (3.39)

$$F_b(\infty)_{\text{droplets evaporated}} = \frac{g \dot{m}_s}{\pi \rho_a} \left(\frac{C_{pss}}{C_{pa}} \left(\frac{T_{oss}}{T_a} - 1 \right) + \left(\frac{M_a}{M_s} - 1 \right) \right)$$

$$\text{for a non-ideal gas with } C_p = C_p(f_s) \text{ only, and } f_s = f_s(x), \quad (3.47)$$

This is the equation needed to calculate the buoyancy flux that can be used in the plume rise equations to estimate the trajectory of the plume from a high velocity source of non-ideal gas.

4 Modifying a Steady Release Rate Model for Transient Releases

For any release rate \dot{m}_s kg/s, pipeline or well blowout source gas mixture, the H₂S release rate Q_s (kg H₂S)/s is

$$Q_s = \chi_s \frac{\dot{m}_s}{\rho_s} \quad (4.1)$$

where

- Q_s = mass release rate of contaminant gas component (kg H₂S/s)
- χ_s = concentration of contaminant (here, H₂S) in the source gas (kg H₂S/m³)
- $\dot{q}_s = \frac{\dot{m}_s}{\rho_s}$, volume release rate of source gas mixture (m³ source gas/s)
- U_c = mass convection velocity (“box speed u” in SLAB) (m/s)
- ρ_s = effective density of the source gas required to produce the same fully-mixed buoyancy flux $F_b(\infty)$ for the high speed non-ideal gas release see Equation (3.40), (kg/m³)

The reason for using the effective density ρ_s of the source gas is that as parcels of high velocity source gas jet mix with atmospheric air, the jet slows down so that total momentum is conserved. The source gas component in the jet mixture rises to its stagnation temperature as jet Mach number slows to zero. In practice, a Mach number less than 0.3 is all that is required for the jet temperature to be within a degree or two of the stagnation temperature. For natural gas mixtures, the speed of sound at stagnation temperature is about 300 m/s, so when the jet has slowed to a centreline velocity less than 100 m/s it can be assumed to be at its stagnation temperature.

In order to simplify calculations, we assume that the transient release is “frozen” in the streamwise direction. This implies that along-wind diffusion is neglected and gives an upper limit for the concentration. The advantage of the frozen release assumption is that the mass flow rate at the downwind receptor has the same equation with time after arrival of the plume as the mass release rate at the source for time after rupture. So, the time "t" after arrival of the plume at

a given downwind location x is the same as the time after the moment of rupture, and the ground level concentration is,

$$\chi_{o,transient}(t) = \frac{Q_s(t)}{\pi U_c \sigma_y \sigma_z} \exp\left(-\frac{h^2(t)}{2\sigma_z^2}\right) \quad (4.2)$$

where the time-after-arrival dependence of $\chi_{o,transient}$ on Q_s and h is shown explicitly. By definition, a “frozen” plume has no along-wind spreading in the x direction, so the beginning and end of the release are not allowed to diffuse in the x direction. This “frozen” plume assumption is conservative because it represents the largest concentration that could occur without the benefit of along-wind plume dispersion.

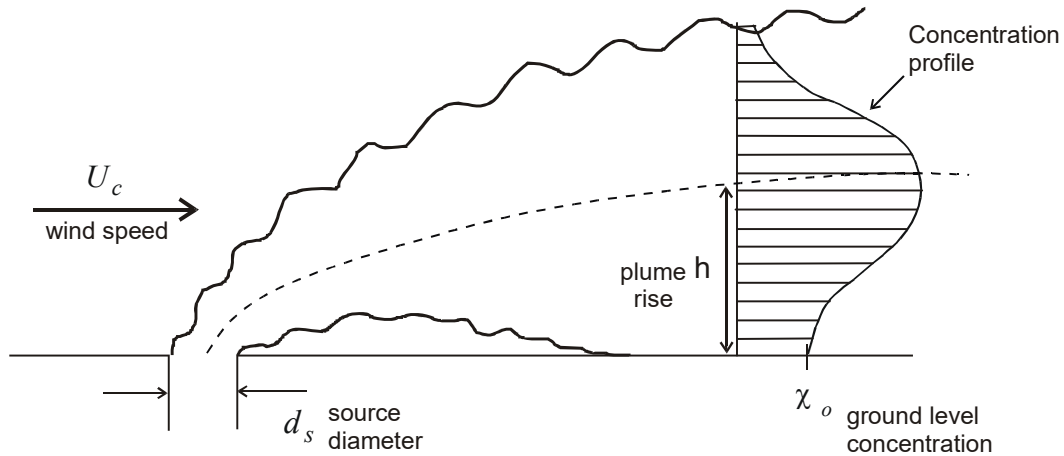


Figure 4-1 Vertical mean concentration profile with ground-level mass reflection

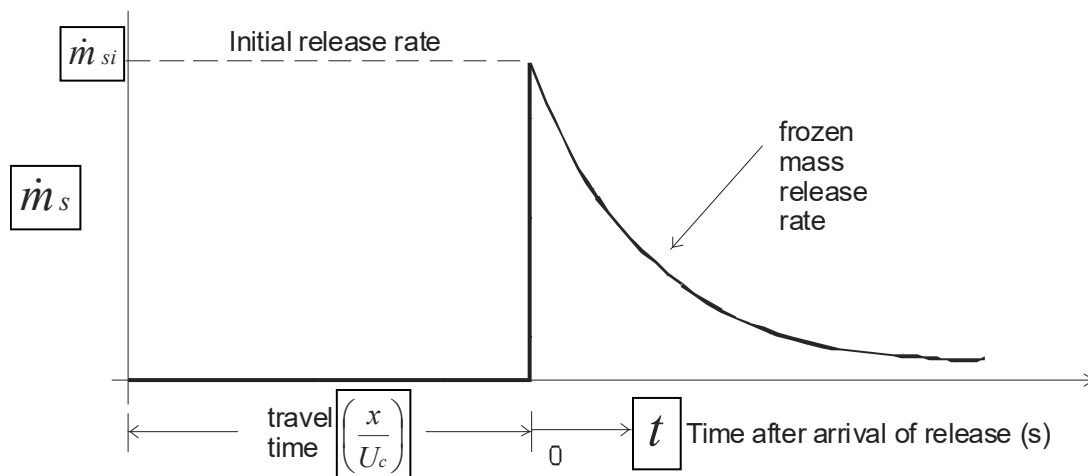


Figure 4-2 "Frozen" mass release profile is unchanged as it is carried downwind

Plume rise h will be a function of both downwind distance x and time t after arrival of the release, because \dot{m}_s determines the plume rise.

The ground level concentration in the frozen transient release at time t after arrival is directly proportional to the mass release rate \dot{m}_s at the same time t after the moment of rupture.

Combining (4.1) and (4.2),

$$\chi_{o,transient} = \frac{\chi_s}{\pi \rho_s U_c \sigma_y \sigma_z} \dot{m}_s \exp\left(-\frac{h^2}{2\sigma_z^2}\right) \quad (4.3)$$

where the parameters \dot{m}_s and h are the time-dependent variables in equation (4.3). Equation (4.3) can be expressed in terms of a steady release with mass release rate $\dot{m}_{si} = \text{constant}$ and plume rise $h_i = \text{constant}$, and a steady release with no plume rise, both of which can be calculated from a steady-state plume model such as SLAB. The steady reference flow is taken as the initial mass release rate \dot{m}_{si} , with h_i calculated from \dot{m}_{si} ,

$$\chi_{o,steady} = \frac{\chi_s}{\pi \rho_s U_c \sigma_y \sigma_z} \dot{m}_{si} \exp\left(-\frac{h_i^2}{2\sigma_z^2}\right) \quad (4.4)$$

Another useful equation is the steady release rate concentration for \dot{m}_{si} , with no plume rise,

$$h_i \equiv 0$$

$$\chi_{o,steady} = \frac{\chi_s}{\pi \rho_s U_c \sigma_y \sigma_z} \dot{m}_{si} \quad (4.5)$$

Now, looking at the steady release solutions (4.4) and (4.5), which our dispersion model is capable of predicting, we can simplify (4.3), (4.4) and (4.5) by defining the x-dependent variable

$$B_s(x) \equiv \frac{\chi_s}{\pi \rho_s U_c \sigma_y \sigma_z} \quad (4.6)$$

where B_s is the ground level concentration per unit volume source flow rate in a plume with no rise, (kg/m³ of air)/(m³/s source gas mixture). In terms of B_s , (4.3) becomes

$$\chi_{o,transient}(\dot{m}_s, h) = B_s \dot{m}_s \exp\left(-\frac{h^2}{2\sigma_z^2}\right) \quad (4.7)$$

$$\chi_{o,steady,with\ rise}(\dot{m}_{si}, h_i) = B_s \dot{m}_{si} \exp\left(-\frac{h_i^2}{2\sigma_z^2}\right) \quad (4.8)$$

$$\chi_{o,steady,norise}(\dot{m}_{si}, h_i=0) = B_s \dot{m}_{si} \quad (4.9)$$

Rewrite (4.7) as

$$\chi_{o,transient} = \frac{\dot{m}_s}{\dot{m}_{si}} B_s \dot{m}_{si} \exp\left(-\frac{h^2}{2\sigma_z^2} \cdot \left(\frac{h}{h_i}\right)^2\right) \quad (4.10)$$

which can be expressed as

$$\chi_{o,transient} = \frac{\dot{m}_s}{\dot{m}_{si}} B_s \dot{m}_{si} \left[\exp\left(-\frac{h_i^2}{2\sigma_z^2}\right) \right] \left(\frac{h}{h_i}\right)^2 \quad (4.11)$$

Where the parameters \dot{m}_s and h are the time-dependent variables in equations (4.10) to (4.14).

Then grouping terms in (4.11)

$$\chi_{o,transient} = \frac{\dot{m}_s}{\dot{m}_{si}} \left(B_s \dot{m}_{si}\right)^{1-\left(\frac{h}{h_i}\right)^2} \left[B_s \dot{m}_{si} \exp\left(-\frac{h_i^2}{2\sigma_z^2}\right) \right] \left(\frac{h}{h_i}\right)^2 \quad (4.12)$$

Comparing (4.12) to (4.8) and (4.9), and making the notation more compact by showing the functional relationships as subscripts

$$\chi_{o,transient} = \frac{\dot{m}_s}{\dot{m}_{si}} \left[\chi_{oi,steady,norise} \right]^{1-\left(\frac{h}{h_i}\right)^2} \left[\chi_{oi,steady,with\ rise} \right] \left(\frac{h}{h_i}\right)^2 \quad (4.13)$$

In standard notation

$$\chi_{o,transient,\dot{m}_s,h} = \frac{\dot{m}_s}{\dot{m}_{si}} \left[\chi_{oi,steady,norise} \right]^{1-\left(\frac{h}{h_i}\right)^2} \left[\chi_{oi,steady,with\ rise} \right] \left(\frac{h}{h_i}\right)^2 \quad (4.14)$$

Equation (4.14) applies to the steady ground level concentration, $\chi_{o,steady}$ for any Gaussian steady release model with constant convection velocity U_c . All we need now is an expression for the plume rise ratio h/h_i in terms of \dot{m}_s/\dot{m}_{si} .

