

Review of Source Term Modelling for Hydrocarbon Releases using Process Dynamic Simulation

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Unlike onshore plants, where the risk of a hazardous release may be dominated by the initial event consequences, the risk profile in offshore plants can also include a significant escalation element. As a result, when considering the potential for escalating events and the impairment of safety critical equipment such as critical structures, escape routes or the temporary refuge, it is necessary to compute the variation of release rate with time, as impairment criteria are time-based. The first stage is to predict the mass flow from an inventory, and model how this will decay against time, taking account of isolation and any depressurisation.

Significant advances have been made in the capability of dynamic process simulators over the last 15 years, to the extent that dynamic simulators such as Aspen HYSYS Dynamics or UNISIM are now used in modelling such safety-critical systems as the response of a protective system to a demand. The use of these models is now widely accepted in the industry. The models carry out rigorous flash calculations and manage heat and mass balance over time, including the ability to remove inventory or add-in energy to simulate fire cases.

The project investigated the difference between the standard equation-based models and a more rigorous dynamic simulation for time-dependent release rates including protective systems such as isolation and blowdown. Three questions were addressed: whether it was feasible to use or overcomplicated dynamic simulation in this way, whether the results matched existing methods, and whether there were areas where the dynamic simulation would give different results. The review concluded that the use of dynamic models was entirely feasible, especially where a model has already been constructed and validated for other use, and while showing good agreement in single phase models, indicates that mixtures with flashing gas may under predict the duration of fire events using equation-based methods.

Keywords: Source Term, Time Dependent, Blowdown, Isolation, Release Rate, Dynamic Risk Analysis

Introduction

While there are many similarities in approach for offshore and onshore risk assessment, one area which gets more attention in the offshore environment is the progression of an event over time. While modern facility design has moved to providing more segregation between the hazardous hydrocarbon processing areas and the accommodation and control areas, the remoteness of many offshore production facilities means that the length of time to ultimate rescue or event termination, and hence exposure to the hazard, is significantly longer than for onshore. Piper Alpha was an archetypal example of this, in that the majority of fatalities occurred in the accommodation as the event escalated, whereas for onshore major accidents, such as at the Texas City Refinery, the fatalities were dominated by those caught up in the immediate explosion.

In the immediate aftermath of the Piper Alpha disaster, there was a significant effort to look at the time-dependence of incidents. Indeed, the entire concept of how Safety Critical Elements are assessed and managed is inherently time-based, with the requirement for survivability and operation over a major accident event included in the design, operation and testing of these elements.

Many of the software packages and modelling tools built to carry out consequence modelling are based on modifications to single-phase source term models to account for multi-phase flow. For instance, for handling gas releases from a production separator, it is not uncommon to carry out an adiabatic flash of the separator down to atmospheric conditions, and then treat the total mass of gas (including the flash gas) as a single-phase inventory.

From a fundamental chemical engineering point of view, the models are generally equation-based, and are not intended to include full thermodynamics of complex chemical systems. However, with the advance in computing power, numerical solution and thermodynamic calculation, changes in mass, energy and flow, (the fundamental building blocks of the mass and energy balance) are routinely handled in dynamic process simulation applications.

There is a risk with using equation-based models in that the fundamental simplifications, made in the past for good reason, may be no longer required, and a more rigorous method may be available to carry out the analysis to give better results, which reflect the reality of an incident more closely. However, there has been a reluctance to move to more advanced modelling, perhaps due to the perceived complexity of dynamic models.

This paper is intended to review the following questions:

- Is it complex to set up a dynamic model for source term modelling processes?
- Does the modelling reflect the equation-based approach in typical modelling scenarios?
- For cases where energy balance is likely to be important, such as flashing liquids, does the modelling differ from the equation-based approach?

Dynamic Process Simulation

Over the last decade the speed at which computers can solve complex problems has increased dramatically. This has led to the ability to use process simulators, such as Honeywell's UNISIM, AspenTech's HYSYS Dynamic, etc. within acceptable run-times. UNISIM and HYSYS share a common historical code-base, and are in wide use across the oil and gas industries. The research was carried out using UNISIM.

