

THEORY

DISCHARGE SCENARIOS

DATE: December 2023

DISC contains models for calculating continuous and instantaneous discharge from a vessel or short pipe. The four sub-models are (a) orifice model (from a vessel leak); (b) short-pipe model; (c) instantaneous model for catastrophic rupture of a vessel; and (d) venting of vapour from a tank during a filling operation. The short-pipe model also allows for the presence of a pump, control valve or compressor.

Reference to part of this report which may lead to misinterpretation is not permissible.





No.	Date	Reason for Issue	Prepared by	Verified by	Approved by
1	Oct 2005	SAFETI NL 6.5	Mike Harper	Oke and Witlox	
2	Jan 2010	Phast 6.6	Jan Stene		
3	April 2011	Phast 6.7	Jan Stene		
4	Aug 2014	SAFETI-NL 6.x	Stene and Witlox	Oke	
5	Nov 2015	SAFETI-NL 7.x	Stene		
6	Oct 2017	Safeti-NL 8.0	Stene		
7	May 2021	Apply new template	D. Vazier		
8	July 2022	Version update	David Worthington		

Date: December 2023

Prepared by: Digital Solutions at DNV

© DNV AS. All rights reserved

This publication or parts thereof may not be reproduced or transmitted in any form or by any means, including copying or recording, without the prior written consent of DNV AS.



ABSTRACT

This report describes the suite of instantaneous and continuous (initial rate) discharge scenarios (DISC) within the software packages Phast and Safeti. The suite comprises four generalised models:

- Orifice model
- Short pipe model
- Instantaneous model
- Vapour vent model

These models describe the expansion from storage conditions to a vessel orifice or short pipe exit. The subsequent expansion to atmospheric conditions is described in the ATEX model. For each of the models, the underlying theory is presented, and a brief indication of how that theory is applied to obtain a solution. The individual scenarios for each of the models are described in detail.

This report also describes an extension of the short-pipe model to allow for the presence of a pump, control valve and compressor at the upstream end of the pipe.

Table of contents

ABSTRACT.....	I
1 INTRODUCTION.....	1
2 ORIFICE MODEL.....	2
2.1 Inputs and Outputs	2
2.2 Model Theory	2
2.3 Method of solution	5
2.4 Use of Bernoulli's Equation	5
3 SHORT PIPE MODEL.....	6
3.1 Inputs and Outputs	6
3.2 Model Theory	7
3.3 Method of Solution	12
4 FIXED FLOW RATE MODELS.....	13
4.1 Introduction	13
4.2 Pumps and compressors - prescribed accidental flow rate	13
4.3 Control valve (vapour and liquid releases)	14
4.4 Testing and verification	20
5 INSTANTANEOUS MODEL.....	1
5.1 Inputs and Outputs	1
5.2 Model Theory	1
6 VAPOUR VENT MODEL.....	3
6.1 Inputs and Outputs	3
6.2 Model Theory	4
7 VERIFICATION.....	6
8 FUTURE DEVELOPMENTS.....	7
APPENDICES.....	2
NOMENCLATURE.....	29
REFERENCES.....	32

1 INTRODUCTION

Hazardous chemicals are frequently stored in vessels. Following a leak in the vessel or in a pipe attached to the vessel, a discharge will occur to the atmosphere. The model DISC is a suite of instantaneous and continuous discharge models. The continuous (non-time varying) models predict the (typically worst-case) initial discharge rate and the release duration if the discharge were to be sustained at this rate.

There are four different models:

- Orifice model. Continuous release rate from a vessel orifice.
- Pipe model. Initial release rate from a short pipe connected to a vessel (including through a relief valve or rupture disk).
- Instantaneous model. The release resulting from a catastrophic rupture of a vessel.
- Vent from vapour space model. Release resulting from a venting of a vapour space during a filling operation.

For each of these (apart from the vapour space model), a subsequent call is made to ATEX to model the final expansion to ambient conditions (e.g. from the vessel orifice or pipe exit). The ATEX model theory document describes this final stage of expansion for all models.

The DISC suite of discharge models is currently included in the Phast consequence modelling package. Note that DISC is applicable only for the scenarios as indicated above and separate discharge models exist in Phast for other discharge scenarios. This includes the model TVDI for time-varying releases from orifices and short pipes. It also includes the models PIPEBREAK and GASPIPE for time-varying releases from long pipelines filled with superheated liquid or vapour.

The orifice and pipe models described above calculate accidental release rates based on the user supplying the stagnation pressure and temperature in the vessel. An extension of these DISC models has been developed for application to pumps, control valves and compressors. For these cases the user will specify a fixed flow rate together with stagnation conditions during normal operation prior to any accident taking place.

This document describes the DISC theory - model input, model output, model theory, and method of solution. Chapter 2 includes the mathematical model for the orifice leak model, Chapter 3 describes the short pipe models, while the "Fixed flow rate" scenarios are covered in Chapter 4. The theory of the instantaneous and vent from vapour space models are given in Chapter 5 and Chapter 6, respectively. Chapter 7 discusses the verification of the DISC model, while the reader is referred to the DISC validation manual¹

¹ for validation of DISC against experimental data. Chapter 8 summarises future developments.

2 ORIFICE MODEL

This continuous (not time-varying) model simulates the release from a small orifice in a vessel. It is an initial-rate discharge model, which predicts the worst-case initial discharge rate and the duration associated with this discharge rate. The chemical stored in the vessel may be vapour, liquid or two-phase.

2.1 Inputs and Outputs

The inputs required by the orifice model are as follows:

- vessel storage data:
 - two of the following: storage pressure P_{st}^{*1} ; storage temperature T_{st} (K); mass liquid fraction η_{st} (-)
 - inventory M_{st} (kg); this is the total chemical mass (vapour + liquid) stored in the vessel
 - scenario flag (used for 2-phase releases only: preferred liquid leak, preferred vapour leak, 2-phase leak)
- (case of liquid storage) sum (ΔH ; m) of liquid head (vertical height between the orifice and the top of the liquid) and pump head².
- orifice area A_o (m²)
- flags
 - flashing suppression flag (to force no change in phase)
 - release phase for 2-phase storage (liquid, vapour, 2-phase)
- (case of > 0) fixed duration (s). Allows a fixed-duration run where orifice diameter is scaled to match required mass release rate

The model returns the following outputs:

- release rate Q (kg/s)
- release duration t_{rel} (s)
- orifice pressure P_o (Pa)
- orifice temperature T_o (K)
- orifice mass liquid fraction (η_{Lo})
- orifice velocity u_o (m/s)
- discharge coefficient C_D (-)

2.2 Model Theory

The orifice model is illustrated in Figure 1, and describes the expansion from pre-release conditions to the orifice. The pre-release or initial conditions are determined from the user specified storage conditions according to the scenario and other settings. Expansion from the orifice to atmospheric conditions is handled by the ATEX (Atmospheric Expansion) model.

¹ For liquids, the specified storage pressure corresponds to the pressure at the top of the liquid.

² The leak scenario is sometimes used to simulate small leaks from pipes with an upstream pump.

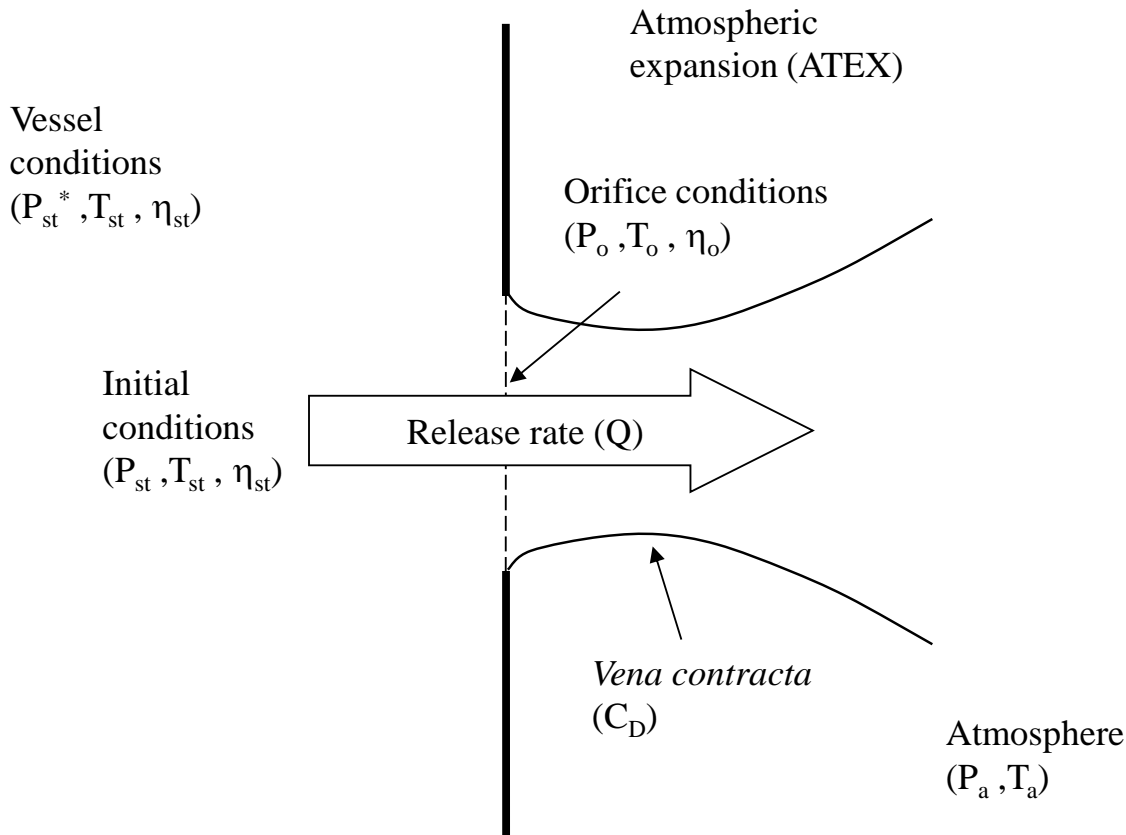


Figure 1. Orifice model

For 2-phase storage, the material can be released as either liquid (orifice below the liquid level) vapour (orifice above liquid level), or 2-phase ('champagne effect' where the vessel is homogenous 2-phase). This is indicated by an input flag.

For liquids, or 2-phase storage to be released as liquid, any liquid head is added to the storage pressure. In these circumstances the initial pre-release state is:

$$P_{st} = P_{st}^* + \rho_L(P_{st}, T_{st})g\Delta H, T_{st}, \eta_{st} \quad (1)$$

The liquid density ρ_L is taken to be that at the top of the liquid³. The following equations are used to determine the orifice conditions. By conservation of energy assuming initially the material is stagnant:

$$h(P_{st}, T_{st}, \eta_{st}) = h(P_o, T_o, \eta_o) + \frac{u_o^2}{2} \quad (2)$$

By conservation of entropy:

$$s(P_{st}, T_{st}, \eta_{st}) = s(P_o, T_o, \eta_o) \quad (3)$$

Note that during this isentropic expansion to the orifice, materials which are initially pure vapour or liquid can be forced to remain so by setting the model input 'Phase change upstream of orifice'. The default setting is 'Disallow liquid phase change', also referred to as the 'metastable liquid' approach. The assumption is that there is insufficient time for changes in phase before the material reaches the orifice⁴.