4.1 Transient-to-Steady Transformation for Purely Buoyant Plumes

For purely buoyant plumes in transitional rise

$$h = \left(\frac{3}{2\beta^2} \right)^{1/3} \frac{F_b^{1/3}}{U_c} x^{2/3} \quad (4.15)$$

where the buoyancy flux F_b is defined as

$$F_b \equiv g \left(\frac{\rho_a - \rho_s}{\rho_a} \right) W_s r_s^2 \quad (4.16)$$

and where

- g = acceleration of gravity (9.81 m/s²)
- r_s = source radius (m)
- ρ_s = effective source gas density see Equation (3.40), (kg/m³)
- ρ_a = ambient air density in the atmosphere (kg/m³)
- W_s = source gas mixture velocity (m/s)

The mass flow from the source can be written,

$$\dot{m}_s = \rho_s W_s \pi r_s^2 \quad (4.17)$$

so that

$$F_b = g \left(\frac{\rho_a - \rho_s}{\rho_a} \right) \frac{\dot{m}_s}{\pi \rho_s} \quad (4.18)$$

So, $h \propto \dot{m}_s^{1/3}$ at a given downwind distance x . Using this in (4.15)

$$\left(\frac{h}{h_i}\right)_{buoyant}^2 = \left(\frac{\dot{m}_s}{\dot{m}_{si}}\right)^{2/3} \quad (4.19)$$

Equation (4.19) applies for purely buoyant plumes (negligible vertical momentum) in transitional rise.

4.2 Transient-to-Steady Transformation for Momentum Jets

For a pure momentum jet (negligible buoyancy) in transitional rise:

$$h = \left(\frac{3}{\beta^2}\right) \frac{F_m^{1/3}}{U_c^{2/3}} x^{1/3} \quad (4.20)$$

where the momentum flux F_m is defined as

$$F_m \equiv \frac{\rho_s}{\rho_a} W_s^2 r_s^2 \quad (4.21)$$

from $\dot{m}_s = \rho_s W_s \pi r_s^2$ in (4.17)

$$W_s = \frac{\dot{m}_s}{\pi \rho_s r_s^2} \quad (4.22)$$

and

$$W_s r_s^2 = \frac{\dot{m}_s}{\pi \rho_s} \quad (4.23)$$

so

$$W_s^2 r_s^2 = \frac{\dot{m}_s^2}{\pi^2 \rho_s^2 r_s^2} \quad (4.24)$$

and the momentum flux becomes

$$F_m = \frac{1}{\pi^2 \rho_s \rho_a} \dot{m}_s^2 \quad (4.25)$$

and, $h \propto \dot{m}_s^{2/3}$ so that the rise ratio is

$$\left(\frac{h}{h_i}\right)_{momentum}^2 = \left(\frac{\dot{m}_s}{\dot{m}_{si}}\right)^{4/3} \quad (4.26)$$

Equation (4.26) applies to transitional rise of vertical momentum jets.

4.3 Characteristic Shapes of Concentration-Time Curves for Transient Releases

Zelensky (2002 private communication) pointed out that there are two characteristic shapes for the $x_{o,transient}$ curves. They are:

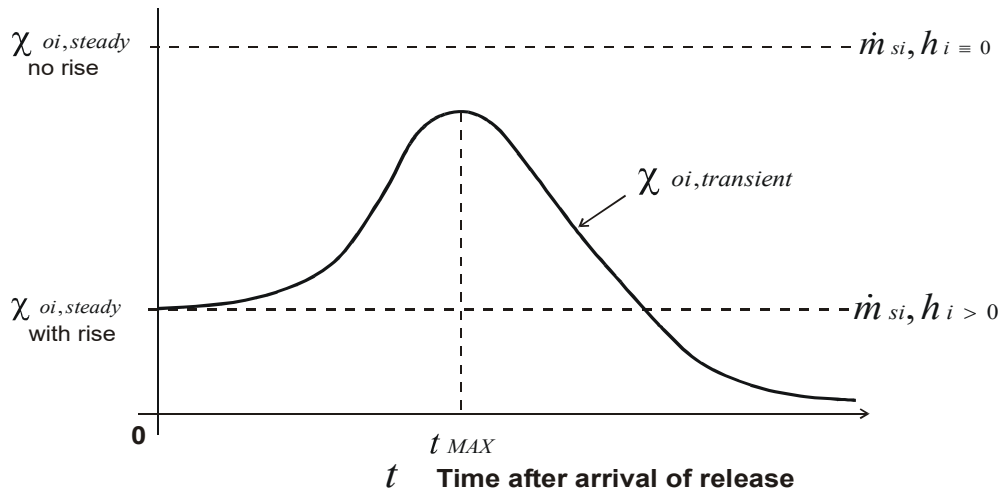


Figure 4-3 Maximum concentration occurs at $t_{MAX} = 0$

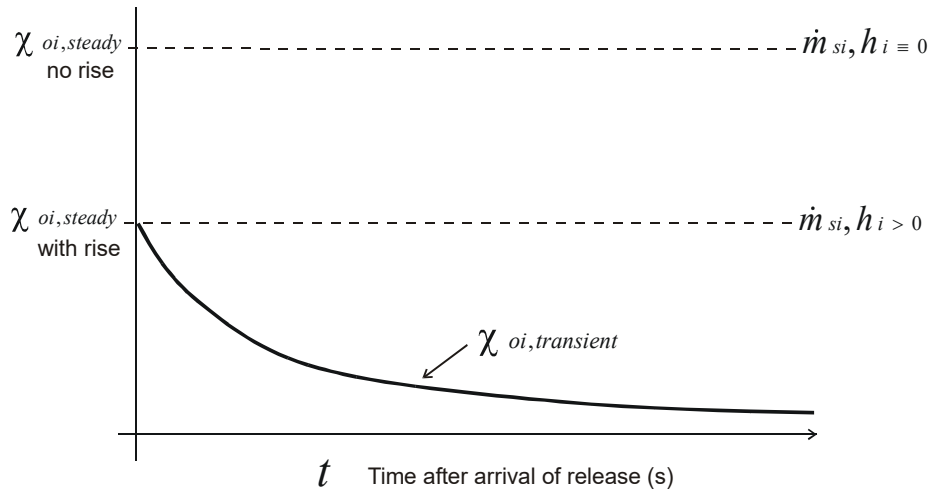


Figure 4-4 Maximum concentration occurs at $t_{MAX} > 0$

What are the conditions that lead to the maximum occurring at $t_{max} > 0$? In the steady concentration terms it is only h/h_i that is a function of time. Note that the initial condition χ_{oi} is at \dot{m}_i and is a steady release. Start by taking the natural logarithm, \ln , of (4.13):

$$\ln(\chi_{o,transient}) = \ln\left(\frac{\dot{m}_s}{\dot{m}_{si}}\right) + \left(1 - \left(\frac{h}{h_i}\right)^2\right) \ln(\chi_{oi, no rise}) + \left(\frac{h}{h_i}\right)^2 \ln(\chi_{oi, with rise}) \quad (4.27)$$

Then, keeping in mind that the two steady solutions are constant with time, take the derivative of

(4.27), noting that $d(\ln y) = \frac{dy}{y}$,

$$\frac{1}{\chi_{o,transient}} \frac{d \chi_{o,transient}}{dt} = \frac{\dot{m}_{si}}{\dot{m}_s} \frac{d}{dt} \left(\frac{\dot{m}_s}{\dot{m}_{si}} \right) - 2 \left(\frac{h}{h_i} \right) \frac{d}{dt} \left(\frac{h}{h_i} \right) \ln(\chi_{oi, no rise}) + 2 \left(\frac{h}{h_i} \right) \frac{d}{dt} \left(\frac{h}{h_i} \right) \ln(\chi_{oi, with rise})$$

Grouping terms

$$\frac{1}{\chi_{o,transient}} \frac{d \chi_{o,transient}}{dt} = \frac{\dot{m}_{si}}{\dot{m}_s} \frac{d}{dt} \left(\frac{\dot{m}_s}{\dot{m}_{si}} \right) - 2 \left(\frac{h}{h_i} \right) \frac{d}{dt} \left(\frac{h}{h_i} \right) \ln \left(\frac{\chi_{oi, no rise}}{\chi_{oi, with rise}} \right) \quad (4.28)$$

The ratio inside the \ln term is defined as

$$R = \frac{\chi_{oi, no rise}}{\chi_{oi, with rise}} \quad (4.29)$$

Using (4.29) in (4.28) and setting the derivative on the left side equal to zero to find the conditions for a maximum to exist yields

$$\ln(R) > \frac{\frac{\dot{m}_{si}}{\dot{m}_s} \frac{d}{dt} \left(\frac{\dot{m}_s}{\dot{m}_{si}} \right)}{2 \left(\frac{h}{h_i} \right) \frac{d}{dt} \left(\frac{h}{h_i} \right)} \quad (4.30)$$

4.4 Finding t_{MAX} for Buoyant Plumes

For buoyant plumes, the square root of equation (4.19) is

$$\left(\frac{h}{h_i} \right)^2 = \left(\frac{\dot{m}_s}{\dot{m}_{si}} \right)^{1/3} \quad (4.31)$$

so

$$2 \left(\frac{h}{h_i} \right) \frac{d}{dt} \left(\frac{h}{h_i} \right) = \frac{2}{3} \left(\frac{\dot{m}_s}{\dot{m}_{si}} \right)^{-1/3} \frac{d}{dt} \left(\frac{\dot{m}_s}{\dot{m}_{si}} \right) \quad (4.32)$$

and this can be used to write the condition for t_{MAX} , where $d(\chi_{o,transient})/dt = 0$ in (4.30) as

$$\frac{\dot{m}_{si}}{\dot{m}_s} \frac{d}{dt} \left(\frac{\dot{m}_s}{\dot{m}_{si}} \right) \left[1 - \frac{2}{3} \left(\frac{\dot{m}_s}{\dot{m}_{si}} \right)^{2/3} \ln R \right] = 0 \quad (4.33)$$

The maximum $\chi_{o,transient}$ occurs for buoyant plumes at the time $t = t_{MAX}$ when

$$\left. \frac{\dot{m}_s}{\dot{m}_{si}} \right|_{t_{MAX}} = \left(\frac{3}{2 \ln R} \right)^{3/2} \quad (4.34)$$

We see that, because $\dot{m}_s/\dot{m}_{si} < 1.0$ for frozen mass release rates from pipelines, that $t_{MAX} > 0$ can only occur for R values that produce

$$\ln R > 1.5 \quad (4.35)$$

which can be solved to show, noting that $e^{3/2} = 4.482$

$$R > 4.48 \quad (4.36)$$

for buoyant plumes

Equation (4.36) gives the condition for which the maximum concentration is “real”, and occurs for times greater than $t = 0$.

4.5 Finding t_{MAX} for Momentum Jets

For momentum jets, the square root of Equation (4.26) is

$$\frac{h}{h_i} = \left(\frac{\dot{m}_s}{\dot{m}_{si}} \right)^{2/3}$$

and if we repeat the derivation for t_{MAX} , in (4.30)

$$2 \left(\frac{h}{h_i} \right) \frac{d}{dt} \left(\frac{h}{h_i} \right) = \frac{4}{3} \left(\frac{\dot{m}_s}{\dot{m}_{si}} \right)^{1/3} \frac{d}{dt} \left(\frac{\dot{m}_s}{\dot{m}_{si}} \right)$$

Then (4.28) with $d(\chi_{o,transient})/dt = 0$ becomes

$$\frac{\dot{m}_{si}}{\dot{m}_s} \frac{d}{dt} \left(\frac{\dot{m}_s}{\dot{m}_{si}} \right) \left[1 - \frac{4}{3} \left(\frac{\dot{m}_s}{\dot{m}_{si}} \right)^{4/3} \ln R \right] = 0 \quad (4.37)$$

The maximum $\chi_{o,transient}$ occurs at time t_{MAX} for momentum jets when

$$\left. \frac{\dot{m}_s}{\dot{m}_{si}} \right|_{t_{MAX}} = \left(\frac{3}{4 \ln R} \right)^{3/4} \quad (4.38)$$

And, again we see because $\dot{m}_s/\dot{m}_{si} < 1.0$ for pipelines, we get $t_{MAX} > 0$ on if

$$\ln R > 0.75 \quad (4.39)$$

then solving this, noting that $\exp(3/4) = 2.117$

$$R > 2.12 \quad (4.40)$$

for momentum jets

Equation (4.40) applies to momentum jets and describes the necessary condition for a maximum to occur at $t > 0$.