Dynamic simulation allows for a process to be modelled in real time, or quicker. Fluctuations can be simulated and it can be seen how well the system will cope with the disruption. Vessels can be modelled with a hold-up inventory and can be emptied with the adjustment of a valve. This allows for a real time simulation of the plant, and is often used to train system operators on how to deal with plant upset, start-up and shutdown.

During dynamic simulation, UNISIM performs a multitude of different calculations per second in the attempt to model the system in as much detail as possible. The calculations aim to model a number of different conditions including: flowrate, pressure, composition, and energy. UNISIM also has many equation of state models that aim to accurately model the flash equilibrium within streams and vessels as they change with time.

Lumped Modelling

One of the major assumptions used within UNISIM is that the system is "lumped". Most engineering problems involve "distributed" systems. A "distributed" system is one that has a gradient associated with it, such as a temperature or a concentration gradient. These gradients occur over the x, y, and z direction and when formed into an equation can be shown to be a series of Partial Differential Equations (PDEs). These PDEs are complicated and take a long time to solve. (Honeywell, 2010)

To save on computational time, UNISIM ignores the dimensional gradients and is only concerned with the change in gradient with time. By making this assumption UNISIM can form Ordinary Differential Equations (ODEs) describing the problem. These are less rigorous than PDEs and allow the system to be solved far quicker. This ignoring of gradient due to positioning is known as "lumped" modelling. Honeywell (2010) claim that lumped modelling gives a solution which "is a reasonable approximation of the distributed model solution"; however, this assumption brings with it a number of issues.

For instance, lumped modelling causes a number of issues when dealing with two-phase flow. UNISIM cannot accurately model both the pressure propagation and the separation of liquid from gas phase within a pipeline. It also does not take into account any shear stresses between the two phases during a release. This is not an issue if one phase is finely dispersed within another, however, it could be an issue in stratified or slug flow. If these flows are known to be present then another software that takes account of these flows, and their shear stresses, should be used.

UNISIM performs a multitude of different calculations every time-step to estimate how the process would react in reality. These involve solution of the mass balance at a global and component level, along with the energy balance, taking into account the dynamic performance of the unit operations, valves, etc. These are simplified into a number of ODEs that are solved using the Implicit Euler method which estimates the solution by rectangular integration. (Honeywell, 2010)

Fluid Packages

A number of different fluid packages are available within UNISIM. Each model has distinct advantages and disadvantages, however, they all are able to model the Vapour Liquid Equilibrium of a select system in detail.

Oil and gas systems are typically a complicated mix of a number of different hydrocarbons which make them difficult to model accurately. Honeywell (2010) strongly suggest a Peng-Robinson (P-R) Equation of State for use with these systems. This is because it has been developed and adapted specifically to cope with the variation of components present in the system. Honeywell (2010) states that P-R is able to deal with a wide range of conditions and can accurately estimate how single, two-phase, and three-phase will cope under these set conditions. This allows UNISIM to accurately model the VLE between the oil, gas, and water system at each time step within the simulation. If another component is added to the simulation, then another fluid package might need to be selected to account for any difficulties the component could bring, such as ionic charges.

Hold-up Model

UNISIM uses the above equations and packages to estimate how the hold-up in each vessel will behave. It calculates how the introduction of feed into a hold-up will affect the hold-up and how it will change with time. This is necessary as any changes in the feed will take time to propagate through the hold-up and into the outlet stream. This model makes the assumption, due to lumped modelling, that each phase within the hold-up is well mixed (Honeywell, 2010). This allows UNISIM to calculate the heat input from the feed and outside the vessel into the holdup. UNISIM can also then calculate the heat exchanged between phases with the aim to model the hold-up in a significant amount of detail.