³ This will underestimate the liquid density ρ_L but the difference will be negligible for common ranges of ΔH

⁴ For large degrees of superheat, this may not be the case as flashing can be observed inside the orifice. However as part of the droplet modelling JIP the metastable liquid assumption was shown to provide accurate results for a relative large range of superheats; see Droplet Size validation Document (Phast Technical Documentation) for details.

The orifice pressure P_o equals the ambient pressure in case of unchoked flow, and is determined from the choke pressure in case of choked flow

$$P_o = \max [P_a, P_c] \quad (4)$$

Here P_c is the choke pressure at the orifice and is defined as the pressure at which the mass flux, G_o , through the orifice is maximised⁵:

$$G_o = \frac{u_o}{v_o} \quad (5)$$

The specific volume is calculated as:

$$v_o = \frac{\eta_o}{\rho_{Lo}} + \frac{(1-\eta_o)}{\rho_{Vo}} \quad (6)$$

The mass release rate, Q^* (kg/s) is then⁶:

$$Q^* = A_o G_o \quad (7)$$

This represents an idealised flow rate, but the frictional effect of convergent flow at the orifice (as represented by the *vena contracta*) effectively reduces this. The convention is to achieve this by reducing orifice cross-sectional area ($A_v < A_o$). The ratio of this reduction is the discharge coefficient, C_D .

$$A_v = C_D A_o \quad (8)$$

$$Q = A_v G_o$$

The method used to calculate the discharge coefficient C_D is included in Appendix B, with values in the range 0.6 to 1. The former value is always used for pure liquids at the orifice.

Finally the release duration, t_{rel} , is

$$t_{rel} = \frac{M_{st}}{Q} \quad (9)$$

For fixed duration runs (*i.e.* where the user input fixed duration > 0) orifice diameter is allowed to vary such that the release rate is sufficient to discharge the inventory in the specified time. As orifice state and mass flux are independent of orifice diameter⁷, we may calculate G_o and C_D as described above, then use Equation (9) to determine release rate Q , and Equation (8) to determine vena contracta diameter.

⁵ VERIFY. To compare with analytical solution (ideal gases), *e.g.* PBRK.

⁶ IMPROVE. Note that for all vapour discharges, the inventory and duration are likely to be overestimates, and this applies for all DISC models. In addition, by releasing the entire inventory as a vapour stream under MC model we effectively release material of a different composition. Ultimately we need to know liquid fraction to specify storage (VI2994, 2991).

⁷ IMPROVE. This is not the case in case of the Phase III JIP droplet size correlation (non-default in Phast), and it will then become necessary to iterate on ATEX.

2.3 Method of solution

The sequence of steps used to determine the orifice conditions is:

1. For a given P_o , temperature and liquid fraction are determined from the isentropic-expansion Equation (3), as described in Appendix A.1.
2. Calculate orifice velocity from conservation-of-energy Equation (2)
3. Calculate the mass flux from Equation (5)
4. The orifice pressure is iterated until the mass flux is maximised, and P_o set according to Equation (4). Normally $P_o = P_a$ for liquids^{8,9}.
5. Calculate C_D and modified Q and A_v from Equation (8)
6. Calculate release duration from Equation (9)

2.4 Use of Bernoulli's Equation

This option is recommended for incompressible liquid flow. Furthermore, occasionally a liquid-liquid isentropic expansion produces unphysical results, causing a temperature increase between the storage and orifice. This arises due to the shape of the liquid entropy curves for saturated liquids at close to the critical pressure. Under these circumstances Bernoulli's equation for incompressible fluids is used to calculate orifice velocity:

$$u_o^2 = 2 \frac{(P_{st} - P_a)}{\rho_{Lst}} \quad (10)$$

We determine orifice state as for the standard model, except we allow no temperature drop ($P_o = P_a$; $\eta_o = 1$; $T_o = T_{st}$). Thus we are assuming negligible pressure effects on liquid density. Steps 2, 3 and 4 in the above algorithm become:

2. Calculate orifice velocity from Equation (10)
3. Set orifice state
4. Calculate mass flux from Equation (5)

⁸ IMPROVE. In fact the mass flux at $P_o = P_a$ and $P_o = P_a + 1 \times 10^4 \text{ N/m}^2$ are calculated, and the one that yields the greatest flux is used. No attempt is made to converge on a maximum.

⁹ IMPROVE. This assumption may not be tenable for flashing liquids with bubble point pressures (P_b), along a given isentrope, higher than P_a . These liquids will "choke" at a pressure (P_c) corresponding to the pressure at which the discharge rate is maximum (see the discussion on "choked flow" in section 3.2.2). A good approximation to P_c is the bubble point pressure along the isentrope (i.e. $P_b(s_{st})$). Note: for liquids $P_b(s_{st}) \approx P_b(T_{st})$.

3 SHORT PIPE MODEL

This continuous (non-time varying) model describes the release from a short pipe attached to a vessel. It can be used to model the full-bore rupture of such a pipe, or alternatively it can be used to model discharge through relief valves or rupture disks. In the latter two cases, the pipe represents the valve tailpipe, while the relief valve itself is represented by a constricted (*i.e.* of smaller diameter than the pipe) orifice at the junction between the vessel and pipe.

3.1 Inputs and Outputs

The inputs required by the pipe model are as follows:

- vessel data:
 - two of storage pressure P_{st}^* (Pa) at the top of the liquid; storage temperature T_{st} (K), or mass liquid fraction η_{st} (-)
 - inventory M_{st} (kg). This input is the inventory inside the upstream vessel. The model also accounts for the fluid mass in the pipe, and the total system inventory is thus the sum of the input vessel inventory and the calculated pipe mass.
 - liquid head ΔH_L (m)
- pipe data:
 - pipe entrance diameter $D_{constriction}$ (m)
 - pipe inner diameter D (m)
 - pipe surface roughness z_0 (m)
 - pipe length L_p (m)
 - pump head ΔH_P (m)
- pipe fittings and bends:
 - frequency (/m) of three valve types: excess flow (f_1), non-return (f_2), and shut-off (f_3) valves
 - number of velocity head losses K_1 , K_2 , K_3 for the three valve types
 - frequency (/m) of pipe couplings (f_{coup}), junctions (f_{unc}) and bends (f_{bend})
- ambient data
 - pressure P_a
 - temperature T_a
 - relative humidity r_h
- scenario data:
 - scenario flag (see below)
 - (relief-valve scenario) ratio of non-equilibrium to equilibrium flow rate R_{neq} (m^{-1})
 - (disk rupture scenario) critical pressure P_{drcrit} (Pa)

The model returns the following outputs:

- pipe exit state
 - pressure, P_e (Pa)
 - temperature T_e (K)
 - mass liquid fraction (η_e)
- release rate, Q (kg/s)
- release duration, t_{rel} (s)
- pipe exit velocity, u_e (m/s)
- discharge coefficient, C_D (-)

3.2 Model Theory

The pipe model is illustrated in Figure 2, and models the release from a short pipe attached to a vessel. At the junction between the vessel and pipe is a constricting orifice ($A_o \leq A_p$). Expansion from the pipe exit to ambient conditions is handled by the ATEX model.

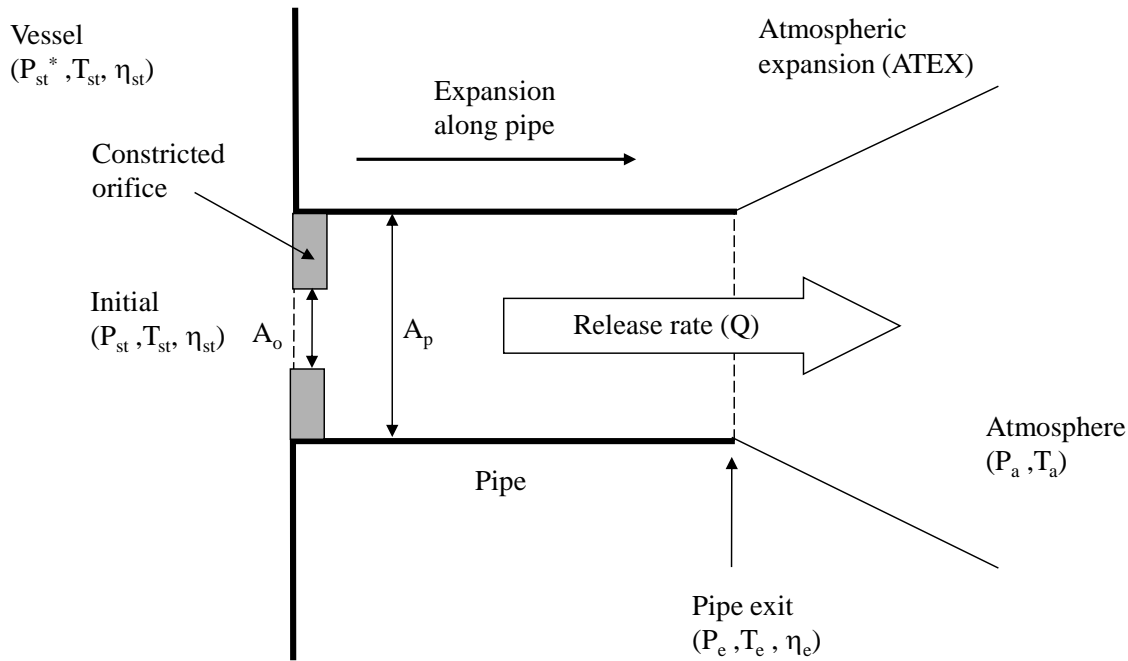


Figure 2. Pipe model

The model assumes the following:

1. At the pipe entrance, the material state is the same as in the bulk vessel (*i.e.* $P_{st}, T_{st}, \eta_{st}$)¹⁰, with P_{st} updated to account for liquid head.
2. Mass flow is conserved along the pipe (*i.e.* velocity at the pipe entrance > 0)
3. Energy is conserved along the pipe, with no heat transfer through the pipe wall.
4. Momentum is conserved along the pipe
5. The cross-sectional area of the pipe is constant along the pipe.
6. Flow lines are parallel at the pipe exit and thus $C_D = 1$.

3.2.1 Scenarios

As with the orifice model, the first stage is to translate the user-specified storage conditions into the initial pre-release conditions at the pipe entrance, according to the model scenario. There are four basic scenarios covered by the pipe model:

Line rupture

Discharge from a vessel through a horizontal short pipe with a full-bore rupture. For 2-phase storage, the material can be released from the vessel as either liquid (pipe entrance below the liquid level) vapour (pipe entrance above liquid level), or 2-phase ('champagne effect' where the vessel is homogenous 2-phase). This is indicated by an input flag. The orifice at the entrance to the pipe is assumed to be the diameter of the pipe ($A_o = A_p$). There may be a pump at the pipe entrance, with a specified pump head ΔH_p .