4.6 Concentration Profiles for Single Exponential Decay of Release Rate \dot{m}_s

An exponential decay is a simple example to illustrate the conditions when the maximum concentration will occur at some non-zero time after the frozen plume arrives. (Recall that a frozen plume has no along-wind spreading.) For an exponential decay of release rate with time constant τ ,

$$\left(\frac{h}{h_i}\right)^2 = \left(\frac{\dot{m}_s}{\dot{m}_{si}}\right)^{2/3} = \exp\left(-\frac{2t}{3}\right) \tag{4.41}$$

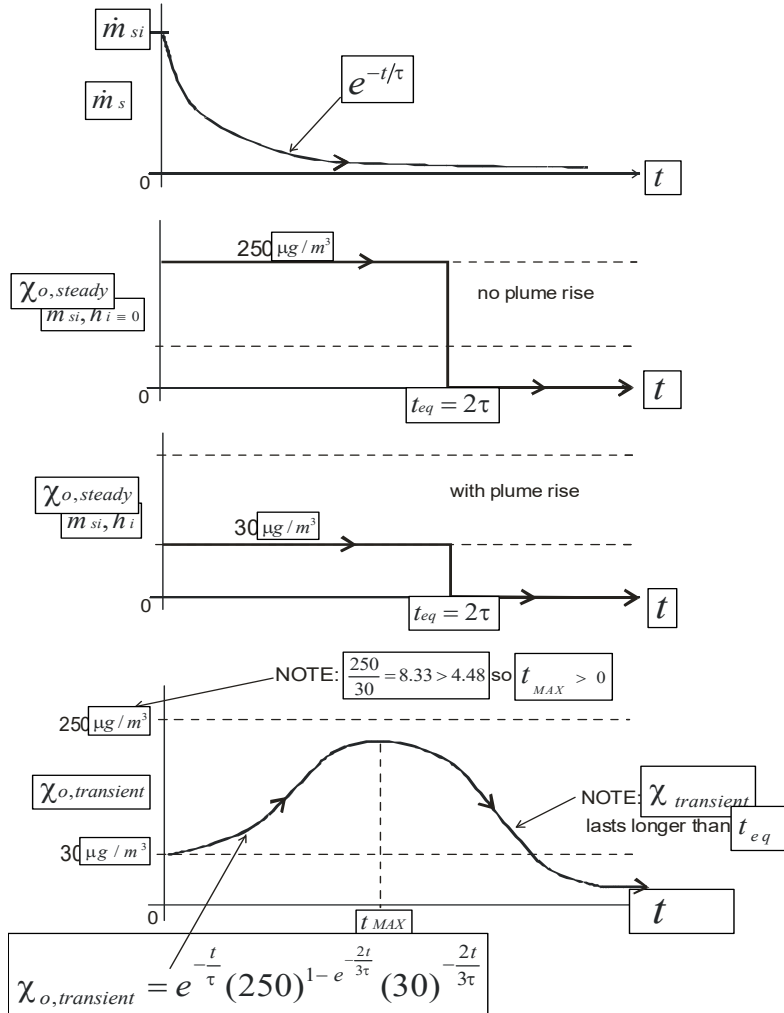


Figure 4-5 Numerical example for combining two steady solutions to generate the transient solution.

4.7 Combined Momentum and Buoyancy Rise

The simplest and most conservative assumption is that the plume rise h from the ground-level release is the maximum of the buoyancy or momentum rise

$$h = MAX [h_{momentum} , h_{buoyancy}] \quad (4.42)$$

The way to handle this for a transient release is to make separate calculations for $\chi_{o,transient}$ for the pure momentum jet component, and for the pure buoyant plume component. Then use whichever of the two calculations produces the smallest concentration, because this will be equivalent to using the larger of the two plume rises.

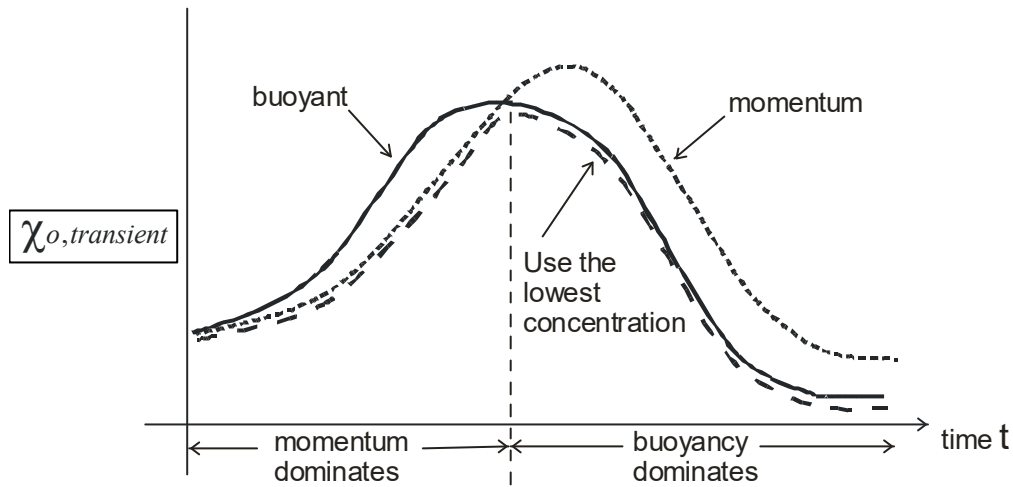


Figure 4-6 *Correct solution for a buoyant momentum jet is the lowest concentration predicted by the purely buoyant plume or the momentum jet.*

4.8 Final Momentum or Buoyant Rise

Momentum jets and buoyant plumes have different functional forms for the dependence of rise on mass release rate once they are far enough downwind to have reached their final rise height. Table 4.1 below summarizes the functional forms for final rise derived by Briggs (1975, 1984).

Table 4-1: Briggs Final Plume Rise Equations

Atmospheric Stability	Stability Class	Buoyant Plumes $\Delta h_{bf} = A_1/U^a$		Momentum Jets $\Delta h_{mf} = A_1/U^a$	
		a	A_1	a	A_1
unstable	A, B or C	3/5	$3.0 \frac{F_b^{3/5}}{H^{2/5}}$ 1984-Eqn 8.101, 1975 Eqn 80	3/7	$2.0 \frac{F_m^{3/7}}{H^{1/7}}$ 1975 Eqn 81 but 2.3 not the 2.0 in Eqn 87
neutral	D	3	$300 F_b$ 1975 Eqn 80 with 300 in text	1	$6.0 F_m^{1/2}$ 1975 Eqn 81
stable windy	E or F	1/3	$2.6 \frac{F_b^{1/3}}{S^{1/3}}$ 1975 Eqn 59 with C2=2.6 from Table 4 Briggs 1965, 1984-Eqn 8.71	1/3	$1.6 \frac{F_m^{1/3}}{S^{1/6}}$ 1975 Eqn 48
stable calm	E or F	0	$5.0 \frac{F_b^{1/4}}{S^{3/8}}$ 1975 Eqn 56	0	$2.5 \frac{F_m^{1/4}}{S^{1/4}}$ 1975 Eqn 57 with 2.5 in text

See 1975 Table 2, first column for plume radius $\ll 1$ turbulence scale for unstable row above.

Using the definitions of momentum flux F_m in (4.21) and buoyancy flux F_b in (4.18) the ratios of

plume rise for instantaneous to initial plume rise at time t are given in Table 4.2. For stable conditions the final plume rise should be taken as the minimum of the two values calculated from the stable, windy and the stable, calm equations, see Briggs (1975, 1984).

Table 4-2: Relation of Final Plume Rise to Mass Flow Rates in Briggs' Equations from Table 4.1 with $F_b \sim m_e$ and $F_m \sim m_e^2$

Atmospheric Stability	Stability Class	Buoyant Plumes $\Delta h_{bf} / \Delta h_{bf, i} = (m_e/m_{ei})^b$	Momentum Jets $\Delta h_{mf} / \Delta h_{mf, i} = (m_e/m_{ei})^m$
		Exponent b	Exponent m
unstable	A, B or C	3/5	6/7
neutral	D	1	1
stable windy	E or F	1/3	2/3
stable calm	E or F	1/4	1/2

4.9 References

- Briggs, G.A. 1975. Plume Rise Predictions. Chapter 3 in Lectures on Air Pollution and Environmental Impact Analyses, American Meteorological Society, Boston, 29 Sept - 3 Oct, 1975, pp. 59-111.
- Briggs, G.R. 1984. Plume Rise and Buoyancy Effects. Chapter 8: in Atmospheric Science and Power Production, D. Randerson (ed.) U.S. Dept. of Energy DOE/TIC-27601, pp. 327-366.

5 Transient Release of Dense Gas Using a Steady Release Rate Model

The box model of the process of dispersion has vertical thickness b_z and horizontal half-width b_y that are defined for a uniform concentration χ_o in the box. In reality the top and side edges of the plume have concentration profiles, and the box model widths b_z and b_y are defined so that the concentration χ_o is the actual concentration at ground level, on the plume centerline.

The concentration χ_o on the plume centerline can be calculated from a mass balance of contaminant,

$$Q_s = \chi_o U_c b_z (2b_y) \quad (5.1)$$

with the mass flow of contaminant from the source Q_s related to the total source mass flow rate \dot{m}_s by

$$Q_s = \chi_s \frac{\dot{m}_s}{\rho_s} \quad (5.2)$$

where

- Q_s = mass release rate of contaminant gas component (kg H₂S/s)
- χ_s = concentration of contaminant (here, H₂S) in the source gas (kg H₂S/m³)
- $\dot{q}_s = \frac{\dot{m}_s}{\rho_s}$, volume release rate of source gas mixture (m³ source gas/s)
- U_c = mass convection velocity (“box speed u” in SLAB) (m/s)
- ρ_s = effective density of the source gas required to produce the same fully-mixed buoyancy flux $F_b(\infty)$ for the high speed non-ideal gas release see Equation (3.40), (kg/m³)

The convection velocity of a dense gas plume is proportional to u_* the friction velocity that drives entrainment, but is usually expressed as the wind speed $U(z_c)$ in the atmosphere at some reference height z_c .