Pressure-Flow Relation

UNISIM utilises a rigorous Pressure-Flow relation, and can estimate pressure drops and flowrates throughout a system. The Pressure-Flow relation is used within pumps, compressors, heat exchangers, and, most importantly, valves. UNISIM is able to calculate the Pressure-Flow (P-F) relation through a number of different methods. For pumps/compressors/heat exchangers the P-F relationship is calculated through heat inputs and work inputs. For valves, which are of prime focus in this paper, UNISIM uses resistance equations based on typical valve equations.

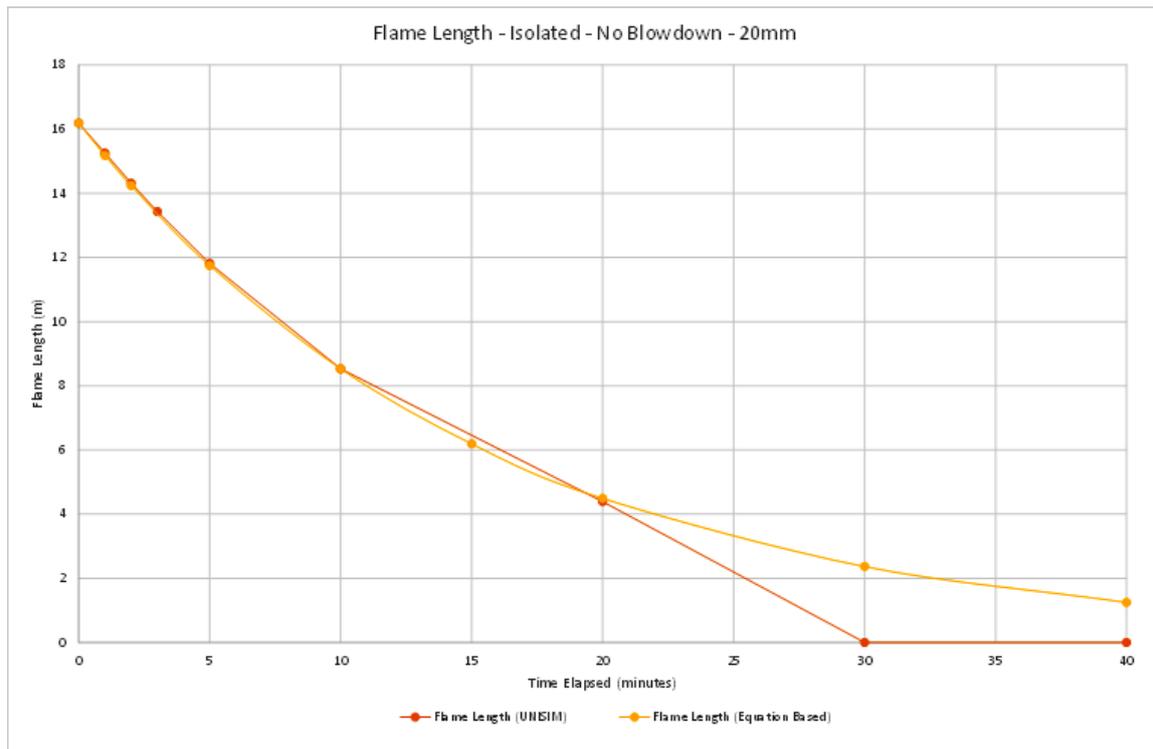


Figure 2. Gas inventory, 20mm hole, no blowdown

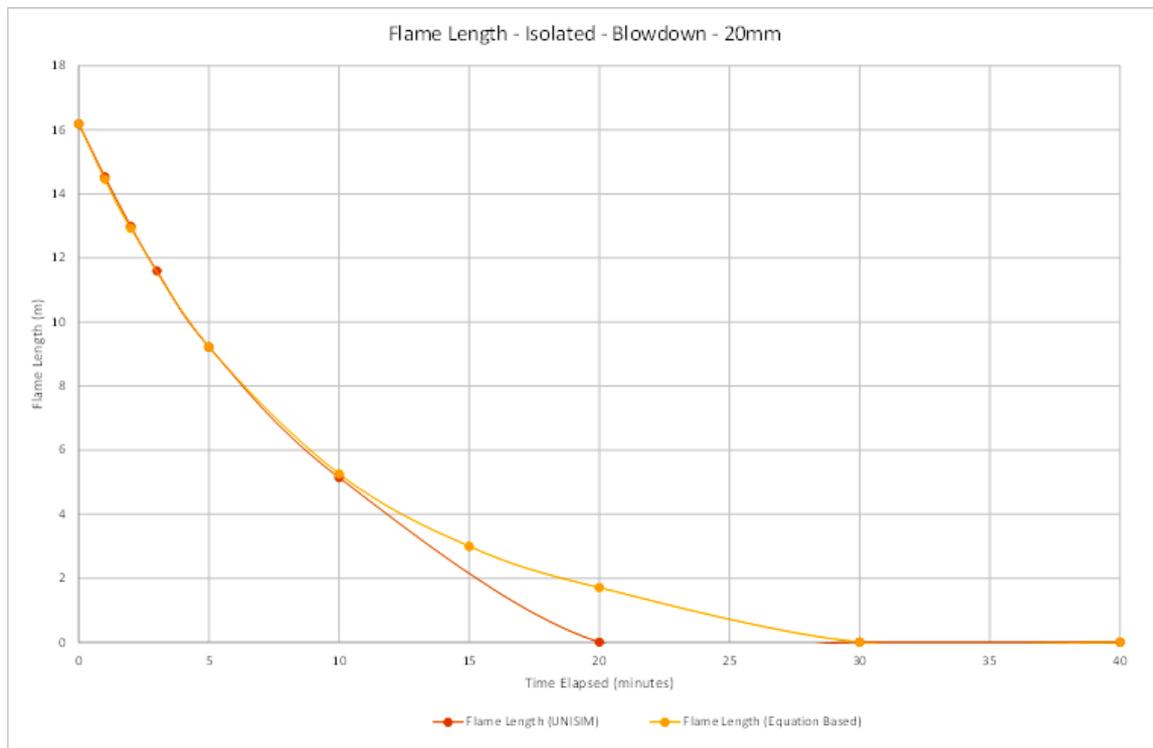


Figure 3. Gas inventory, 20mm hole, blowdown in line with API521

The dynamic model showed very good agreement with the equation, and deviates only when flow becomes non-choked. The deviation shown in the results illustrates that to get to low flame sizes, it is important to account for the transition to non-choked flow: however, this is well understood, and comparison carried out with the PHAST results matched very well.

It is concluded from this phase of the work that the dynamic modelling approach is valid, in line with fundamental single phase modelling, and consistent with the understanding of gas-system behaviour from research and the resultant equations.

Multi-phase Inventories

Hydrocarbon processing generally involves dealing with a complex mixture of hydrocarbons of different molecular weights, typically accompanied by water, CO₂, and other components, such as H₂S, Nitrogen etc. As multicomponent mixtures, the composition and quantity of any phase is determined not just by the temperature and pressure, but also by the mixture composition. In the case of a release, for example in the gas phase of a separator, the initial composition of the release would be the flash gas in the separator, but as the event proceeds, the pressure in the inventory drops, and additional gas would flash from the liquid and add to the gas inventory.

The prediction of the behaviour of the fluids during flashing generally requires a good fluid characterisation, including how the heavier components are modelled, and an appropriate equation of state. This is carried out to a degree, but most equation-based release models do not attempt to carry out this out. Rather, the practice has generally been to determine the total gas inventory by flash calculation, and then treat the release as a single-phase release in line with the methods shown above.

In order to compare these, a typical three phase separator was chosen, with the following dimensions, and operating conditions.