Relief valve

¹⁰ JUSTIFY. This is the only assumption by which the model makes sense, though its validity is questionable. How can there have been an increase in velocity (see assumption 2) between the stagnant vessel interior and the pipe entrance without a pressure drop? To avoid this would require consideration of pipe entrance (orifice) pressure, P_o , and an additional expansion from P_{st} to P_o .

A relief valve at the top of a vessel (Figure 3) lifts due to overpressuring of a large vapour-space vessel, or liquid swelling of a small vapour-space vessel. The discharge occurs through the constricting relief valve at the entrance to the pipe (with orifice area $A_o \leq A_p$) and then along the length of a short tailpipe. For 2-phase storage, the material can be released from the vessel as either vapour (overpressuring of a large vapour space vessel) or as a homogeneous 2-phase¹¹. Liquid vessels cannot use this scenario.

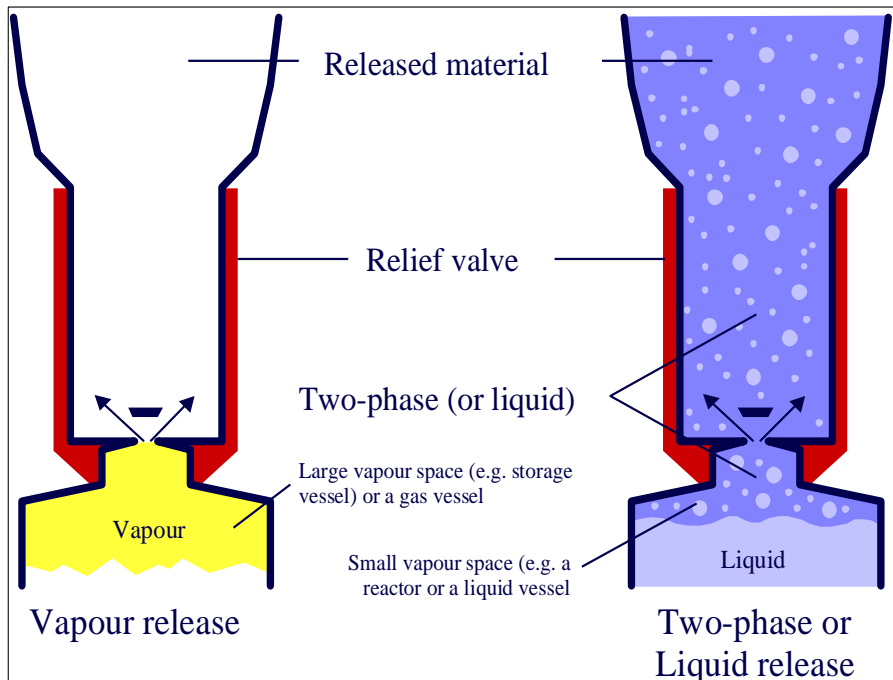


Figure 3. Relief valve scenario.

The relief valve is modelled as a short tailpipe after an constricted orifice. Overpressuring results in a vapour discharge (left), whereas liquid swelling (right) results in a liquid or two-phase discharge.

Disk rupture

This scenario (Figure 4) models the release through a burst rupture disk and along a short tailpipe. The release can be caused either by overpressuring of a large vapour space vessel (storage disk rupture) or liquid swelling or over-filling of a small vapour space vessel (reactor disk rupture). Discharge occurs through the disk seat (assumed not to be constricting, $A_o = A_p$). For 2-phase storage, the material can be released from the vessel as vapour (overpressuring of a large vapour space vessel) or as a homogeneous 2-phase¹². Liquid vessels cannot use this scenario.

¹¹ IMPROVE. It would be possible to have logic determining which phase was released based on the liquid fraction (e.g. > 0.95 was by definition a small vapour space and released 2-phase). However, this would require exposure of liquid or volume fraction in the interface.

¹² If the storage pressure is less than a specified threshold value ($P_{st} < P_a + P_{crit}$) this will be modelled as a vapour release.

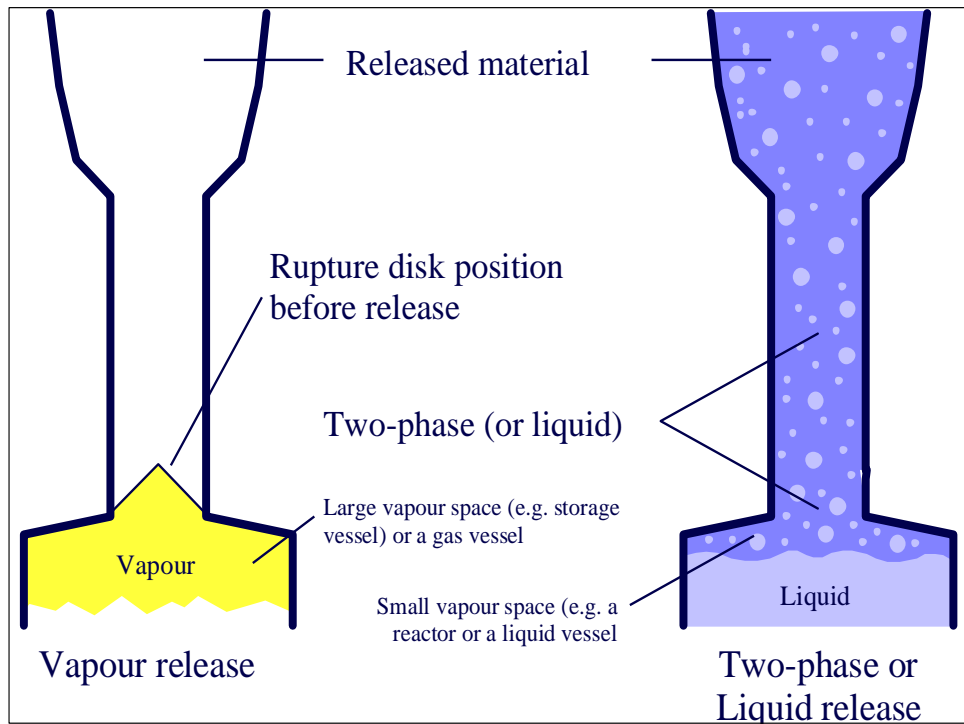


Figure 4. Rupture disk scenario.

Vapour and 2-phase discharges occur for as for the relief valve scenario, but the disk seat is the same diameter as the tailpipe pipe.

3.2.2 Model Development

As for the orifice model, for liquid releases (*i.e.* line rupture scenario only) the storage pressure is increased by the total head ($\Delta H = \Delta H_L + \Delta H_p$)¹³ as described for the orifice model (1). The storage temperature is kept constant. No head is added for vapour or 2-phase releases.

The basic conservation equations (mass, energy, momentum) for a differential length of pipe, dl , are:

$$\frac{dG}{dl} = 0 \quad (11)$$

$$0 = \frac{dh}{dl} + u \frac{du}{dl} \quad (12)$$

$$dP + G^2 dv = -\frac{4\tau_o}{D} dl \quad (13)$$

where τ_o is the shear stress at the pipe wall opposing the flow; G is the mass flux through the pipe; v is the specific volume; and D the diameter of the pipe. Thus the flow is adiabatic.

Analysis

The Fanning friction factor, f , is defined as:

¹³ IMPROVE. For full bore line ruptures, pump head should probably be disallowed (VI2466).

$$f = \frac{2\tau_o v}{u^2} \quad (14)$$

Eliminating τ_o from Equation (13) gives:

$$dP + G^2 dv = -2 \frac{fG^2 v}{D} dl \quad (15)$$

Dividing the momentum equation (15) through by G^2/v gives:

$$dF = \frac{dP}{G^2 v} + \frac{dv}{v} = -\frac{2f}{D} dl \quad (16)$$

We now integrate along the pipe from the exit to the initial pressure and derive a dimensionless expression for the frictional resistance for the whole pipe length¹⁴:

$$F_{friction} = -\frac{4}{D} \int_{L_p}^0 f dl = \frac{2}{G^2} \int_{P_e}^{P_{st}} \frac{dP}{v} - 2 \ln \left(\frac{v_e}{v_{st}} \right) \quad (17)$$

The integral $\int f dl$ is necessary, as f is not constant along the pipe due to the presence of fittings, valves, etc. Note that this integral is not computed, but its value $F_{friction}$ is determined empirically from model inputs (see below).

Evaluation of the right hand side of Equation (17) given G requires that we know v as a function of P . The energy at the entrance to the pipe is given by:

$$E_i = h_{st} + \frac{(Gv_{st})^2}{2} \quad (18)$$

Where E_i is the initial energy, and h_{st} and v_{st} the known initial specific enthalpy and specific volume at stagnation conditions ($P_{st}, T_{st}, \eta_{st}$). We now determine the state at any given P_e by applying conservation of energy, by doing an isoenergetic expansion to P_e ($h + \frac{1}{2}u^2 = \text{constant}$) according to the method described in Appendix A.2. From this v_e can be determined using standard equation of state methods.

Choked flow

At the pipe exit the flow may be choked such that $P_e = P_c > P_a$ with P_c as the choke pressure. The choke condition is best understood by rewriting Equation (15) using $du = Gdv$, and $G = u/v$:

$$\frac{dP}{dl} \left(1 + G^2 \frac{dv}{dP} \right) = -2 \frac{fG^2 v}{D} \quad (19)$$

As $dv/dP \rightarrow -1/G^2$, then $dP/dl \rightarrow -\infty$. It is not possible to go beyond this point, and therefore if this condition is satisfied it must be at the pipe exit. The condition for the choke is therefore

$$\frac{dv}{dP} = -\frac{1}{G^2} \quad (20)$$

From Equation (16) we can therefore say that at the choke $dF/dP = 0$. It is this condition used in the model to determine the choke pressure.

Pipe frictional resistance

¹⁴ Note this includes an additional $\times 2$ factor, corresponding with the PHAST 6.4 model (has $4fL/D$ term, etc). This formulation effectively decreases the importance of frictional terms not subject to this multiplier – valves, etc (see below).

Pipe frictional resistance $F_{friction}$ is calculated from model inputs according to empirical correlations in the literature. It is expressed as a sum of contributions from pipe walls, fittings and valves, and losses on entrance to the pipe:

$$F_{friction} = F_{wall} + F_{fit} + F_{valve} + F_{entry} \quad (21)$$

The contribution of the pipe walls is based on the Fanning friction coefficient, f , for a straight pipe of roughness z_0 ¹⁵ from Equation 3.11 in Coulson and Richardson (1977)²:

$$F_{wall} = \frac{4fL}{D} (1 + DL_e f_{bend}) \quad (22)$$

$$f = \frac{2}{[3.2 - 2.5 \ln(z_0/D)]^2} \quad (23)$$

Note the first part of the right-hand expression is the equivalent to the integral of Equation (17) for a uniform length L of straight pipe. The second is a correction to account for the presence of pipe bends, which are each assumed to add a number, L_e , of pipe diameters (fixed at $L_e = 10^{16}$) to the effective pipe length. f_{bend} is the frequency of (assumed 90°) bends along the pipe. Thus a 10m long, 0.2m diameter pipe with two bends will have an effective length of 14m¹⁷.