Combining (5.1) and (4.1), denoting the transient release concentration where $\dot{m}_s = \dot{m}_s(t)$,

$$\chi_{o,transient} = \frac{\chi_s \dot{m}_s}{2b_y b_z \rho_s U_c} \tag{5.3}$$

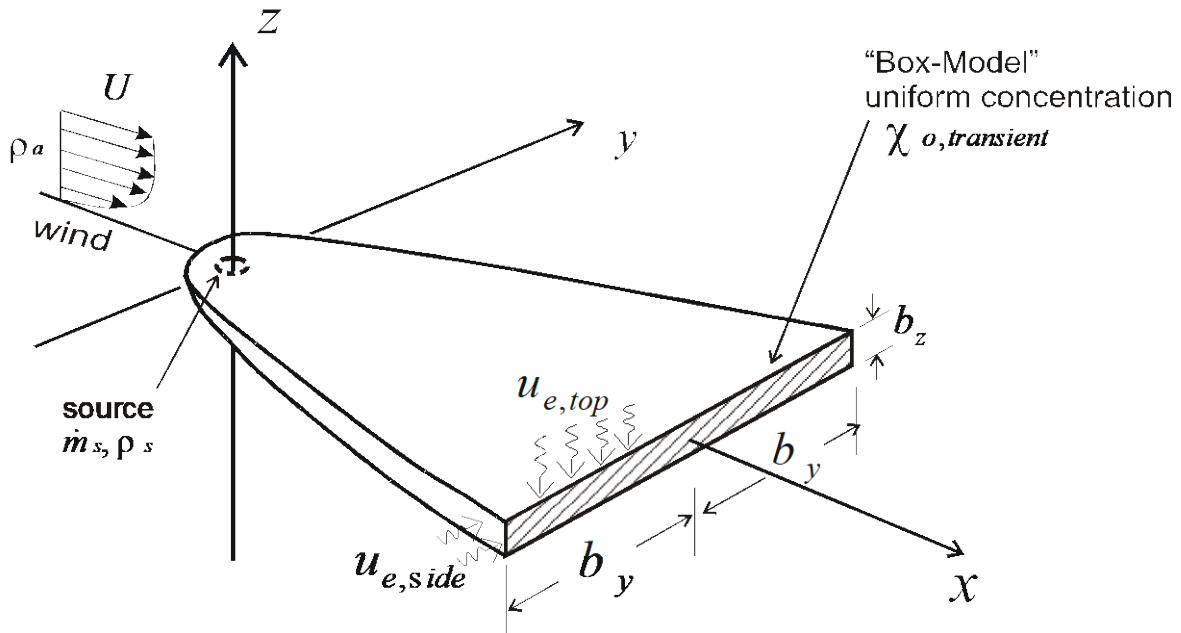


Figure 5-1 Dense plume with gravity slumping causing density-driven crosswind spreading

where

- $u_{e,top}$ = turbulent air entrainment velocity into the top of a dense plume (m/s)
- $u_{e,side}$ = turbulent air entrainment velocity into the sides of a dense plume (m/s)

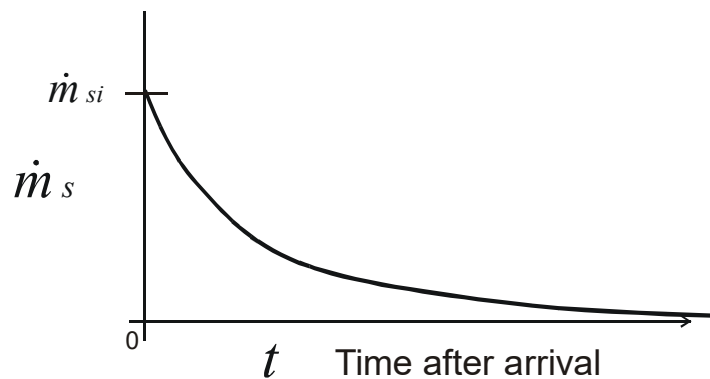


Figure 5-2 "Frozen" time-varying mass release rate arrives unchanged at downwind receptor

The source has a mass release rate \dot{m}_s that varies with time, where \dot{m}_s is kg/s of source gas. In the passive limit where density does not affect b_y and b_z , we get a Gaussian plume with

$$2b_y b_z \rightarrow \pi \sigma_y \sigma_z \quad (5.4)$$

For dense plumes with effective source density $\rho_s > \rho_a$, gravity produces a downward force on the plume that forces b_z to slump downward, which causes b_y to spread in the crosswind direction in order to maintain the required cross-section plume area. This means that as ρ_s increases, b_z decreases and b_y increases. The plume cross sectional area $2b_y b_z$ may increase, decrease, or even remain unchanged by this dense-plume slumping effect.

The cross sectional area $2b_y b_z$ is quite easy to calculate for a constant density plume at ρ_s with no dilution by entrainment. In reality, the process is complicated by turbulent air entrainment at entrainment velocity u_e into the top and sides of the plume. This increases the mass in the plume, and decreases the rate of slumping of b_z and gravity spreading of b_y . As a further complication the turbulent entrainment velocity $u_{e,top}$ depends on u_* the friction velocity, and on a Richardson number Ri_* based on u_* , and **not** on the windspeed U_c itself. Britter proposed that air entrainment should be a function of this friction Richardson number Ri_* , with

$$u_{e,top} = \frac{\alpha_e u_*}{1 + B_* Ri_*} \quad (5.5)$$

Where B_* is a constant, and the “friction” Richardson number, based on the turbulent friction velocity u_* is

$$Ri_* \equiv \frac{g \left(\frac{\rho - \rho_a}{\rho_a} \right) b_z}{u_*^2} = \frac{g'_s \dot{q}_s}{2b_y u_*^2 U_c} \quad (5.6)$$

where ρ is the local diluted density at distance x, and the effective gravitational acceleration g'_s at the source is

$$g'_s \equiv g \left(\frac{\rho_s - \rho_a}{\rho_a} \right) \quad (5.7)$$

where g is the acceleration of gravity, 9.81 m/s^2 , $\rho_s \text{ kg/m}^3$ is the density of the source gas mixture, and $\rho_a \text{ kg/m}^3$ is the density of atmospheric air. Equations (5.5) and (5.6) lead to a complicated calculation for crosswind width b_y and vertical thickness b_z , with the competing effects of plume growth by entrainment into the sides of the plume increasing b_y , and the density-driven slumping of b_z also contributing to increasing b_y . At the same time, density-driven slumping of b_z is being partially cancelled or even reversed by the entrainment of air into the top of the plume. This density-driven coupling between b_z and b_y , makes it impossible to find a simple equation for the cross-sectional area $2b_y b_z$. What happens in a particular case can be deduced from Britter-McQuaid workbook Figure 8,

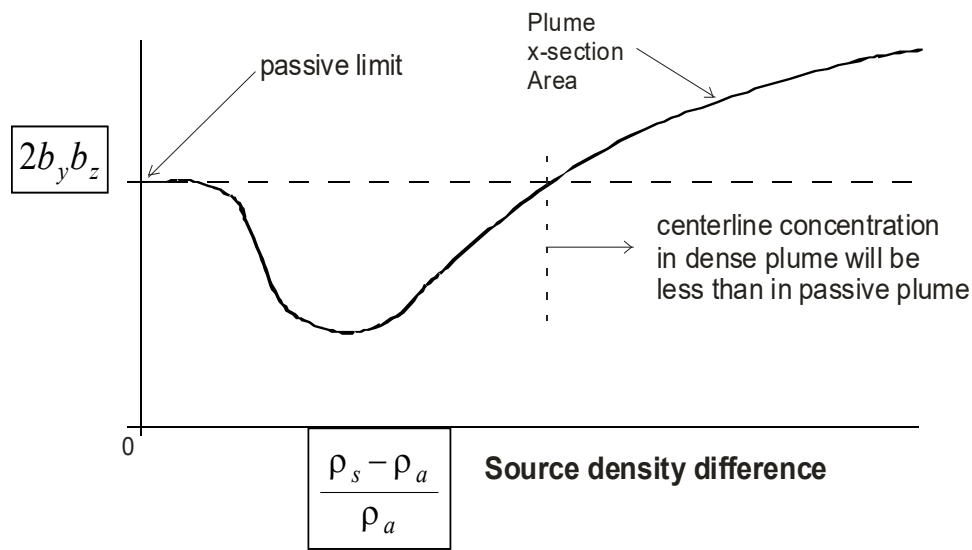


Figure 5-3 *Dense releases can have both larger and smaller cross-section areas than a passive plume for U_c , χ_s , q_o and the downwind distance all at fixed values*

5.1 Estimating the Effect of Density using Britter and McQuaid's Correlations

Britter and McQuaid (1988) used dimensional analysis to find groups of easily-measured variables against which experimental data from full-scale atmospheric could be plotted to determine distance to a given concentration. They found that the ratio of centerline volume concentration

$$C_o \equiv \frac{\chi_o}{\rho_s}, \left(\frac{m^3 H_2S}{m^3 mixture} \right) \quad (5.8)$$

to the source concentration C_s with units $m^3 H_2S$ per m^3 of source gas,

$$C_s = \frac{\chi_s}{\rho_s} \quad (5.9)$$

is

$$\frac{C_o}{C_s} = \frac{\chi_o}{\chi_s} \quad (5.10)$$

As shown in (5.10) the ratio of volume concentrations, C , is the same as the ratio of mass concentrations χ for a quasi-ideal gas with a constant compressibility factor Z . The concentration ratio in (5.10) is the inverse of the source to receptor dilution factor. Britter and McQuaid's dimensional analysis led them to propose that for a continuous steady release this concentration ratio should correlate with the variables shown in (5.11),

$$\frac{C_o}{C_s} = f \left(\frac{x}{(q_s/U_{ref})^{1/2}}, \phi \right) \quad (5.11)$$

where

$$\phi \equiv \left(\frac{g_s'^2 \dot{q}_s}{U_{ref}^5} \right)^{1/5} = \frac{g^{0.4} \left(\frac{\rho_s - \rho_a}{\rho_a} \right)^{0.4} \dot{q}_s^{0.2}}{U_{ref}} \quad (5.12)$$

Britter and McQuaid (1988) then plotted experimental data for constant values of C_o/C_s and drew smooth curves through the points at selected downwind distances, as shown below. Britter (private communication) has pointed out that the curves were drawn manually with a drafting curve, and do not represent any specific mathematical functional form or equation.

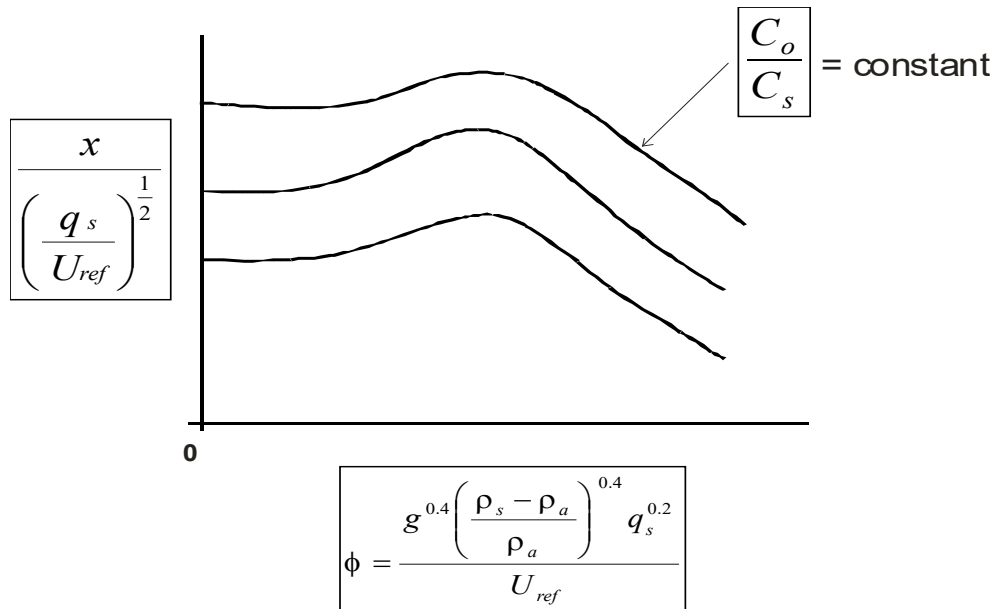


Figure 5-4 Concentration correlation variables from Figure 8 in the Britter-McQuaid (1988) workbook

In the following analysis, it will be shown how the plume cross-sectional area $2b_y b_z$ can be estimated directly from Britter and McQuaid's empirical curves. First, use (5.3) for the concentration in a transient release rate $\dot{m}_s = \rho_s \dot{q}_s$ ($\text{kg } H_2S$)/s, to express the source-to-receptor concentration ratio in (5.8) as

$$\frac{C_o}{C_s} = \frac{\dot{q}_s}{2b_y b_z U_c} \quad (5.13)$$

Then, solving for plume cross sectional area

$$2b_y b_z = \left(\frac{\dot{q}_s}{U_c}\right) \frac{C_s}{C_o} \quad (5.14)$$

Next, assume the effect of density difference can be separated in a function $F(\phi)$ from all the other variables, turbulence scale S_a , surface roughness z_o , and turbulent friction velocity u_* that affect $2b_y b_z$ in a function $G(x, S_a, z_o, u_*)$

$$2b_y b_z \equiv \frac{G^2 x^2}{F^2} \quad (5.15)$$

where

$$\begin{aligned}
 F(\phi) &= \text{effect of density on } 2b_y b_z \\
 G(x, S_a, z_o, u_*) &= \text{effect of atmospheric turbulence scale } S_a, \\
 &\quad \text{surface roughness } z_o \text{ and friction velocity } u_* \text{ on } 2b_y b_z
 \end{aligned}$$

The key assumption here is that, at a given distance x , the effects of density difference can be separated in $F(\phi)$ from **all** the other parameters that influence the plume cross-sectional area $2b_y b_z$. This separation of variables is the way in which a simple function for the effect of density on $2b_y b_z$ will be found.