Table 1. Horizontal Three Phase Separator Data

Description	Value
Volume	18.85m ³
Diameter	2m
Length	6m
Oil Volume (Height)	40% (0.8423m)
Water Volume (Height)	8% (0.1602m)
Pressure	35Bara
Weir Height	0.7m
Weir Position	4m

The separator was assumed to be processing a typical offshore oil, such as could typically achieve Forties Pipeline Specification in a conventional 2 or 3 stage separation train. The fluid was characterised including heavy ends in line with normal process engineering modelling practice.

A significant number of runs were carried out again, but the following results illustrate the findings overall.



Figure 4. 20mm Hole, Multiphase Inventory, No Blowdown

Figure 4 illustrates the general outcome of all the multi-phase releases. The initial release rate is identical. However, the dynamic model outflow rate drops more quickly at the start of the event, dipping below the equation-based line. This is in turn reversed later in the model, where the time to reach 2 m flame length is increased. On examination in more detail, this is in line with expectations, as the gas inventory actually present at the start of the release does not include the gas that would flash over the incident, and hence the pressure will drop more quickly. However, the gas will be liberated over time with the dropping pressure, and the overall mass released will be very similar.

For the same case, with an API-521 blowdown, the same effect is visible as shown in figure 5 below.

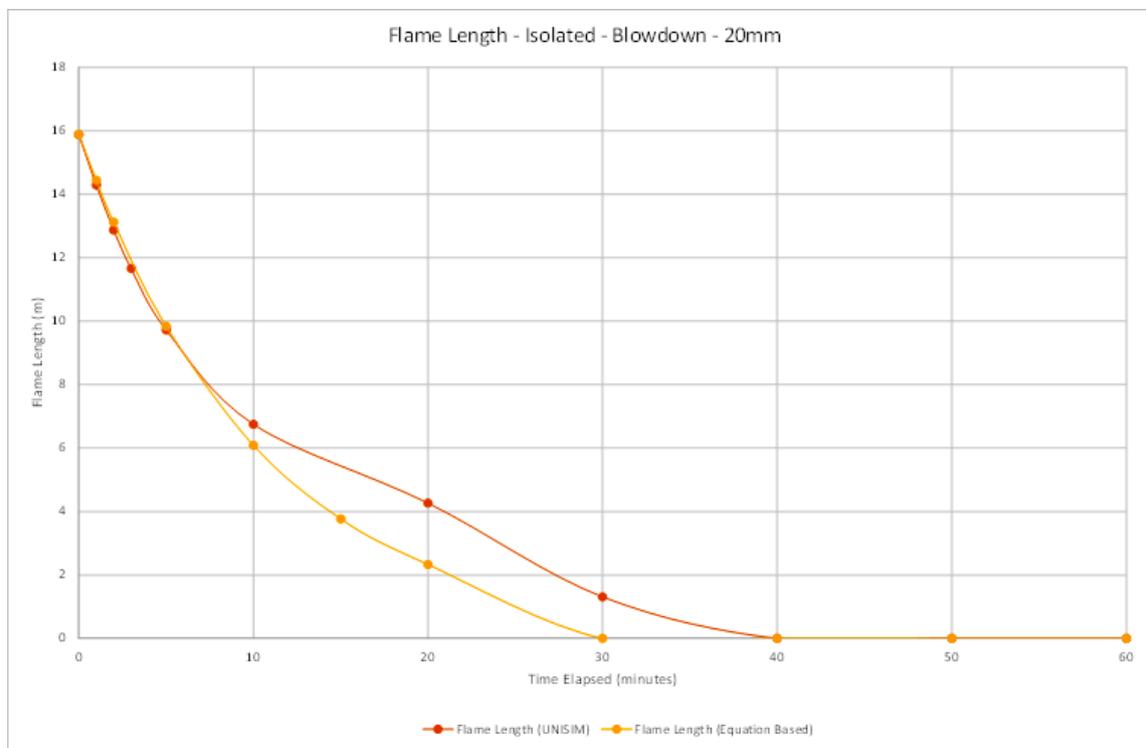


Figure 5. 20mm Hole, Multiphase Inventory, API521 Blowdown

In both cases, there is an appreciable increase in the time to reach a 2 m flame length of approx. 5-10 minutes. While this is arguably a small number, given the other uncertainties built into most QRA's, it is potentially of concern in that the simpler models under-predict duration, and hence may give an incorrect conclusion when survivability of equipment or structures is of particular concern.