The contribution, F_{valve} , of valves is:

$$F_{valve} = \sum_{i=1}^3 N_i K_i \quad (24)$$

N_i is the number of valves of type i , and K_i is the number of velocity heads lost for one valve of type i . Currently 3 types of valves can be specified, conventionally used in PHAST to refer to excess flow ($i=1$), non-return ($i=2$) and shut-off ($i=3$) valves.

The contribution, F_{fit} , of fittings is calculated as in Equation (24), except that the K values are hard-coded¹⁸ in the model ($K_{coup} = 0.04$, $K_{junc} = 1.0$):

$$F_{fit} = N_{coup} K_{coup} + N_{junc} K_{junc} \quad (25)$$

The number of velocity heads lost through entrance to the pipe is taken from Vennard and Street (1982)³, page 536:

$$F_{entry} = \frac{1}{(kC_v)^2} - 1 \quad (26)$$

C_v is the 'coefficient of velocity', and is determined as per the method described later for discharge coefficient in Appendix B. This approach differs from standard literature but is justified in Appendix E. The factor k is used to model the increase in frictional losses on entering the pipe through the constricted orifice of a relief valve. The factor k ¹⁹ is defined as:

$$k = \min \left[R_{neq} \frac{A_o}{A_p}, 1 \right] \quad (27)$$

where A_o and A_p are the cross sectional areas of the relief valve orifice and pipe respectively. The smaller this ratio of areas (*i.e.* the more constricting the orifice), the smaller the discharge coefficient and therefore the greater the frictional losses. R_{neq} is a safety factor to allow for possible under-estimation of the constricting orifice (used to allow for over-drilling in the relief valve scenario). For all apart from the relief valve scenario, orifice and pipe area are equal, and thus $k = 1$.

¹⁵ DOC. See GASPIPE/PIPEBREAK theory manual for some discussion on surface roughness (range of values) and Fanning Friction Factor. See also book by Fannelop and other references.

¹⁶ This value is consistent with Perry and Green (1984), Fig. 5-45 (smooth bend, radius of curvature / pipe diameter ~ 3).

¹⁷ Tabulated values are available, *e.g.* Coulson and Richardson (1977).

¹⁸ Values from page 5-38 of Perry and Green (1984).

¹⁹ JUSTIFY. This is of unknown origin.

3.3 Method of Solution

The overall sequence of steps in solving the pipe model is as follows:

1. Determine initial state according to scenario and other inputs
2. Establish maximum flux, G_{max} , through the pipe according to the orifice model^{20,21}
3. Calculate empirical pipe friction
 - a. Determine coefficient of velocity, C_v , according to the discharge coefficient method.
4. Iterate to find G (where $G_{min} \leq G \leq G_{max}$) such that the empirical and thermodynamically calculated friction along the pipe are equal^{22,23}
 - a. Determine energy of the fluid at entrance to pipe (from initial state and G)
 - b. Solve Equation (17) for pipe friction
5. Perform isoenergetic flash between initial and exit pressures, and determine exit velocity, release rate and release duration.

The core of the pipe model is clearly the solution of Equation (17) for a given flux G . Let I be the integral in Equation (17) required to determine pipe friction:

$$I = \int \frac{dP}{v} \quad (28)$$

$$\frac{dI}{dP} = \rho$$

The differential equation dI/dP is solved by the standard Kutta-Merson numerical method, where $\rho(P)$ is obtained by an isoenergetic expansion from P_i to P . Each step of the solver yields an intermediate pressure P_n ($P_e \leq P_n < P_i$; $n = 1, 2, \dots$) and solution I_n , and from these the total friction along the pipe F_n (between P_i and P_n) can be determined.

The condition for the choke pressure is that $dF/dP = 0$. Therefore once we reach n such that $F_n < F_{n-1}$ we are past the choke. In this case we can approximate the curve of $F = f(P)$ close to the choke by fitting a quadratic to the three points F_n , F_{n-1} and F_{n-2} ; its maximum will therefore represent the choke pressure P_c .²⁴

The algorithm can sometimes (especially for condensing gas releases) take overlarge steps along the pipe, resulting in too low a choke pressure and too high (*i.e.* supersonic) exit velocity. A warning is raised if exit velocity exceeds by 10% sonic velocity for an ideal gas, c :

$$c = \sqrt{\frac{\gamma RT}{M_w}} \quad (29)$$

Where γ = ratio of specific heats, and M_w is the molecular weight.

The mass dM in a pipe segment of length dl is given by

²⁰ A pipe model parameter controls whether the model will cap the flow rate using this orifice calculation, and whether flashing is allowed or suppressed for the orifice model. The pipe model can run in uncapped mode where the orifice flow rate is ignored.

²¹ Note that only the mass flux is used from this calculation: other orifice outputs are ignored apart from in determination of the coefficient of velocity.

²² JUSTIFY If $G > G_{max}$ then P_c was set using some questionable logic (VI5926). We now use P_c at G_{max} .

²³ In SAFETI 6.4, G was determined by interpolation once the value had been bracketed, but this was done wrongly leading to an underestimation in flux (VI3023)

²⁴ This could be evaluated more accurately by converging on the solution using a root finder. However, as the integral has to be calculated anyway, it is much more computationally efficient to use this information to determine the choke rather than nesting inside another iteration loop.

$$dM = \frac{\pi}{4} D^2 \rho(P, T) dl.$$

4 FIXED FLOW RATE MODELS

4.1 Introduction

This chapter deals with situations where the analyst wants to prescribe a fixed flow rate as a model input rather than the flow rate being a model-calculated value as in the previous chapters. The situation of a fixed flow rate known a priori may arise when certain flow control devices are in operation such as pumps, compressors or control valves. The analyst may also want to prescribe the accidental flow rate upfront to study the impact of a release of a given size.

A scenario with a prescribed “accidental flow rate” is described in Section 4.2 for orifice leaks and line rupture scenarios. Here the stagnation pressure or liquid fraction is calculated so as to produce the requested flow rate. Section 4.3 introduces both vapour and liquid short-pipe scenarios with a “control valve” upstream.

4.2 Pumps and compressors - prescribed accidental flow rate

There could be situations where the analyst would like to prescribe the accidental flow rate rather than this flow rate being calculated by the model. This situation is supported by the DISC orifice scenario and the short-pipe scenario (full-bore rupture at end of short pipe). The “prescribed accidental flow rate” scenario may be applied for the following cases:

- The presence of a pump (liquid storage) at the upstream end of a pipe for liquid releases with a fixed flow rate prescribed²⁵.
- A vapour production system (e.g. for control flow system; vapour storage) with a fixed flow rate prescribed. Alternatively the “control valve system” can be applied with the stagnation pressure P_{st} set as the compressor discharge pressure.

The relevant modelling is described here, and key points to note include:

- The prescribed accidental flow rate Q_{fixed} is user input instead of the stagnation pressure P_{st} . The stagnation temperature T_{st} must also be input. Otherwise input data are as for the normal orifice and short-pipe scenarios.
- These calculations can currently only be carried out in pseudo-component (PC) mode

The following will be carried out by the model when prescribing an accidental flow rate:

- For cases with $T_{st} < T_{critical}$ (stagnation temperature less than critical temperature):
 - The program first evaluates the flow rate $Q(P_{sat}(T_{st}))$ based on the saturated vapour pressure presuming both pure vapour initially in the vessel [$Q_{v,sat}$] and pure liquid initially in the vessel [$Q_{L,sat}$], with $Q_{v,sat} < Q_{L,sat}$
 - Cases²⁶:
 - $Q_{fixed} > Q_{L,sat}$: the stagnation state will be liquid. The program will iterate over the stagnation pressure $P_{st} [P_{sat}(T_{st}) < P_{st} < P_{max}]$ at the height of the hole to determine the value for which $Q(P_{st}) = Q_{fixed}$. Here P_{max} is an upper limit²⁷ on the pressure.
 - $Q_{fixed} < Q_{v,sat}$: the stagnation state will be vapour. The program will iterate over the stagnation pressure $P_{st} [P_a < P_{st} < P_{sat}(T_{st})]$ to determine the value for which $Q(P_{st}) = Q_{fixed}$
 - $Q_{v,sat} < Q_{fixed} < Q_{L,sat}$: the stagnation pressure equals the saturated vapour pressure $P_{sat}(T_{st})$ and the stagnation state is two-phase. In this case homogeneously mixed two-phase fluid will be

²⁵ An alternative approach to modelling a pump at the upstream end is described in **Error! Reference source not found.**

²⁶ There are added DISC output to indicate data associated with the specified fixed flow rate, i.e. vapour, liquid or two-phase stagnation state, and the associated stagnation pressure at the height of the hole. In the Phast product implementation, two-phase stagnation states are not allowed, i.e. either vapour (compressor) or liquid (pump) stagnation states.

²⁷ A maximum pressure of 800 bar is imposed; it is considered unlikely that the pressure will be higher than 800 bar when there is a pump operating. Ideally, however, the upper pressure limit should be the pressure at which the liquid turns solid, but this pressure is not available from the Phast property system.

released, and the program will iterate over the stagnation liquid mass fraction η_{st} to determine the value for which $Q(\eta_{st}) = Q_{fixed}$

- b) For cases with $T_{st} > T_{critical}$:
- Release phase will always be vapour
 - Iterate over the stagnation pressure P_{st} to determine the value for which $Q(P_{st}) = Q_{fixed}$, with $P_a < P_{st} < P_{max}$, where P_{max} is an upper limit for the pressure.

4.3 Control valve (vapour and liquid releases)

This section considers the case when a control valve is presumed to be located at the upstream end of a pipe, immediately downstream of a connected vessel; see Figure 5. The user inputs the flow rate and control valve opening during normal operation of the pipeline. Following a full-bore rupture the control valve is assumed to respond in such a manner as to maintain the same flow rate as prior to the rupture. This is achieved by imposing a constriction diameter at the start of the pipe while maintaining a constant upstream pressure P_{st} , and the details of this approach are described in this section.

Note that the control valve scenario is not meant to model actual controller action or the dynamic response of a real system to the closing or opening of a control valve following a disturbance event, i.e. pipe rupture. Instead, the scenario is intended to apply an appropriate constriction so as to satisfy certain user-defined system properties like upstream and downstream pressure, fixed flow rate, and the pipe roughness.

Input data are as follows:

- All data as usual for DISC including upstream pressure P_{st} , temperature T_{st} and pipe length x_B between vessel and rupture location.
- Additional input:
 - o flow controller set-point flow rate Q_{fixed}
 - o (optional input) initial control valve constriction diameter $D_{constriction}$; here the control valve can initially be fully open ($D_{constriction}=D$) or partially closed ($D_{constriction}<D$)
 - o pipe roughness²⁸ z_0

4.3.1 Initial steady-state conditions prior to accidental pipe rupture

Two different cases are considered, i.e. a fully-open control valve ($D_{constriction}=D$) or partially closed ($<D$). For a fully open valve, the modelling is fully consistent with the line rupture scenario (pipe entry force modelling distributed along the pipe). For partially closed valves, two separate stages are considered for expansion from stagnation to downstream-valve conditions (isothermal), and from downstream-valve to pipe exit conditions (conservation of energy).