The justification for expressing the effect of density, $F(\phi)$, as a separate function is because Britter and McQuaid's curves for each C_o/C_s with varying $x/(\dot{q}_s/U_{ref})^{1/2}$ locations, all have very nearly the same shape on their Figure 8, reproduced above. The reason for multiplying G by x in the definition of (5.15), is to make both functions G and F dimensionless. Then, using (5.15) in (5.14) and rearranging to express the result in Britter and McQuaid's variables,

$$\frac{x^2 G^2}{F^2} = \left(\frac{\dot{q}_s}{U_c} \right) \frac{C_s}{C_o} \quad (5.16)$$

solving (5.16) for $x/(\dot{q}_s/U_{ref})^{1/2}$, and showing the functional forms of F and G

$$x \left(\frac{\dot{q}_s}{U_c} \right)^{-1/2} = \frac{F(\phi)}{G(x, S_a, z_o, u_*)} \left(\frac{C_o}{C_s} \right)^{-1/2} \quad (5.17)$$

So, the vertical axis on Britter and McQuaid's graphs can be used to define a density-only function $F(\phi)$

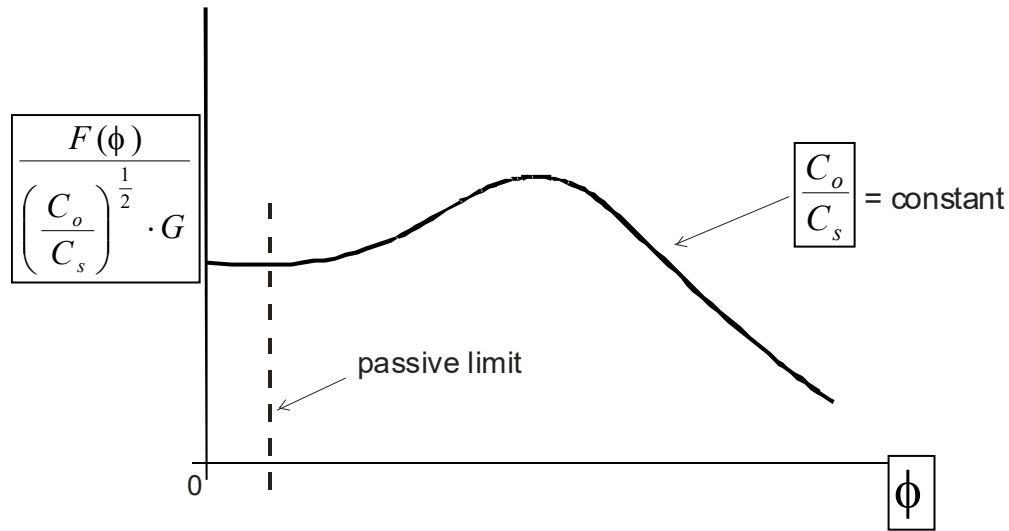


Figure 5-5 Transformed correlation variables for adjusting passive plume models to find dense plume centerline concentrations

This assumes all the curves for different C_o/C_s can be collapsed to a single curve using $(C_o/C_s)^{1/2} G$. Next, multiply (5.14) by x^2 , transpose and take the square root to get Britter and McQuaid's variable $x / (\dot{q}_s / U_{ref})^{1/2}$ used as the vertical axis on their plots.

$$x \left(\frac{\dot{q}_s}{U_{ref}} \right)^{-1/2} = \frac{x}{(2b_z b_z)^{1/2}} \cdot \left(\frac{C_o}{C_s} \right)^{-1/2} \cdot \left(\frac{U_{ref}}{U_c} \right)^{1/2} \quad (5.18)$$

where $U_{ref} = U$ at z_{ref} a fixed height above the ground. Then put (5.15) into (5.16) to separate the density difference variable, $F(\phi)$, from all others,

$$x \left(\frac{\dot{q}_s}{U_{ref}} \right)^{-1/2} = \frac{F(\phi)}{G(x, S_a, z_o, u_*)} \cdot \left(\frac{C_s U_{ref}}{C_o U_c} \right)^{1/2} \quad (5.19)$$

Then, Britter and McQuaid's plots (see their Figure 8) can be used to find $F(\phi)$. Normalizing $F(\phi)$ by its value $F(\phi = 0)$ for a passive plume,

$$x \left(\frac{\dot{q}_s}{U_{ref}} \right)^{-1/2} = H(x, S_a, z_o, u_*, \frac{C_o}{C_s}) \cdot \frac{F(\phi)}{F(\phi = 0)} \quad (5.20)$$

with H defined in (5.21) from the values in (5.19),

$$H(x, S_a, z_o, u_*, \frac{C_o}{C_s}) \equiv \frac{F(\phi=0)}{G} \left(\frac{C_s}{C_o} \cdot \frac{U_c}{U_{ref}} \right)^{1/2} \quad (5.21)$$

This definition of H implies that U_c/U_{ref} is not a function of ϕ , but only of the atmospheric wind profile $U(z)$ that depends on S_a, z_o and u_* , and on the distance x and concentration ratio C_o/C_s . In fact, U_c does depend on density, but so does C_o/C_s , so we hope that U_c/U_{ref} is uniquely defined for a given dilution C_o/C_s .

5.2 Finding $F(\phi)$ from Britter and McQuaid's Plots

Britter and McQuaid's curves for different C_o/C_s do not collapse into a single curve when normalized by $F(\phi=0)$. However, the curve shapes are very similar. Here, the curve at the largest dilution, $C_o/C_s = 0.002$, a dilution of 500:1, was used to represent the range of concentrations of interest. For a source concentration of 35% H_2S , a 500:1 dilution is a concentration $C_o = 1430 \text{ ppm}$, so even the largest dilution curve from Britter and McQuaid is at the upper concentration limit of the range of interest for H_2S .

Using (5.20) and analysing Britter and McQuaid's, Figure 8, the function we want to fit has the following properties:

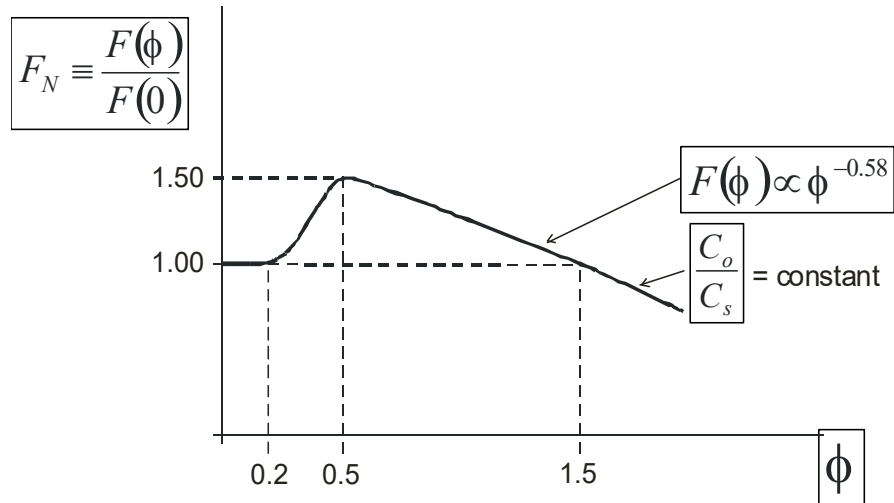


Figure 5-6 Asymptotic behaviour of density correction function F

which can be expressed quantitatively as the conditions:

$$\begin{aligned}
 F_N(0.2) &= 1.0 \\
 F_N(0.5) &= 1.5 \\
 \frac{dF_N}{d\phi}(0.5) &= 0 \quad (\text{maximum at } \phi=0.5) \\
 F_N(1.5) &= 1.0 \\
 F_N(\phi) &= \phi^{-0.58} \quad (\text{for } \phi \geq 1.0) \\
 \frac{\partial F_N}{\partial \phi}(0) &= 0 \quad (\text{flat for } \phi < 0.2)
 \end{aligned}$$

After several approximating functions were tested, a very good fit to these requirements was found by trial and error to be:

$$F_N = \frac{F(\phi)}{F(\phi=0)} = \frac{1 + 6.0\phi^3 e^{-4.0(\phi-0.1)^2}}{(1 + 0.05\phi^6)^{0.1}} \quad (5.22)$$

Which yields, the following values for the approximating function in (5.22),

$$\begin{aligned}
 F_N(0.2) &= 1.05 \\
 F_N(0.66) &= 1.49 \quad \text{at its maximum} \\
 F_N(1.5) &= 0.96
 \end{aligned}$$

Equation (5.22) is a distorted Gaussian hump multiplied by a $\phi^{-0.6}$ decay. The ϕ^3 distorts the Gaussian and broadens the roll-off on the right side as shown below.

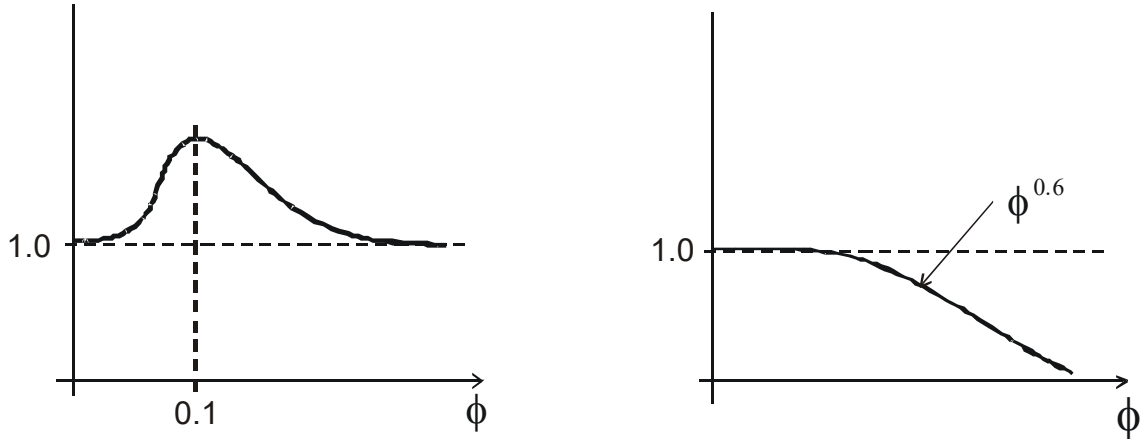


Figure 5-7 Approximating functions for semi-empirical F_N function

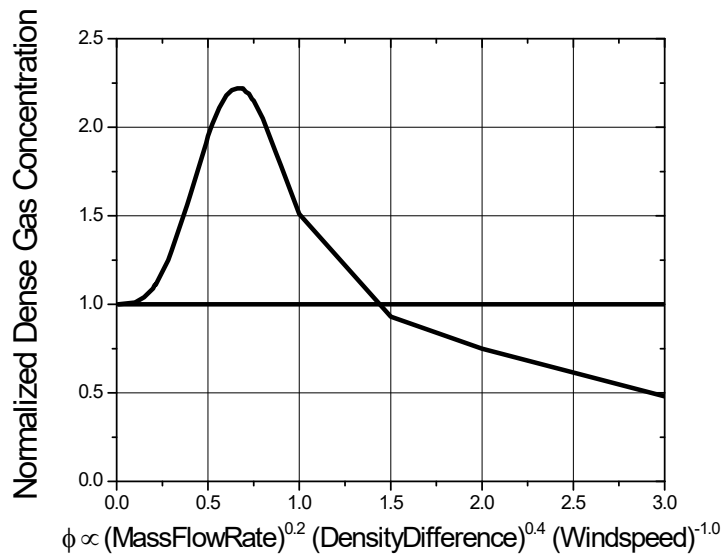


Figure 5-8 Numerical values of concentration $C_0 \sim F_N^2$ from Equation (5.16) using the density adjustment function $F_n(\phi)$ from Equation (5.22)

5.3 Transient Releases of Dense Gas

The major feature of the density adjustment function $F_N(\phi)$ is that it depends only on source release rate and density parameters in ϕ , in (5.12) and is **independent** of downwind location x . In this section we will show how to apply $F_N(\phi)$ to transform steady release dense plume

concentrations calculated with a model such as SLAB to account for dense gas effects in a transient release of a dense gas mixture.