Conclusions

This paper presents a subset of the results obtained from a six-month research topic and is intended to present the answers to three questions as presented initially. The key conclusions are:

1. Dynamic process simulators, such as UNISIM, can be readily used to carry out source term modelling. Where a model already exists, then for relatively low marginal cost, the model can be modified to incorporate source term modelling.
2. For single phase isolated releases, there is close agreement between the equation-based and dynamic modelling, providing confidence in the modelling approach, as similar mass release rates are obtained using two different methods.
3. For multi-phase inventories such as oil-gas-water mixtures, the dynamic model predicted longer incident durations than the traditional modelling approach. The durations were longer for a range of operating conditions, starting points and variations in operation of blowdown, shutdown systems etc. Based on these results, it is proposed that dynamic simulation approaches should be considered, especially for cases where a longer incident duration would have significant risk impact through escalation or impairment of SCEs.

The project was undertaken as a research project as part of the Masters degree in Chemical Engineering at University of Edinburgh. It is noted that the current phase of research focused only on the source-term modelling, and that the inherent uncertainties in the overall risk assessment process may relegate this finding to a second order effect. This has not been tested as part of this analysis, but may form the basis for future study.

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Appendix: Fundamentals of Modelling of Release Rates and Durations

Gas Releases

Most releases above the liquid level in a vessel are assumed to be pure gas releases. This is based on an assumption that most of the droplets within the gas phase have had significant time to settle out by the time they reach an outlet, which is indeed the case in most vessels. The equations seen below aim to model gas only releases and how the release develops with time.

When attempting to model the release rate of the leak in question the first calculation undertaken is to determine whether the flow will be choked or non-choked. Choked flow occurs as described below for general gases.

$$\frac{P_{atm}}{P_o} < \left(\frac{2}{\gamma + 1}\right)^{\frac{\gamma}{\gamma - 1}} \quad (1)$$

The ratio is approximately 2 for typical hydrocarbons, i.e. when the pressure upstream is above 2 bara or 1 barg, the flow will be choked. Choked flow is the point when flowrate through an orifice will not increase with a decreasing downstream pressure (C.J.H. van den Bosch, 2005). At this point the velocity of the gas through the orifice is equal to the speed of sound and the only way of increasing the flowrate is by increasing the density of the gas flowing through it. Below this limit, flow will be non-choked. This most commonly occurs when the pressure upstream of the valve is increased which in turn increases the density of the gas and hence the flowrate through the valve.

As the downstream pressure has no effect on the choked flowrate of the orifice it is removed from the flowrate equation. The accepted initial flowrate equation for choked flow is given below (C.J.H. van den Bosch, 2005).

$$\dot{m}_o = A \cdot C_d \cdot \left[\frac{P_o \gamma}{v_o} \left(\frac{2}{\gamma + 1}\right)^{\frac{\gamma + 1}{\gamma - 1}} \right]^{\frac{1}{2}} \quad (2)$$

This equation is used to calculate the initial flowrate through an orifice.

One of the terms in equation 2, v_o is the specific volume of the released gas. This is equal to the inverse of the density, which can be calculated from the ideal gas law.

$$PV = nRT \quad (3a)$$

$$\rho = \frac{P}{R \cdot T} \quad (3b)$$

The assumption of ideality in oil and gas systems where there are a number of different components often held at high pressures can give significant differences in predicted flowrates.