It can be shown that the final steady-state conditions do not depend on the prescribed value of $D_{constriction}$ prior to the rupture. However the initial state calculations are carried out to ensure no phase changes occur along the pipe, i.e. vapour remains vapour or liquid remains liquid.

Initially fully-open control valve

The following is applied in case the control valve is fully open during normal operation of the pipe:

- For the initial state (prior to the breach) either liquid flow must apply across the entire pipe (no flashing²⁹), or vapour flow applies across the entire pipe. Further details are given below for the vapour and liquid cases.
- If pipe roughness z_0 is specified and the calculated $P(x_B) < P_a$, then issue a model error and terminate the calculations as the specified upstream pressure P_{st} is too low to maintain the specified flow rate Q_{fixed} .
- As part of future development, it may be possible to specify P_B instead of the pipe roughness. We must then have $P_A > P_B > P_a$, and the implied roughness z_0 from the calculated Fanning friction coefficient f is output and to be checked by the user whether reasonable.

Initial liquid state

²⁸ Future development may allow specification of downstream pressure P_B instead of the pipe roughness

²⁹ In reality it is possible for two-phase flow to exist along the length of the process line, but this would not be typically expected for a transport pipeline under typical operating conditions.

Assumptions include:

- The fluid remains pure liquid throughout the pipe³⁰.
- Isothermal conditions prevail along the entire pipeline length
- The liquid density remains constant along the pipe, $\rho_L = \rho_L(P_{st}, T_{st}) = \rho_{Lst}$ along the pipe, i.e. the minor effect of pressure variation along the pipe is ignored³¹.

The initial steady-state conditions are now set as follows:

- Set uniform pipe velocity along pipe from mass conservation: $u = Q_{fixed}/(A_p \rho_{Lst})$
- Analytically solve momentum equation (13):

$$P(x) = P_{st} - 2 \frac{f \rho_{Lst} u^2}{D} x \quad (31)$$

Here x is the distance along the pipe, and D the internal pipe diameter.

- In case the pipe roughness z_0 is specified, the Fanning friction coefficient f is set from z_0 using Equation (23). Future development may allow specification of P_B , and then f (and hence pipe roughness z_0) can be derived from Equation (31) as follows

$$f = \frac{D [P_{st} - P_B]}{2 \rho_{Lst} u^2 x_B} \quad (32)$$

The thus calculated roughness needs to be checked by the user whether it is reasonable. If the calculated $P(x_B) < P_a$, then a model error is issued and the calculations terminated as the specified upstream pressure is too low to maintain the specified flow rate.

Initial vapour state

Use GASPIPE initial solution (isothermal assumption – see Section 2.6 in the GASPIPE theory document⁴). Assuming ideal gas³², the pressure along the pipe during initial steady-state can be calculated by

$$P(x) = \sqrt{P_A^2 - 4 \frac{f R T_{st} (\rho_A u_A)^2}{D \hat{M}} x} \quad (33)$$

Here R is the universal gas constant and \hat{M} is the molecular weight of the gas, whereas the density $\rho_A = \rho_V(P_{st}, T_{st})$ and the velocity at the upstream end of the pipe is given by $u_A = Q_{fixed}/(A_p \rho_A)$

In case the pipe roughness z_0 is specified, the Fanning friction coefficient f is set from z_0 using Equation (23). In case P_B is specified, f (and hence pipe roughness z_0) can be derived from Equation (33) as follows:

$$f = \frac{\hat{M} D (P_{st}^2 - P_B^2)}{4 R T \rho_A^2 u_A^2 x_B} \quad (34)$$

Initially partially-closed control valve

As shown in Figure 5a the overall fluid expansion is considered in two stages:

- From valve constriction area to full pipe area immediately downstream of valve ($P_{st} \rightarrow P_{valve}^{final}$ ³³)
- From full pipe area immediately downstream of valve to the pipe downstream end B ($P_{valve}^{final} \rightarrow P_B$)

³⁰ If $P(x_B) < P_{sat}$, then a model error will be issued and calculations terminated.

³¹ Default EOS behaviour for evaluation of liquid density in DISC and TVDI is saturated liquid density anyway, i.e. pressure-independent liquid density.

³² Non-ideal gas effects as incorporated in the Gaspipe mode are currently not considered since the final steady state is not affected by the initial steady state.

³³ Note that P_{valve}^{final} includes any pressure-recovery effects that may occur downstream of the constriction.

The first stage $P_{st} \rightarrow P_{valve}^{final}$:

- The initial control valve constriction diameter $D_{constriction}$ and normal operating flow rate Q_{fixed} are prescribed. An error is given when the “accidental” throughput (from the standard DISC orifice scenario based on orifice diameter = $D_{constriction}$) is less than Q_{fixed} . This is a necessary but not sufficient requirement due to frictional losses along the pipe.
- Isothermal flow conditions apply during normal operating conditions, so $T_{st} = T_{valve}^{final}$; no phase change occurs (vapour remains vapour, liquid remains liquid²⁹).
- Assume zero initial velocity at the constriction area: $u_{st}=0$.
- Impose conservation of mass and momentum to determine the pressure P_{valve}^{final} [$P_B < P_{valve}^{final} \leq P_{st}$ if P_B specified, and $P_a < P_{valve}^{final} \leq P_{st}$ if roughness z_o specified], liquid fraction η_{valve}^{final} and velocity u_{valve}^{final} .
- Note that the fundamental equations for mass and momentum conservation along the pipe are given in Section 3.2.2 by Equation (11) and Equation (13), respectively.
- The mass flow rate is constant along the pipe, and at the point where the control valve expansion completes, mass conservation may be expressed as

$$Q_{fixed} = \rho(P_{valve}^{final}, T_{st}; \eta_{valve}^{final}) u_{valve}^{final} A_p . \quad (35)$$

- For the short pipe scenario described in Section 3.2.2, the momentum equation (13) is further manipulated and integrated along the pipe to the pipe exit to yield Equation (17). Equivalent considerations are made here, though integrating to the end of the control valve expansion zone rather than the pipe exit, yielding³⁴

$$F_{friction} = F_{entry} = 2 \left(\frac{A_p}{Q_{fixed}} \right)^2 \int_{P_{valve}^{final}}^{P_{st}} \rho(P, T_{st}; \eta_{st}) dP - 2 \ln \frac{\rho(P_{st}, T_{st}; \eta_{st})}{\rho(P_{valve}^{final}, T_{st}; \eta_{valve}^{final})} . \quad (36)$$

The only friction considered here is due to the initial control valve constriction. This initial constriction may be seen as equivalent to the constriction considered for the relief valve scenario described in Section 3. On this basis we therefore adopt the same correlation for the evaluation of the associated friction³⁵ – see Equation (25) and Equation (26).

- If liquid remains liquid ($\eta_{valve}^{final} = 1$) or vapour remains vapour ($\eta_{valve}^{final} = 0$), then Eq. (36) is solved for P_{valve}^{final} and thereafter Eq. (35) is solved to obtain u_{valve}^{final} ; if liquid becomes two-phase [$P_{valve}^{final} = P_{sat}(T_{st})$], a fatal error is issued: “Two-phase effects currently not handled for initial state of control valve scenario”.
- For incompressible liquids³⁶, density is constant and therefore Eq. (36) simplifies and gives this explicit solution for the control valve pressure:

$$P_{valve}^{final} = P_{st} - \frac{F_{entry} Q_{fixed}^2}{2 A_p^2 \rho_{st}} . \quad (37)$$

The second stage $P_{valve}^{final} \rightarrow P_B$:

³⁴ In the derivation of Equation (36) there is an assumption of constant cross-sectional fluid flow area A_p . In reality however, the cross-section flow area varies in the integration from the constricted valve opening to the fully expanded pipe flow.

³⁵ There are questions marks around how the pipe entry friction term is evaluated in the DISC model for relief valve scenarios – see Appendix E.

³⁶ By default liquid density in Phast is evaluated as the saturated liquid density. This means that the liquid density is not pressure dependent but only temperature dependent, and so the liquid density remains constant in the isothermal expansion from pipe upstream to immediately downstream of the control valve.

- Starting from the now known data immediately downstream of the valve, subsequently equations along the pipe can be solved completely analogous as for the above case of a fully-open control valve, presuming no phase change along the pipe.
- For liquid this explicitly means³⁷:

$$P(x) = p_{valve}^{final} - 2 \frac{f \rho_{Lst} u^2}{D} x \quad (38)$$

and

$$f = \frac{D [p_{valve}^{final} - p_B]}{2 \rho_{Lst} u^2 x_B} \quad (39)$$

- For vapour this explicitly means:

$$P(x) = \sqrt{\left(p_{valve}^{final}\right)^2 - 4 \frac{f R T_{st} (\rho_A u_A)^2}{D \hat{M}}} x. \quad (40)$$

and

$$f = \frac{\hat{M} D \left(\left(p_{valve}^{final}\right)^2 - p_B^2 \right)}{4 R T \rho_A^2 u_A^2 x_B}. \quad (41)$$

³⁷ Assume negligible distance between upstream end of pipe to the "final valve" state.