First, factor the transient concentration equation (5.3) into a steady-release with the initial release rate \dot{m}_{si} at $t = 0$, multiplied by additional terms.

$$(\chi_{o,transient})_{dense} = \frac{\chi_s \dot{m}_{si}}{2b_{yi} b_{zi} \rho_s U_{ci}} \left(\frac{2b_{yi} b_{zi}}{2b_y b_z} \right) \left(\frac{U_{ci}}{U_c} \right) \left(\frac{\dot{m}_s}{\dot{m}_{si}} \right) \quad (5.23)$$

where the lead term on the right side of (5.23) is just the steady concentration,

$$\chi_{oi, steady dense} = \frac{\chi_s \dot{m}_{si}}{2b_{yi} b_{zi} \rho_s U_{ci}} \quad (5.24)$$

Then, the ratio of plume cross section areas is found by using (5.14) at a fixed x location where the function G , defined in (5.15), is constant

$$\frac{2b_{yi} b_{zi}}{2b_y b_z} = \left(\frac{F_N(\phi)}{F_N(\phi_i)} \right)^2 \cdot \frac{x_i}{x} \cdot \frac{G_i}{G} \quad (5.25)$$

Then, because only the mass flow changes between the initial condition and the final condition in (5.24) we must have

$$\frac{x_i}{x} = 1.0 \quad \text{and} \quad \frac{G_i}{G} = 1.0$$

so the last two terms on the right side of (5.24) always cancel out. Unfortunately, there is no way to estimate U_{ci}/U_c in (5.23) without knowing the plume thickness b_{zi} at the initial mass release rate, and the thickness b_z at the current mass release rate. So, we must assume that

$$\frac{U_{ci}}{U_c} = 1.00 \quad (5.26)$$

Combining (5.23), (5.24) and (5.25) the final equation for the steady to transient transformation of a ground level dense plume is,

$$(\chi_{o,transient})_{dense} = \left(\frac{\dot{m}_s}{\dot{m}_{s_i}} \right) \left(\frac{F_N(\phi)}{F_N(\phi_i)} \right)^2 (\chi_{o,steady})_{dense\ at\ \dot{m}_{s_i}} \quad (5.27)$$

where $F_N(\phi)$ and $F_N(\phi_i)$ are from (5.22), and $(\chi_{o,steady})_{dense\ at\ \dot{m}_{s_i}}$ is calculated from a steady dense plume model such as SLAB. It is important to note that because ϕ defined in (5.12) depends only on source release rate, density difference and windspeed, the function $F(\phi)$ is independent of x and all dependence on downwind distance must come from the steady-state dense gas concentration $(\chi_{o,steady})_{dense\ at\ \dot{m}_{s_i}}$.

In (5.12), with $\dot{q}_s = \dot{m}_s / \rho_s$ and the definition of g' from (5.7):

$$\phi = \left(g^2 \left(\frac{\rho_s - \rho_a}{\rho_a} \right)^2 \frac{\dot{m}_s}{\rho_s U_{ref}^5} \right)^{1/5} \quad (5.28)$$

so that Britter and McQuaid's ϕ is only very weakly time-dependent because

$$\phi \propto \dot{m}_s^{1/5}$$

so as \dot{m}_s varies by a factor of 100, ϕ only varies by a factor of 2.51. Because $F_N(\phi) \propto \phi^{-0.6}$ for large ϕ , we see at large values of ϕ , the function $F_N(\phi)$ only varies by a factor of 1.74 when the mass release rate varies by a factor of 100.

5.4 References

Britter, R.E. and McQuaid, J. 1988. Workbook on the Dispersion of Dense Gases. Health and Safety Executive, U.K. Contract Research Report #17, 1988, 129 pages.

6 Accounting for Fluctuations in Toxic Load and Odour

The model in this chapter will allow concentration fluctuations to be included in a simple spreadsheet model of atmospheric dispersion of toxic or odorous gas release. The objective here is to provide a method for adjusting toxic load \bar{L} that is proportional to $\overline{\chi}^n$, the mean concentration $\overline{\chi}$ to an exponent n , to account for the fact that the concentration during an exposure does not stay constant at the mean value, but in fact fluctuates by factors of four or more about the mean.

The concentration fluctuation model described below requires only the mean concentration $\overline{\chi}$ calculated by a dispersion model, and the toxic load or odour exponent n from empirical models of toxic or odour response of people to concentrations of the gas in question. To achieve this simplicity some assumptions must be made about the nature of fluctuation concentrations in atmospheric dispersion. The following sections show how a few reasonable assumptions produce the desired adjustment factor.

6.1 Frequency of Occurrence of Concentrations

Wilson (1995) p50 recommends the log-normal pdf (probability density function) as a good fit to observed concentration fluctuation data for the instantaneous concentrations χ in laboratory and full-scale atmospheric plumes. The log-normal describes the non-zero concentrations $\chi > 0$ that are observed within the plume for a fraction of time γ , and the integral of the log-normal pdf over all concentrations $\chi > 0$ is γ , interpreted here as the probability of finding a non-zero concentration at any instant. The intermittent time periods when the concentration $\chi = 0$ are expressed as a delta function (a “spike”) at $\chi = 0$, with an area in the delta function of $(1 - \gamma)$, which is the probability of finding a zero concentration at any instant. The parameter γ is confusingly called the “intermittency factor” even though it denotes the non-zero fraction of concentrations.

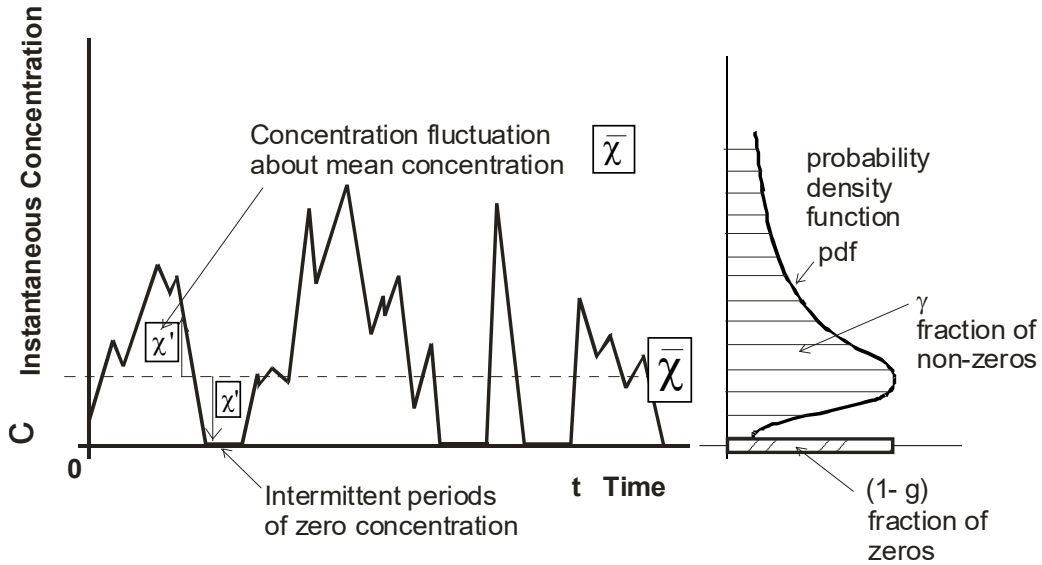


Figure 6-1 Probability distribution of concentration fluctuations at a receptor location

The mean toxic load \bar{L} for an exposure to time-varying instantaneous concentration χ is defined as,

$$\bar{L} = \int_0^{\infty} \chi^n dt \quad (6.1)$$

This is just the n^{th} moment of the concentration,

$$\bar{L} = \overline{\chi^n} \cdot t_{\text{exposure}} \quad (6.2)$$

where t_{exposure} is the exposure time in a steady release, and $\overline{\chi^n}$ is the n^{th} moment of the fluctuating concentration. The objective of this chapter is to relate this n^{th} moment to the mass mean concentration $\bar{\chi}$ that is calculated by an atmospheric dispersion model.

6.2 Concentration n^{th} Moment for Intermittent Log-Normal Fluctuations

For a log-normal pdf, it can be shown that the mean n^{th} moment $\overline{\chi^n}$ of concentration for use in toxic load is related to the n^{th} power of the mean concentration $\bar{\chi}^n$ by the intermittency factor γ and the concentration fluctuation intensity i :

$$\overline{\chi^n} = \gamma \frac{(n-1)(n-2)}{2} (1+i^2)^{\frac{n(n-1)}{2}} \overline{\chi}^n \quad (6.3)$$

where

- $\overline{\chi}$ = mean concentration (kg H₂S / m³)
- $\overline{\chi}^n$ = nth power of mean concentration
- $\overline{\chi^n}$ = mean of nth moment used in toxic load ((kg H₂S / m³)ⁿ)
- γ = fraction of time concentration is non-zero, $\chi > 0$
- χ' = $(\chi - \overline{\chi})$ instantaneous concentration fluctuation about the mean $\overline{\chi}$ (kg H₂S / m³)
- $\overline{\chi'^2}$ = $(\overline{(\chi - \overline{\chi})^2})$, concentration fluctuation variance, ((kg H₂S / m³)²)
- χ_{rms} = $(\overline{\chi'^2})^{\frac{1}{2}}$ root-mean-square (standard deviation) of concentration fluctuations about the mean (kg H₂S / m³)
- i = $\frac{\chi_{rms}}{\overline{\chi}}$, concentration fluctuation intensity including zero periods

Wilson (1995) p139, derives an exact equation that relates the intermittency factor γ to the total fluctuation intensity i .

$$\gamma = \frac{1 + i_p^2}{1 + i^2} \quad (6.4)$$

Knowing the “total” fluctuation intensity i that includes the intervals with zero concentration, and the “conditional” intensity i_p with zero concentrations removed allows us to find the intermittency factor γ using (6.4). The conditional fluctuation intensity i_p removes the intervals of zero concentration from the concentration-time graph in Figure 6.1, and uses the non-zero concentrations to form an in-plume mean $\overline{\chi_p}$ and standard deviation $\chi_{p,rms}$ of concentration about this conditional mean. (Note that the concentrations used are “conditional” upon them being greater than zero, hence the term “conditional intensity”.)

6.3 Total Concentration Fluctuation Intensity i at Ground Level

The total concentration fluctuation intensity i at ground level depends primarily on two factors:

- Whether the ground level receptor is exposed to the lower fringes of an elevated plume whose axis height $z = h$ is high above the ground (typically $h > 2\sigma_z$); or to the on-axis fluctuations of a plume whose axis is near or at ground level (typically $h < \sigma_z$).
- Whether the atmosphere is stable, with a large amount of vertical wind shear dU/dz , in Pasquill-Gifford Classes E and F; or with less wind shear in Pasquill-Gifford Classes A, B, C, or D.

The total fluctuation intensity i for an elevated plume can be several times larger than a ground-level source, and high wind shear in stable weather conditions can produce ground level intensities several times smaller than in unstable or neutral conditions.