When calculating the densities for a system the gas law including the compressibility factor should be used to calculate density.

$$PV = nzRT \quad (4a)$$

$$\rho = \frac{P}{z \cdot R \cdot T} \quad (4b)$$

Towards the end of a release the flow will reduce until it reaches a point where equation 1 will no longer be true and the flow will become non-choked. At this point the downstream pressure will have an effect on the release rate and as such has to be included in any flowrate calculations. After this point the flow will remain in a non-choked state until the pressure in the vessel/pipeline has reached atmospheric pressure.

$$\dot{m}_o = A \cdot C_d \cdot \left[\frac{P_o}{v_o} \left(\frac{2\gamma}{\gamma-1} \right) \left(\frac{P_{atm}}{P_o} \right)^{\frac{2}{\gamma}} \left\{ 1 - \left(\frac{P_{atm}}{P_o} \right)^{\frac{\gamma-1}{\gamma}} \right\} \right]^{\frac{1}{2}} \quad (5)$$

The equation for non-choked flow can be seen below.

Liquid Only Releases

Liquid-only releases occur where the leak source is below the liquid level and have significantly higher flowrates than gas-only releases. The equation for non-choked liquid flow (C.J.H. van den Bosch, 2005) as the equation used for modelling flowrate which has been widely studied to be:

$$\dot{m}_o = C_D A_l [2\rho(P_o + \rho gh - P_{atm})]^{\frac{1}{2}} \quad (6)$$

The liquid releases equation is based on the Bernoulli equation, thus takes account of the differences between the internal pressure, a combination of the physical pressure of the system and the liquid head, and the external pressure.

The true initial liquid release rate of a leak would be found by inputting the initial conditions into equation (6) above.

The vessels modelled for this paper held an oil, gas and water mixture at high pressures. The oil in question, when flashed to atmospheric pressure, would partially vaporise and produce more gas which would feed any gaseous leak further. This means that upon the release of oil into the atmosphere, gas would be formed from the oil and be released. This process of the release of gas occurs after the orifice. This is due to the compression of the orifice preventing gas from forming, and allows the flashing liquid to be modelled as a purely liquid flow.

Modelling of Variations with Time

The above release equations (2, 5, and 6) give an estimate of the initial release rate of the system. Once these have been calculated the changes in flowrate, pressure and temperature with time need to be estimated. This can be done by defining the total releasable inventory and using this to estimate how quickly the system will reach ambient conditions.

Flowrate Variation with Time

For a gaseous, or two-phase, flowrate exiting through a leak the following equation is used to estimate the reduction in flowrate with time (Naser Badri, 2013).

$$Q(t) = Q_o e^{-\left(\frac{Q_o t}{M}\right)} \quad (7)$$

This curve matches with the general release rate curves obtained through experimentation.

Flowrate Variation with Non-Isolated Inventory

In the case of an instantly isolated system the total releasable inventory is relatively simple to calculate. However, for a non-isolated inventory, or a situation where isolation is activated after a certain time then the releasable inventory is more difficult to calculate. For example in a situation where no isolation is initiated the whole plant could potentially be assumed to be releasable inventory. In cases like these there are a number of methods that can be used to calculate releasable inventory.

One simplification is to assume the process isolates in sections. In this case the leak would have the combined inventory of all the connected vessels within that section of plant. This seems like an acceptable assumption as all the connected vessel's inventory will eventually exit the system through the leak.

However there is no gauge of how much inventory is available to be released through the leak at any given time. The valves between vessels could let the whole inventory through to the leaking vessel instantly or extremely slowly through a small leak. This assumption treats both these scenarios the same way and assumes that all the inventory from all vessels is available for release at any time. In essence this method assumes many vessels, and their inventory, combine into one large vessel, with a large inventory. This could potentially lead to issues when dealing with non-isolated process releases.

A second simplification is to assume that the flowrate remains constant until the vessel has been isolated (Naser Badri, 2013).

$$Q(t) = Q_o \quad (8)$$

If the release is modelled in this way then upon isolation of the vessel flowrate will begin to follow equation 7 above.