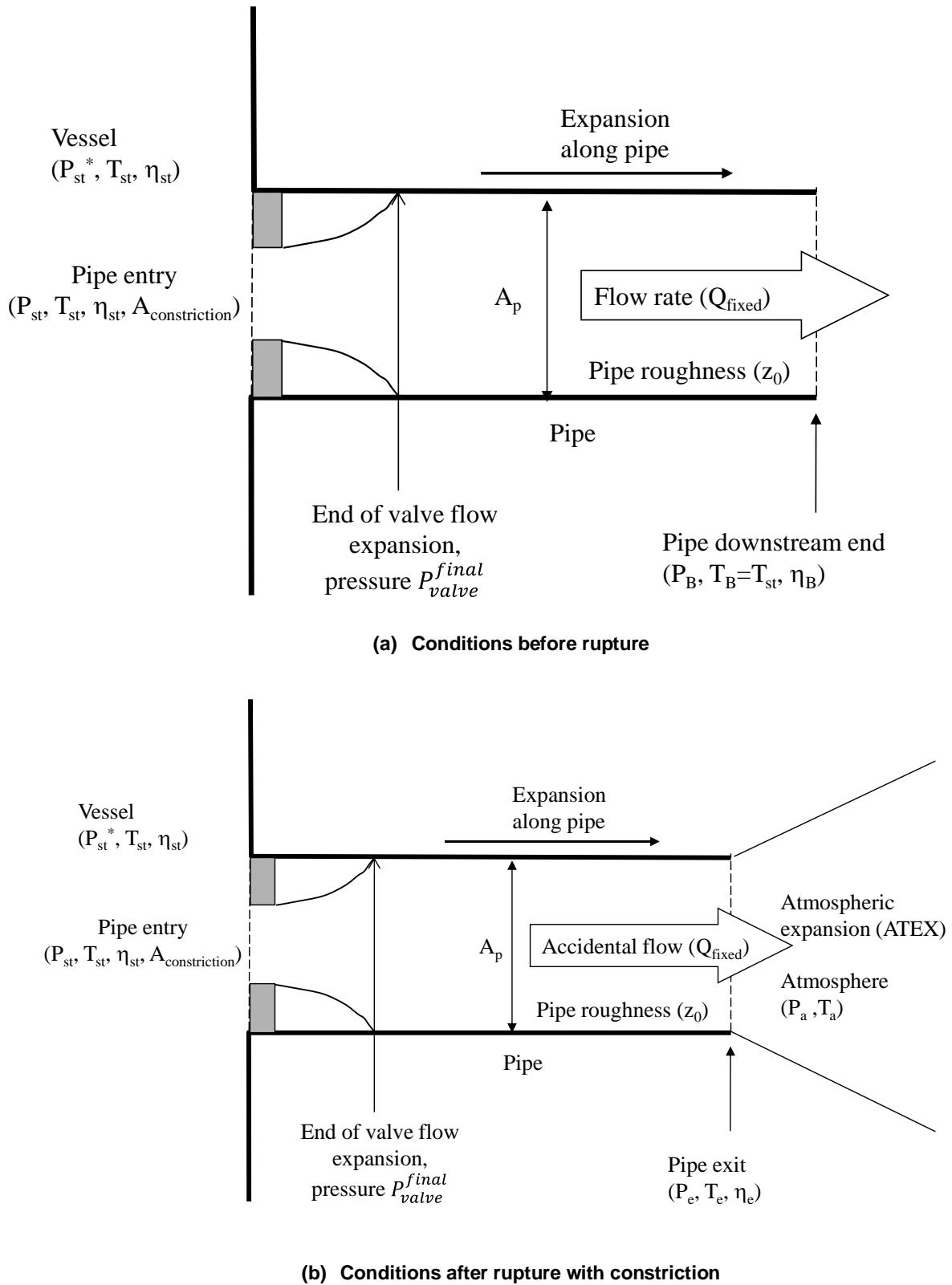


Figure 5. Pipe model with control valve at upstream end

4.3.2 Final steady-state conditions after accidental pipe rupture

We consider the scenario where a full-bore rupture has occurred and that a constricting control valve is in operation during the final steady-state flow in the pipe. The upstream pressure P_{st} and temperature T_{st} remain the same after the rupture, while the control valve is assumed to operate in such a way as to maintain the same flow rate after the rupture, namely Q_{fixed} . In Figure 5b it can be seen that the overall fluid expansion is considered in three stages:

1. From valve constriction area to full pipe area immediately downstream of valve ($P_{st} \rightarrow P_{valve}^{final}$)
2. From full pipe area immediately downstream of valve to the pipe rupture plane ($P_{valve}^{final} \rightarrow P_e$)
3. From the pipe exit to atmospheric pressure ($P_e \rightarrow P_a$)

The final stage 3 is a standard application of the atmospheric expansion model ATEX, so the focus here will be on the first two stages. The key idea is to evaluate data immediately downstream of the valve by using a root solver to find P_{valve}^{final} such that the accidental flow rate equals the prescribed fixed flow rate: $G(P_{valve}^{final}) A_p = Q_{fixed}$, where A_p is the pipe cross-section area and G the flux (kg/s/m^2). The adopted solution method to achieve this consists of the following steps:

1. Given stagnation conditions (P_{st}, T_{st}) and guessing P_{valve}^{final} , determine conditions immediately downstream of the valve [temperature T_{valve}^{final} , liquid fraction η_{valve}^{final} and velocity u_{valve}^{final}] by imposing conservation of energy and conservation of mass (not momentum):

$$h(P_{st}, T_{st}, \eta_{st}) = h(P_{valve}^{final}, T_{valve}^{final}, \eta_{valve}^{final}) + \frac{[u_{valve}^{final}]^2}{2} \quad (42)$$

$$Q_{fixed} = A_p \rho(P_{valve}^{final}, T_{valve}^{final}, \eta_{valve}^{final}) u_{valve}^{final} \quad (43)$$

- In case the conditions immediately downstream of the valve correspond to either pure vapour or pure liquid, the above two equations are solved for T_{valve}^{final} and u_{valve}^{final} . In case these conditions correspond to two-phase conditions, $T_{valve}^{final} = T_{sat}(P_{valve}^{final})$ and the equations are solved for η_{valve}^{final} and u_{valve}^{final} . See Appendix A.2 for further details on the solution to the above equations.
 - Note the assumption that the upstream energy equals the enthalpy, i.e. no kinetic energy so $u_{st}=0$.
2. Solve pipeline equations (assuming iso-energetic thermodynamic trajectory) to determine the mass flow-rate (GA_p) satisfying the system of equations described in Section 3.3 (basically carry out an accidental short pipe calculation but *without the pipe entry friction F_{entry} and with positive velocity u_{valve}^{final}*).

Note that the control valve constriction diameter after the full-bore rupture is not explicitly calculated.

4.4 Testing and verification

To assess the model implementation of the control device logic some targeted testing has been carried out and is described in this section. The case of a line-rupture scenario is considered involving a 50 m long pipe with 6" diameter (0.154m) and pipe roughness 457 μ m. The tests include cases with both ethane and propane stored at a temperature of 20°C. Further key scenario data is given in the subsections below.

4.4.1 Pump and compressor tests

A set of tests with pump and compressor action for ethane pipes has been carried out and is based on the modelling as described in Section 4.2. The specified fixed flow rate is varied between 0.01 kg/s and 400 kg/s. The stagnation pressure is calculated based on the specified input fixed flow rate³⁸.

The storage pressure, storage liquid fraction and pipe exit pressure are plotted in Figure 6 as a function of the fixed flow rate. We note that:

- Flow rates up to around 110 kg/s are achieved with storage pressures giving a gaseous fluid state; this regime corresponds to compressor action.
- Flow rates from around 110 kg/s up to around 165 kg/s are achieved with saturated storage pressure and liquid fractions increasing from 0 to 1. In the product implementation two-phase storage is disallowed and an error would therefore be produced for flow rate inputs in this range.
- Flow rates above 165 kg/s are achieved with storage pressures giving a liquid fluid state; this regime corresponds to pump action.

³⁸ MDE_Test_Disc_ACC-ethane_vary_fixedRate.xls

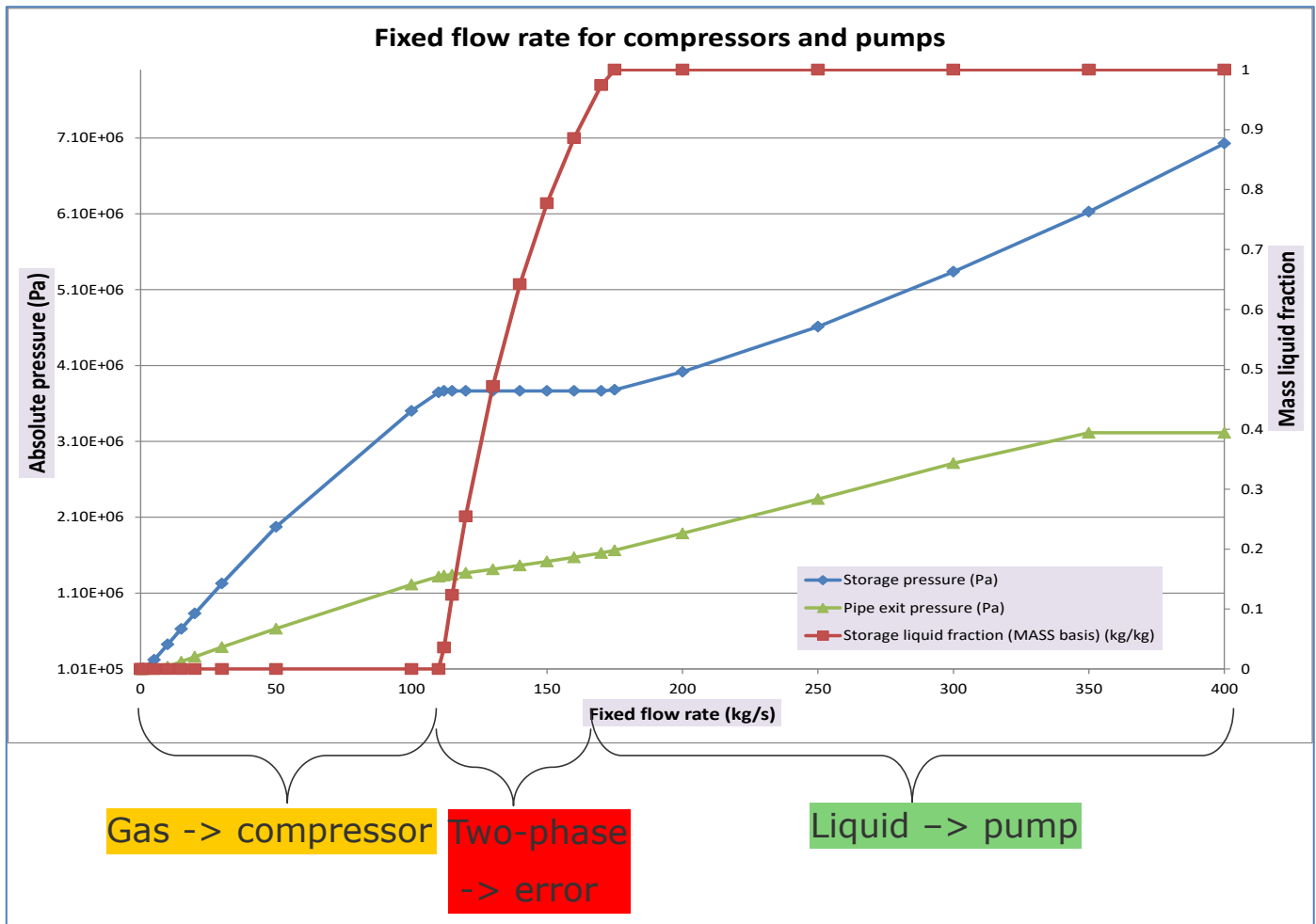


Figure 6: Pump and compressor action for varying fixed flow rates.

4.4.2 Control valve tests

In this section we turn our attention to line rupture scenario with a control valve present at the upstream end of the pipe. A vapour pipe³⁹ with ethane stored at 10 bara and 20°C and a liquid pipe⁴⁰ with propane stored at 40 bara and 20°C were both studied. The impact of varying the fixed flow rate specified for control valve scenarios was studied with results shown in Figure 7 and Figure 8 for the vapour and liquid cases, respectively. Key observations:

- Figure 7 and Figure 8 show that the maximum fixed flow rate happens when there is no pressure drop across the control valve.
- Figure 7 shows that there is a transition from unchoked to choked flow when the fixed rate exceeds around 8 kg/s.
- Figure 8 shows results for the propane pipe. The storage fluid phase and the phase throughout the pipe during normal flow is liquid for all fixed flow rates. However, after rupture the situation changes:
 - The liquid flashes across the control valve up until about 100 kg/s
 - The liquid flashes in the pipe up until about 250 kg/s
 - For flow rates higher than around 250 kg/s the fluid remains liquid throughout the pipe after rupture
- There is an upper limit on what fixed flow rate would give a successful model run. Specifying a too high flow rate will give one of the following two model errors:

³⁹ MDE_Test_Disc_CV-ethane_vary_fixedRate.xls

⁴⁰ MDE_Test_Disc_CV-propane_vary_fixedRate.xls

- o DISC error 40:

"Pressure after rupture downstream of control valve, %1%Pressure%, higher than pipe inlet pressure - too high fixed flow rate specified".