Accurate estimates of the total fluctuation intensity require the use of complex models for the along-wind evolution and dissipation of concentration fluctuations. For a simplified spread-sheet based screening model this complicated analysis will be avoided by considering only the case of a near-ground level release in stable atmospheric conditions. Under these conditions, the total fluctuation intensity at ground level on the plume centerline is estimated to be $i_{ref} \sim 0.25$ for an exposure time (referred to as the “averaging time”) of $t_{avg,ref} = 3$ minutes. The total fluctuation intensity i at *longer* exposure (averaging) times can be calculated from the equation in Wilson (1995, page 101),

$$\frac{i^2 + 1}{i_{ref}^2 + 1} = \frac{\sigma_y}{\sigma_{y,ref}} = \left(\frac{t_{avg}}{t_{avg,ref}} \right)^{0.2} \quad (6.5)$$

Here, the 0.2 power law for mean concentration and crosswind plume spread has been used to express the effect of averaging time on fluctuation intensity. For an averaging time of 60 minutes the recommended 3 minute average of $i_{ref} = 0.25$ in (6.5) produces an intensity $i = 0.97$. This is consistent with Hanna, Drivas and Chang (1996) p111 who recommend an exponential pdf (for which $i_p = 1.00$ at all times) and an intermittency factor of $\gamma = 1.0$ to produce $i = 1.00$ for 60 minute averages.

6.4 Relating Conditional Fluctuation Intensity i_p to Total Fluctuation Intensity i

The conditional in-plume intensity (with zeros removed) is much easier to characterize than the intermittency factor γ itself. Based on water channel and full-scale atmospheric fluctuation data the following functional form is used to relate i_p and i , with empirical factors $i_{p\infty}$ and exponent a ,

$$i_p = \frac{i}{\left(1 + \left(\frac{i}{i_{p\infty}}\right)^a\right)^{\frac{1}{a}}} \quad (6.6)$$

where the in-plume fluctuation intensity $i_p \rightarrow i_{p\infty}$ as the total intensity (including zeros), $i \rightarrow \infty$ in the highly intermittent outer fringes of the plume where $\gamma \rightarrow 0$.

Wilson (1995), with access to a few sets of wind tunnel and full scale field data, chose $i_{p\infty} = 1.4$ and $a = 2.0$. Hilderman (2003), used a much larger data set with several thousand measurements of i and i_p for elevated and ground level releases, and elevated and ground level receptors in water channel plume dispersion experiments. From this large data set he found that $i_{p\infty}$ depends on both the receptor and source positions in x and z . Values of $i_{p\infty}$ ranged widely; from $0.5 < i_{p\infty} < 5$, with smaller values for both the source and the receptor at ground level. All receptors were well-fit by $a = 3.0$.

The limit $i_{p\infty}$ that occurs in the outer fringes of a plume where the intermittency factor $\gamma \rightarrow 0$, $i_{p\infty} \rightarrow 0$ was found by Hilderman (2003) to be primarily dependent on the history of normalized wind shear $(\sigma_z / U)(\partial U / \partial z)$ that the plume has experienced as it travels from the source height h to the receptor near ground level. In order to represent wind speeds in all atmospheric stability classes, a power-law (rather than a log-law) mean wind velocity profile with exponent p , is assumed.

$$U = U_{met} \left(\frac{z}{z_{met}} \right)^p \quad (6.7)$$

where z_{met} is the height of the nearby meteorological tower at which the windspeed U_{met} is measured, and z is the height of the receptor above ground level. The exponent p in Table 6.1 was determined by Irwin (1979) for the Pasquill-Gifford Stability Classes, and various terrain roughness.

Table 6-1: Windspeed Power Exponent "p" for Varying Terrain Roughness, from Irwin (1979)

Stability Category		Exponent p in $U = U_{ref} (z/z_{ref})^p$		
		$z_o = 0.01$ m	$z_o = 0.10$ m	$z_o = 1.0$ m
A	very unstable	0.05	0.08	0.17
B	moderately unstable	0.06	0.09	0.17
C	weakly unstable	0.06	0.11	0.20
D	neutral	0.12	0.16	0.27
E	moderately stable	0.34	0.32	0.38
F	very stable	0.53	0.54	0.61

Hilderman (2003) proposes a relation for $i_{p\infty}$ that is a complicated function of the averaged non-dimensional wind shear $(\sigma_z / U)(\partial U / \partial z)$ at the heights of the source and of the receptor. This function can be simplified by assuming that the receptor is at a "near" ground level location of $z = 0.1\sigma_z$, and that the source height h for an elevated source is "high" above ground level where the wind shear $(\partial U / \partial z)$ is much smaller than at the receptor. With these two assumptions, the conditional fluctuation intensity $i_{p\infty}$ for a "near ground level" receptor is calculated from

$$i_{p\infty} = \frac{1.9}{(1 + B_i p)^{\frac{1}{6}}} \quad (6.8)$$

with $B_i = 25$ for a ground-level source, and $B_i = 13$ for a "very high" elevated source where $h > 4\sigma_z$. The suggested functional relation for i_p is (6.6) with $a = 3.0$, so that

$$i_p = \frac{i}{\left(1 + \left(\frac{i}{i_{p\infty}}\right)^3\right)^{\frac{1}{3}}} \quad (6.9)$$

where the value of $i_{p\infty}$ can be calculated from (6.8) using the values of the windspeed exponent p from Table 6.1. Some typical values are:

- Range of $i_{p\infty}$ for a Ground Level Source $B_i = 25$
Very stable air, dense urban roughness: Class F, $z_o = 1.0$ m, $p = 0.61$ so $i_{p\infty} = 1.2$
Very unstable air, smooth rural roughness: Class A, $z_o = 0.01$ m, $p = 0.05$ so $i_{p\infty} = 1.6$
- Range of $i_{p\infty}$ for a Very High Elevated Source $B_i = 13$
Very stable air, dense urban roughness: Class F, $z_o = 1.0$ m, $p = 0.61$ so $i_{p\infty} = 1.3$
Very unstable air, smooth rural roughness: Class A, $z_o = 0.01$ m, $p = 0.05$ so $i_{p\infty} = 1.7$

Considering the inherent uncertainties in estimating conditional statistics (with zero concentration periods removed), the ranges above have relatively constant values of conditional intensity $i_{p\infty}$ over a wide range of atmospheric stability and terrain roughness. To keep the concentration fluctuation model simple, it is recommended that a single constant value of $i_{p\infty}=1.5$ be used for the screening model. With this value, equation (6.9) becomes

$$i_p = \frac{i}{\left(1 + \left(\frac{i}{1.5}\right)^3\right)^{\frac{1}{3}}} \quad (6.10)$$

This should be used to calculate the value of i_p for estimating the intermittency factor γ in (6.4)

6.5 Fluctuation Factor $K_{fluctuation}$ to Include Fluctuations in Calculation of Mean Toxic Load

What is needed is a factor $K_{fluctuation}$ that can be multiplied by the mean concentration $\bar{\chi}$ to account for the contribution of peak and zero concentrations to the mean integrated toxic load exposure factor \bar{L} , so that (6.1) is written as

$$\bar{L} = \int_0^{\infty} (K_{fluctuation} \bar{\chi})^n dt \quad (6.11)$$

This can be written as

$$\bar{L} = K_{fluctuation}^n \int_0^{\infty} \left(\bar{\chi}^n\right) dt \quad (6.12)$$

Comparing this with Equation (6.2) and equating to Equation (6.3)

$$K_{fluctuation}^n \equiv \frac{\overline{\chi^n}}{\chi^n} = \gamma^{\frac{(n-1)(n-2)}{2}} (1+i^2)^{\frac{n(n-1)}{2}} \quad (6.13)$$

from which the effective concentration $\chi_{effective}$ for calculating the mean toxic load \bar{L} is

$$\chi_{effective} = K_{fluctuation} \overline{\chi} \quad (6.14)$$

which is used in the toxic load integral to calculate the average toxic load, where the adjustment factor is

$$K_{fluctuation} = \left(\gamma^{\frac{(n-1)(n-2)}{2}} (1+i^2)^{\frac{n(n-1)}{2}} \right)^{\frac{1}{n}} \quad (6.15)$$

Equation (6.8) is used to find the intermittency factor γ for use in (6.15) for the mean n^{th} moment of concentration. First, the total fluctuation intensity i at ground level on the plume centerline is estimated to be $i_{ref} = 0.25$ for 3 minute averages, and adjusted to the actual exposure time (actual averaging time) using (6.5). This total fluctuation intensity includes both the variability caused by fluctuations during any one release event AND the fluctuations caused by event-to-event variability that would occur in a large ensemble of identical repeated events. Then, this value of i is used as an input in (6.10) to calculate the conditional fluctuation intensity i_p , that removes the intermittent periods of zero concentration. Next, both i and i_p are used in (6.4) to calculate the intermittency factor γ . Finally, put i and γ in (6.15) to get the n^{th} moment $\overline{\chi^n}$ needed to calculate the average toxic load \bar{L} in (6.12) for an exposure to fluctuating concentrations.

6.6 Example for Toxic Load from Hydrogen Sulphide

For example, consider a release of hydrogen sulphide with two different toxic load exponents, $n=2.5$ for the Triple-Shifted Rijnmond toxic load model, and $n=4.36$ for the AEGL toxic load exponent recommended by the U.S. EPA. Table 6.2 shows values for the effective concentration adjustment factor $K_{fluctuation}$ for a range of in-plume concentration intensities. This factor is used

to get the effective concentration $\chi_{effective}$ in (6.14) needed for the toxic load with fluctuations included.

Table 6-2: Calculated Concentration Adjustment Factors $K_{fluctuation}$ for Estimating Average Toxic Load Near Ground Level

Averaging Time t_{avg} (minutes)	Fluctuation Intensity i	Conditional Fluctuation Intensity i_p	Intermittency Factor γ	Triple-Shifted Rijnmond $n = 2.50$ $K_{fluctuation}$	U.S. EPA AEGL $n = 4.36$ $K_{fluctuation}$
user input	Eq. (6.5)	Eq. (6.10)	Eq. (6.4)	Eq. (6.15)	Eq. (6.15)
3	0.25	0.25	1.00	1.05	1.11
5	0.42	0.42	1.00	1.13	1.31
10	0.59	0.58	0.99	1.25	1.64
15	0.68	0.66	0.98	1.33	1.87
30	0.83	0.79	0.96	1.47	2.31
45	0.91	0.85	0.94	1.56	2.61
60	0.97	0.89	0.93	1.62	2.83
71	1.00	0.92	0.92	1.66	2.97
75	1.01	0.93	0.92	1.67	3.02
90	1.05	0.95	0.91	1.72	3.18
120	1.11	0.99	0.89	1.79	3.44
131	1.12	1.00	0.88	1.81	3.52
180	1.19	1.04	0.86	1.89	3.83

6.7 Application to Estimating Time-Averaged Odour Intensity

All the values above are for toxic load. The same equations may be applied to odour annoyance intensity I_{odour} when odour is expressed as a power n of the concentration.

$$I_{\text{odour,average}} = \left(\frac{K_{\text{fluctuation}} \bar{\chi}}{\chi_{\text{I,ref}}} \right)^n \quad (6.16)$$

where $\bar{\chi}$ is the time averaged mean concentration, and the factor $K_{\text{fluctuation}}$ is the adjustment factor to convert the n^{th} moment $\bar{\chi}^n$ of concentration for use in odour annoyance to the n^{th} power of the mean concentration $\bar{\chi}^n$ that can be calculated by a plume dispersion model. The reference concentration $\chi_{\text{I,ref}}$ is the threshold at which the odour intensity I_{odour} takes on its reference value of unity, usually denoting that the odour is perceived as “very faint”. The value of the adjustment factor $K_{\text{fluctuation}}$ is calculated from (6.13). The odour annoyance intensity in (6.16) is the intensity averaged over same length of time as the mean concentration averaging time for $\bar{\chi}$, typically, the one hour interval for which most dispersion models are designed.