Flowrate Variation with Blowdown Systems Enabled

Most high pressure systems will have blowdown systems installed on them to minimise the flowrate of any unsafe releases from process equipment. If these are installed they will typically be activated at the same time as isolation activates. Once blowdown has started the total mass leaving the vessel via the leak and the blowdown route increases significantly, quickly reducing the pressure and minimising the release rate from the leak (B. Hekkelstrand, P. Skulstad, 2004). This effect can be modelled in a similar way to equation 7 above (Naser Badri, 2013).

$$Q(t) = Q_L e^{-\left(\frac{Q_T}{M}(t-t_b)\right)} \quad (9)$$

Due to the exponential term having a higher value than equation 7 the reduction in leak flowrate is greater than when the system is not performing blowdown. This equation is used in place of equation 7 once the blowdown system is activated.

Pressure Variation with Time

As well as calculating the reduction of the flowrate within a vessel there are equations available to predict the change in pressure and temperature in the vessel.

Pressure drops are estimated in a similar way to the flowrate reduction equations above. Similar assumptions are made to estimate the total releasable inventory in the case of a non-isolated system. The equation used to determine pressure drop in the vessel over time can be seen below (Naser Badri, 2013).

$$P(t) = P_o e^{-\frac{Q_o t}{M}} \quad (10)$$

In a similar way to equation 9, the pressure drop equation above can be modified to take into account any blowdown systems installed on the vessel. The pressure drop with time is estimated using equation 10 could be also used with equations 2, 5, 6 to determine the flowrate at each selected time.

Temperature Variation with Time

Finally, the temperature profile of the system can also be estimated. The temperature of the gas within the vessel is dependent on the Joule-Thomson effect; as a gas expands it cools down. This effect can be modelled using the equation below.

$$\frac{T_2}{T_1} = \left(\frac{P_2}{P_1}\right)^{\frac{\gamma-1}{\gamma}} \quad (11)$$

The above equation uses the initial temperature, the gas ratio of specific heats Cp/Cv, and the pressure profile to determine the temperature of the system at any time. The initial temperature is set by the operating conditions and the gas ratio is assumed to remain at initial conditions. This leaves the pressure profile as the only factor that determines the estimated temperature profile. This equation does not take into account the heat lost through the walls of the vessel or from the heat of vaporisation of the oil fraction and as such can be, in a number of scenarios, inaccurate.

Determination of Exit Temperature

Similarly to equation 11, the temperature at the point of release can also be calculated. Again, the temperature at the outlet is controlled by the Joule-Thompson effect and can be calculated using the equation below (C.J.H. van den Bosch, 2005).

$$\frac{T_{exit}}{T(t)} = \left(\frac{P_{exit}}{P(t)}\right)^{\frac{\gamma-1}{\gamma}} \quad (12)$$

This equation can be useful when estimating the temperature of any flare tips and the potential damage they could sustain from low temperature operation.

Calculation of Flame Length

Once the release rates have been calculated they are then used to estimate an expected flame length (C.J.H. van den Bosch, 2005).

$$Flame\ length\ (m) = A \cdot Q^B \quad (13)$$

A and B are constants that are changed depending broadly on the type of material released.

Nomenclature

Symbol	Description	Units
P_{atm}	Atmospheric Pressure	Pa
P_o	Vessel Pressure	Pa
γ	Ratio of Specific Heats (C_p/C_v)	-
m_o	Initial Mass Release Rate	kg/s
A	Area of Leak	m^2
C_d	Discharge Coefficient	-
C_v	Discharge Coefficient for Valve in UNISIM	-
v_o	Specific Volume	m^3/kg
V	Volume	m^3
n	Number of Moles	moles
R	Gas Constant	$m^3PaK^{-1}mol^{-1}$
T	Temperature	K
z	Compressibility Factor	-
ρ	Density	kg/m^3
g	Acceleration due to Gravity	m/s^2
h	Height of Liquid	m
P_{exit}	Pressure at Exit	Pa
P_{back}	Back Pressure	Pa
Q	Release Rate (at time t)	kg/s
Q_o	Initial Release Rate	kg/s
T	Time Elapsed	s
M	Total Mass Inventory Released	kg