This means that the specified flow rate cannot be maintained after the rupture as there cannot be a pressure increase from stagnation to after the control valve.

- o DISC error 41:

"Phase change along pipe not allowed during normal flow for control valve scenario"

This means that the required pressure drop to satisfy the specified fixed flow rate is so high that the pressure at the pipe end is not high enough to maintain liquid phase.

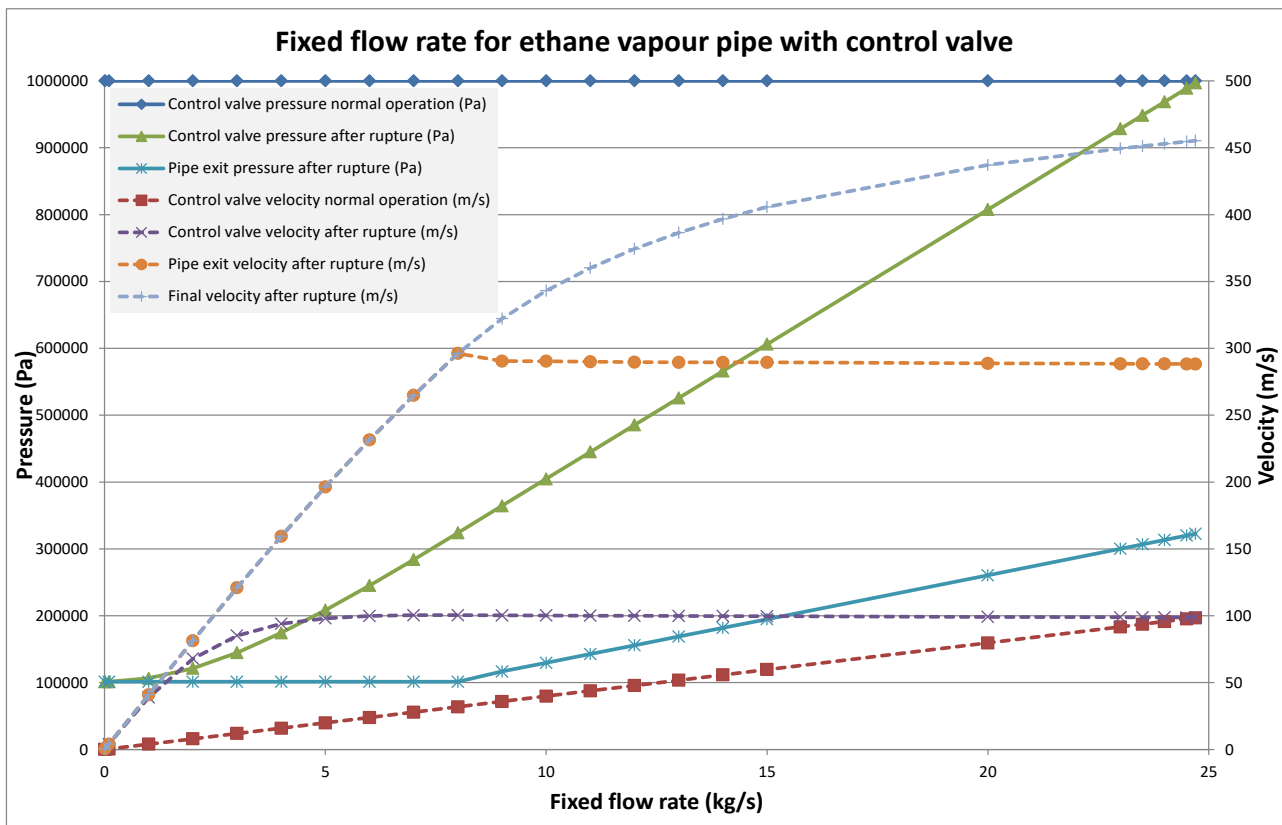


Figure 7: Effect of increasing fixed flow rate for an ethane vapour pipeline with control valve.

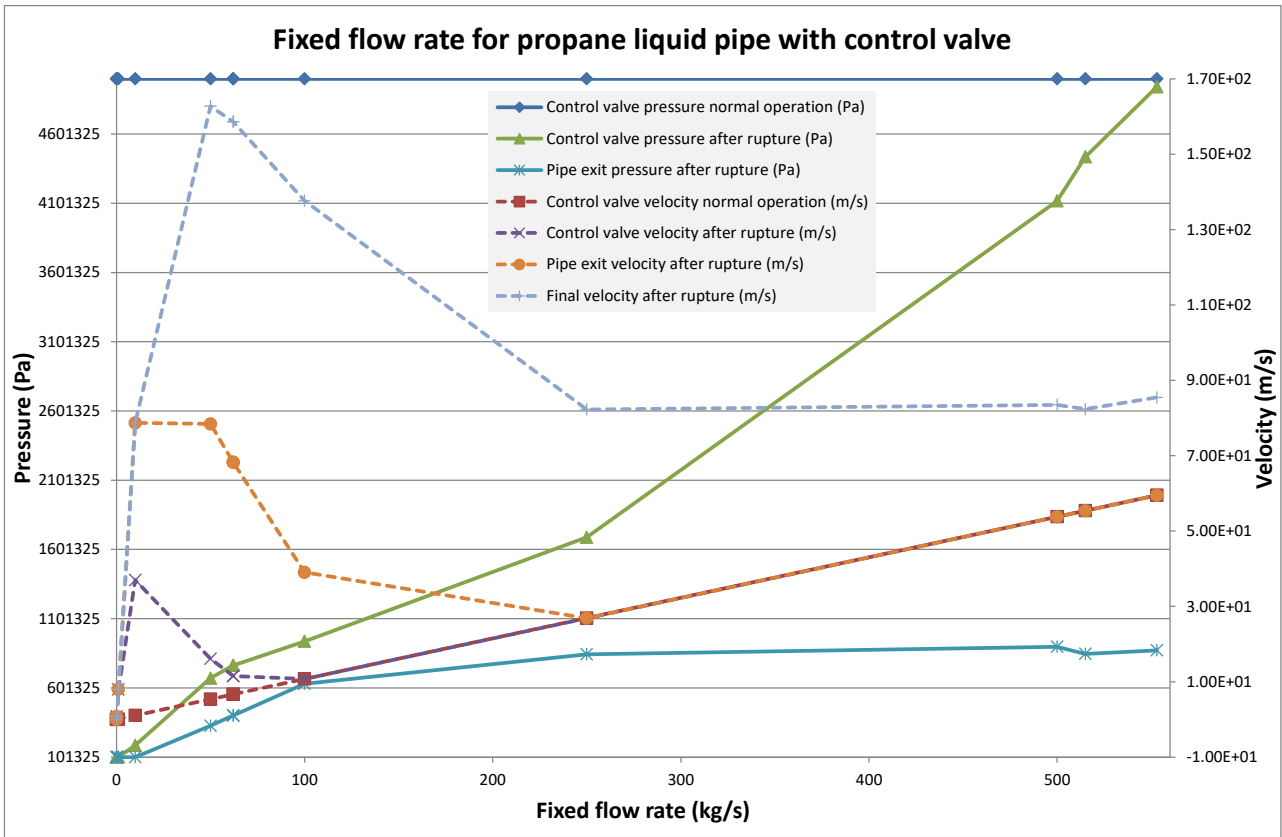


Figure 8: Effect of increasing fixed flow rate for a propane liquid pipeline with control valve.

5 INSTANTANEOUS MODEL

5.1 Inputs and Outputs

The inputs required by the instantaneous model are:

- Storage pressure, P_{st} (Pa)
- Storage temperature, T_{st} (K), or mass liquid fraction, η_{Lst} (-)
- Liquid head, ΔH_L (m)

The following are returned from the model:

- Pre-release pressure, P_i (Pa)

5.2 Model Theory

This model is used to describe the instantaneous release of an entire vessel inventory due to, for example, a catastrophic rupture. Essentially the model comprises only one stage: the expansion from initial conditions to atmospheric (Figure 9). As such, it is described largely in ATEX. Note that the ATEX expansion is done differently to that for the continuous models.

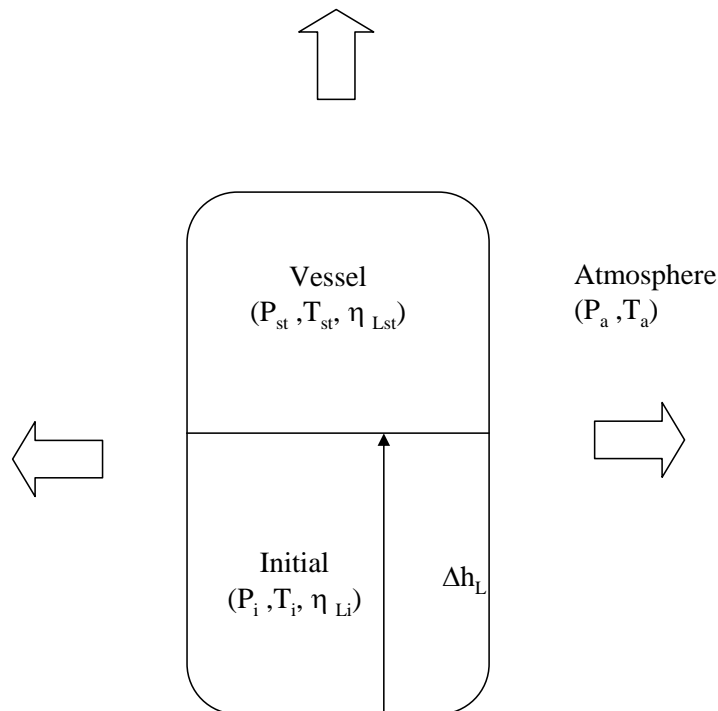


Figure 9. Instantaneous model

The only aspect of the model not described by atmospheric expansion is the determination of the initial state from the user-specified storage state. For 2-phase storage the liquid phase is released, and liquid head is added for all but pure vapour vessels^{xii}:

$$P_i = P_{st} + \rho_L(P_{st}, T_{st})g \frac{\Delta H_L}{2} \quad (44)$$

$$T_i = T_{st}$$

^{xii} IMPROVED. In SAFETI liquid head cannot be added for pressurised releases, but in the model this is now possible.



The storage pressure is therefore assumed to be the 'average' pressure of the stored liquid.

This model cannot be used with the JIP droplet correlation which is based on continuous releases from orifices.

6 VAPOUR VENT MODEL

This model describes the release of vapour from an unpressurised vessel containing liquid and vapour, for example during a filling operation (see Figure 10). The lower part of the vessel is filled with component liquid, while the upper part of the vessel is assumed to be a vapour mixture consisting of saturated component vapour and air. During the filling operation, the liquid inflow volumetric rate and storage temperature are assumed to be constant.