For example, many unpleasant odours have values of the exponent n of about 0.25. Using a typical user-input value of a 60 minute averaging time, the conditional fluctuation intensity $i_p = 0.89$, Table 6.2 shows that the resulting intermittency factor is $\gamma = 0.93$. Then, in (6.15), the adjustment factor $K_{\text{fluctuation}} = 0.64$. This gives the surprising result that the average odour intensity $I_{\text{odour,average}}$ over the time period for which the mean concentration is calculated will be only 64% of the odour intensity that is estimated from the hourly averaged concentration. This decreased odour annoyance is mainly due to the periods of intermittent zero concentrations that occur $(1-\gamma) = (1-0.93) = 0.07$, which is 7% of the time. *Whether people will actually perceive these zero odour periods as a reduction in odour annoyance has not yet been tested in a real odour exposure situation.*

6.8 Fraction of Time a Specified Odour or Toxic Threshold Concentration is Exceeded

For fluctuating concentrations that are intermittently zero for a fraction of the time $(1 - \gamma)$, and non-zero for a fraction γ of the time, the conditional statistics with the zero periods removed are denoted by the subscript “ p ” which means “in-plume” as opposed to the out-of-plume zero readings. For the in-plume (non-zero concentrations) the equations for the recommended log-normal probability distribution are, for a specified threshold concentration χ^*

$$P_p(\chi^*) = \frac{1}{\sqrt{2\pi} \sigma_{\ln p} \chi^*} \exp \left[\frac{- \left(\ln \left(\frac{\chi^*}{\chi_{50,p}} \right) \right)^2}{2 \sigma_{\ln p}^2} \right] \quad (6.17)$$

where the variables with subscript are always evaluated for the “conditional” time series with zero concentration intervals removed, see Wilson (1995) p. 50 (where the first χ^* is missing due to a typographical error). The conditional median (50th percentile) value of the non-zero concentrations is

$$\chi_{50p} = \frac{\bar{\chi}_p}{(1 + i_p^2)^{0.5}} \quad (6.18)$$

the conditional mean concentration (with the periods of zero concentration removed) is always larger than the overall mean $\bar{\chi}$ that is predicted by dispersion models,

$$\bar{\chi}_p = \frac{\bar{\chi}}{\gamma} \quad (6.19)$$

where γ is the fraction of time the concentrations are non-zero (that is, the fraction of time the plume is present at the fixed receptor location.) The log standard deviation of the non-zero concentrations is given by the definition

$$\sigma_{\ln p} = \left[\ln(1 + i_p^2) \right]^{0.5} \quad (6.20)$$

Then, for the cumulative distribution $P_{c < c^*}$ of observing a concentration less than χ^*

$$P_{\chi < \chi^*} = (1 - \gamma) + \frac{\gamma}{2} \left(1 + \operatorname{erf} \left(\frac{\ln \left[\frac{\chi^*}{\chi_{50p}} \right]}{\sqrt{2} \sigma_{\ln p}} \right) \right) \quad (6.21)$$

where $\operatorname{erf}(\dots)$ is the error function. The marginal distribution function $P_{c > c^*}$ that represents the fraction that exceeds the threshold χ^* is

$$P_{\chi > \chi^*} = \gamma \left[1 - \frac{1}{2} \left(1 + \operatorname{erf} \left(\frac{\ln \left[\frac{\chi^*}{\chi_{50p}} \right]}{\sqrt{2} \sigma_{\ln p}} \right) \right) \right] \quad (6.22)$$

This exceedence probability is just the joint (combined) probability

$$P_{\chi > \chi^*} = \left(\begin{array}{l} \text{fraction, } \gamma, \text{ of} \\ \text{concentrations} \\ \text{greater than} \\ \text{zero} \end{array} \right) \left(\begin{array}{l} \text{fraction of} \\ \text{concentrations} \\ \text{greater than zero that} \\ \text{exceed threshold } \chi^* \end{array} \right) \quad (6.23)$$

so we see that the presence of intermittent zero concentrations for $(1 - \gamma)$ of the time, plays an important role in determining the fraction of time a specified threshold concentration χ^* will be exceeded.

6.9 References

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Appendix 3 Selection of the Drag Coefficient for Uncontrolled Sour Gas Releases

Appendix 3

Selecting the Drag Coefficient

Background

The jet at the D-zone may expand as a result of drag forces. Drag forces result from friction, temperature differences and obstacle interactions. Friction and temperature can be considered components of turbulent entrainment of ambient air. Jet obstruction or interaction with obstacles can result in two drag forces: skin friction and form drag. Although the skin friction drag force can be determined analytically for a simple surface such as a flat plate, interaction with multiple obstacles such as assorted pipes and square bars cannot be determined with certainty. Form drag results from a rigid obstacle in the free jet stream creating a pressure cavity. Form drag can be readily understood in association with the aeronautical characteristic (i.e., streamlined versus blunt body) of the obstacle rather than the ambient flow past the obstacle.

In the model of sonic releases, drag effects are divided into three groups:

- drag effects, including ambient friction, that leads to turbulent entrainment of air, energy dissipation and dispersion;
- drag effects, including jet interaction (skin friction) with the ground, gravity flow and temperature, that leads to changes in jet momentum and energy;
- drag effects, including combined skin friction (without heat input) and form drag, that leads to an effective instantaneous change in momentum.

Turbulent entrainment and jet interaction (ground friction, gravity and temperature) are formulated within the SLAB dense gas model. However, the instantaneous momentum drag is included in the Wilson (1981) model and is a user selected input variable to the source initial conditions. An instantaneous change in momentum results in a change in the effective source size but assumes there is no entrainment. Because the instantaneous momentum drag cannot be determined analytically for most practical situations, some guidance is provided in the following sections for selecting the appropriate input to the AERH2S model.

The instantaneous momentum drag is described by the model input variable, C_D , and may have a value between 0 and 1. A value of $C_D=0$, represents no loss of momentum and therefore no initial change in plume size. A value of $C_D=1$, represents all of the jet momentum has been transferred to the environment obstacle without otherwise changing the jet energy.

The selection of the drag coefficient, C_D , requires some consideration of the specific release being analyzed. The predicted downwind concentrations may be sensitive or non-sensitive to the selection of C_D , and therefore, only through interpretation of the model results after iterating on several C_D values, can the appropriate value be determined. A worst-case prediction is not guaranteed by selecting $C_D=0$ nor $C_D=1$. A worst-case prediction is not necessarily the most realistic prediction. It is therefore important that

description of the results contain an adequate description of the assumptions about the source and the reasoning behind the final selection of C_D .

Pipeline Ruptures

For pipeline ruptures, the instantaneous momentum drag is used to characterize the loss of momentum resulting from interaction with the crater at the source of the release jet. The appropriate drag input to the model depends upon pipeline size, pressures and depth. Consider for example, in Figure 1A the release may be considered to have a large drag, $C_D \leq 1$, because of the large interaction with the crater. The plume downwind of such a release would be considered to be completely dominated by ambient wind conditions. In Figure 1C, the initial rupture has removed most or all the surrounding earth and therefore there is no crater to deflect the source jet. In this case, a selection of $C_D \geq 0$ is appropriate, because the release would be considered to be negligibly impacted by the crater and the jet would completely dominate over the ambient wind. Situations may be present that are between the two extremes and is represented in Figure 1B. In this case, a selection of $C_D \approx 0.5$ may account for some loss of the source momentum due to some crater interaction.

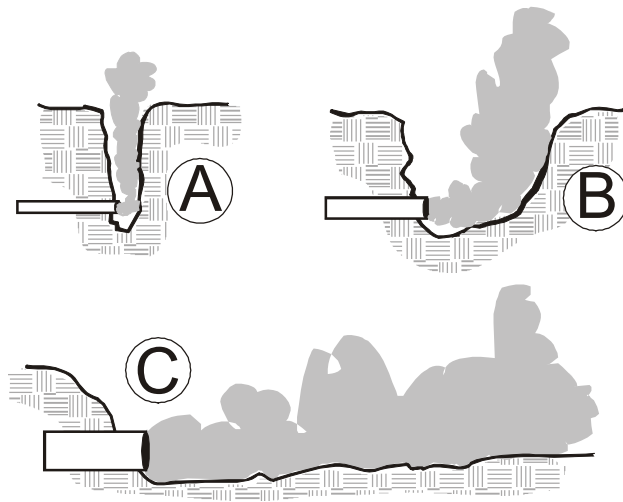


Figure 1: Schematic of a pipeline rupture for (A) small size/pressure (B) medium size/pressure, and (C) large size/pressure

Well Releases

For well releases, the instantaneous momentum drag is used to characterize the loss of momentum resulting from interaction with obstacles such as the rig structure, piping, etc. Source characterization for releases from wells requires careful consideration of the following (for example):

- is the release vertical or horizontal;
- is the rig present or absent;
- is the rig present for the entire release duration;

- is the Christmas tree present or absent;
- are there significant liquids present that may impact the assumed gas phase release; or
- is it possible for the drill plate to be blown out of the way of the jet such that the release flows through the top structure or is contained below the rig flooring.

Several photographic examples of well blowouts (Figure 2) have been adapted from internet sources that illustrate some of the likely complexities the simple C_D term accounts for. A selection of $C_D \geq 0$ may be appropriate for release that is either vertical or horizontal from a Christmas tree where there are no obstructions nearby. A selection of $C_D \leq 1$ may be appropriate where it is expected that the release occurs during drilling and interaction with a rig structure is likely.

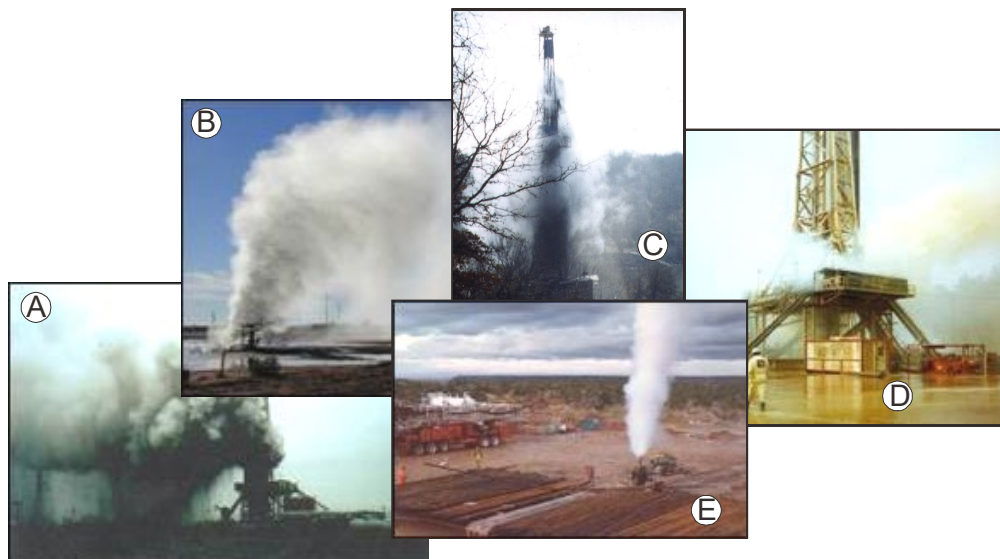


Figure 2: Internet examples of well blowouts illustrating obstructed flows (A,C,D) and unobstructed flow (B,E)

General Recommendations

The selection of the most appropriate C_D cannot be determined in isolation of a critical assessment of the source conditions. However, an estimate of $C_D = 0.5$ can be used to make initial estimates using the AERH2S model. Limited sensitivity testing of the AERH2S model suggests that conservative estimates of the EPZ may result using:

- for dense pipeline releases, $C_D \leq 0.5$, and
- for dense or buoyant well releases, $C_D \leq 0.5$.