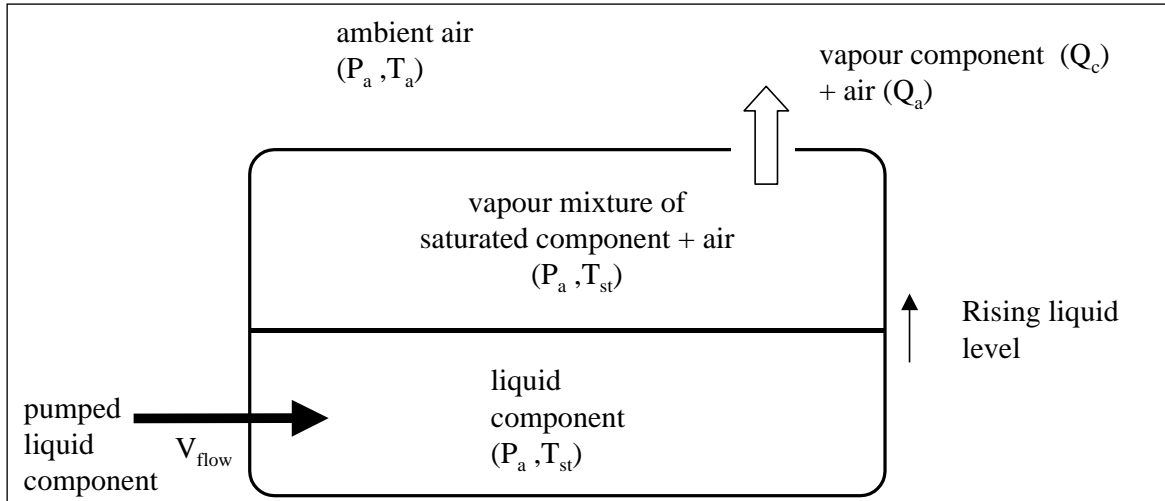


Figure 10. Vapour vent model

6.1 Inputs and Outputs

The model requires as inputs:

- storage data: temperature T_{st}^{xlii} (K), initial inventory M_{st} (kg)^{xliii};
- filling operation: component liquid volumetric flow rate V_{flow} (m³/s)
- exit area A (m)
- ambient data: pressure P_a (Pa), temperature T_a (K), relative humidity r_h^{xliv}
- component and ambient properties (e.g. vapour pressure, molecular weight etc.)

It returns as outputs the following release data:

- humid air mass flow rate, Q_a (kg/s)
- component vapour mass flow rate, Q_c (kg/s)
- duration, t_{rel} (s)
- velocity, u_f (m/s)
- temperature, T_f (K)

^{xlii} CORRECTED. The air in SAFETI 6.4 and earlier releases was assumed to be at ambient rather than storage temperature (VI6134).

^{xliii} JUSTIFY. Theory later on is only correct if M_{st} is the initial mass of component vapour (excluding component liquid; VI2991). A more useful input would be the initial volume of the mixture vapour V_{st}^{vap} . The release duration would then simply be $t_{rel} = V_{st}^{vap}/V_{flow}$ (ignoring any volume arising from liquid evaporation).

^{xliv} CHECK. Ambient data should ideally correspond to values at the top of the vessel. They are currently simplistically set equal to the ambient data at the reference height. Currently, relative humidity is not used by the model (VI3162).

6.2 Model Theory

Assumptions

The lower part of the vessel is filled with component liquid, while the upper part of the vessel is assumed to be a vapour mixture consisting of saturated component vapour and air. The following further assumptions are adopted:

- The vessel is unpressurised with the pressure of the vapour mixture (and the top of the liquid) equal to the atmospheric pressure P_a .
- The vapour mixture consists of saturated component vapour and air, where the humidity of the air is assumed to be equal to that of the ambient air outside the vessel.
- Prior to the filling operation commencing, the vessel is open to the atmosphere and the temperature inside the vessel is T_{st} . During the filling operation, the storage temperature T_{st} is assumed to remain constant^{xlv}.
- During the filling operation, the liquid inflow volumetric rate is constant. The vapour outflow volumetric rate is assumed to be equal to the liquid inflow volumetric rate, effectively ignoring the change in the total volume for the vapour mixture because of evaporation of the liquid component.

Release composition

The vapour mixture consists of saturated component vapour and humid air, and therefore the volume fractions y_c^f , y_a^f and mass fractions η_c^f , η_a^f of component and humid air in the released vapour mixture are as follows

$$y_c^f = \frac{P_v^c(T_{st})}{P_a}, \quad y_a^f = 1 - y_c^f \quad (45)$$

$$\eta_c^f = \frac{y_c^f M_w^c}{y_c^f M_w^c + y_a^f M_w^a}, \quad \eta_a^f = 1 - \eta_c^f = \frac{y_a^f M_w^a}{y_c^f M_w^c + y_a^f M_w^a} \quad (46)$$

where $P_v^c(T_{st})$ is the saturated vapour pressure at the vessel temperature T_{st} , M_w^c the molecular weight of the component and M_w^a the molecular weight of humid air

Release flow rates

The vapour mixture outflow volumetric rate is assumed to be equal to the liquid component inflow volumetric rate V_{flow} . Thus according to Equation (45) the component vapour and air mass discharge rates (m^3/s) are given by

$$V_c^{out} = y_c^f V_{flow}, \quad V_a^{out} = y_a^f V_{flow} \quad (47)$$

The total mass discharge from the vessel is the sum of component vapour and air mass discharge rates (kg/s):

$$Q = Q_c + Q_a \quad (48)$$

Here the component, air mass discharge rates Q_c, Q_a are set as product of the vapour, air volumetric flow rates and the component, air vapour densities^{xlvi, xlvi}:

$$Q_c = V_c^{out} \rho_v^c [P_v^c(T_{st}), T_{st}] = \frac{P_v^c(T_{st})}{P_a} V_{in} \rho_v^c [P_a, T_{st}] \quad (49)$$

^{xlv} JUSTIFY. However the UDM receives treats this a separate streams of material and air, the former at T_{st} , the latter at T_a . Thus the air temperature will typically change between discharge and dispersion.

^{xlvi} CORRECTED. Various problems with the vent from vapour space component and air release rates have been applied in SAFETI 6.5 (VI7519, 6851, 2988).

^{xlvi} Dry rather than humid air is used for density calculations (VI3162).

$$Q_a = V_a^{out} \rho_a(P_a - P_v^c(T_{st}), T_{st}) = \left[1 - \frac{P_v^c(T_{st})}{P_a} \right] V_{in} \rho_a(P_a, T_{st}) \quad (50)$$

Multi-component modelling

Where the improved multi-component modelling is used, the composition of the vapour phase in the tank is initially unknown. Raoult's Law is used to determine the vapour phase partial pressures and thus mole fractions (y_i) of components in the mixture:

$$y_i = \frac{P_v^i(T_{st})}{P_a} x_i \quad (51)$$

Where x_i is the mole fraction of component i in the bulk mixture (assumed to also be the composition of the liquid), and the mole fraction of air $y_a = 1 - \sum y_i$.

In a manner analogous to pseudo-component logic, the mass flow rates Q_c^i for component i (including air):

$$Q_c^i = V_{in} y_i \rho_v^i[P_a, T_{st}] \quad (52)$$

Other release data

The velocity of the release is set from the ratio of the total volumetric discharge rate ($=V_{flow}$) and the exit area A :

$$u_f = \frac{V_{flow}}{A} \quad (53)$$

The release duration is:

$$t_{rel} = \frac{M_{st}}{Q_c} \quad (54)$$

The release temperature T_f is set equal to the storage temperature T_{st} .

Since the vessel is unpressurised (exit pressure = ambient pressure), no atmospheric expansion takes place upon release and consequently ATEX is not used.

Method of Solution

1. Calculate mass flow rates Q_c and Q_a
 - 1.1. For the old pseudo-component modelling, this is explicitly calculated from Equations (49) and (50)
 - 1.2. For the new multi-component modelling, the composition is varied until a flash results in pure vapour, *i.e.* until the dew point pressure equals ambient pressure.
2. Calculate final velocity, u_f , from Equation (53)
3. Calculate release duration, t_{rel} , from Equation (54)
4. Set final temperature $T_f =$ storage temperature, T_{st} .

7 VERIFICATION

The orifice, short pipe and instantaneous DISC models have all been verified using manual calculations for a number of common scenarios (A-E, Table 1)

Scenario	A	B	C	D	E
Material	Ammonia	Methane	Chlorine	HC mixture	LNG
Storage phase	Liquid	Vapour	2-phase	2-phase	Liquid
Pressure (Pa)	1.1×10^5	1.0×10^6	5×10^5	3×10^5	5×10^6
Temperature (K)	230	160	na	na	180
Liquid mass fraction	na	na	0.95	0.8	n/a
Inventory (kg)	5,000	500	1,000	5,000	750
Orifice diameter (m)	0.025	0.05	0.1	0.025	0.01
Liquid head (m)	3	na	0	0	1.5
Pipe diameter	0.1	0.05	0.2	0.2	0.1
Pipe length	10	4	20	100	20

Table 1. Base scenarios for testing and verification

Using independent property system calculations at initial and orifice pressure and temperature, the model as documented here is applied using spreadsheet calculations. The results are then compared with the model run outputs.

All outputs agreed to within 0.1%.

Verification of the post-expansion outputs as calculated by ATEX is reported in that model's documentation.

8 FUTURE DEVELOPMENTS

The following further work is recommended:

- Review specific areas where the theoretical basis of the models is uncertain, including discharge coefficients, the treatment of relief valve and addressing several of the footnotes in the current document.
- Expose model features not currently supported in SAFETI, such as 2-phase leaks for line ruptures.
- In addition to releases from sharp-edge orifice, consider extending the orifice scenario to non-circular orifices⁵.
- In addition of full-bore ruptures at the end of the pipe, allow for partial leaks.
- Validation against additional experiments; see the DISC validation document for details¹.

APPENDICES

Appendix A. Flash calculations for discharge models

The discharge models use three types of flash calculations: isentropic (expansion from storage to orifice conditions), isenthalpic (expansion to atmospheric conditions – see ATEX) and isoenergetic (expansion along a pipe). The fixed enthalpy flash method of solution is exactly the same as for the fixed entropy flash, and is not documented further. These PC flashes differ from standard flash calculations described in the FLAS model, specifically in the use of ‘forced’ flashes (where the flashed phase is forced to remain pure vapour or liquid) and the assumption of pure component logic.

A.1 Fixed Entropy

Inputs and Outputs

The isentropic expansion requires the following inputs:

- specific entropy, s (J kg^{-1})
- pressure, P (Pa)

It returns the following outputs

- temperature, T (K)
- liquid fraction, η_L (-)
- phase

Description

Note the description below relates to flashes that use pure component logic. Rigorous multicomponent flashes are done as described in the Property System Theory document.

In terms of vapour (s_V) and liquid (s_L) entropies, the total entropy is:

$$s = \eta_L s_L(P, T) + (1 - \eta_L) s_V(P, T) \quad (55)$$

Some scenarios (especially the Leak scenario) force vapour or liquid discharges to remain the same phase after expansion, in which cases the liquid fraction is set to one or zero. For non-forced phases, liquid fraction must be determined. As liquid entropy is less than vapour entropy, whether the final state in single phase or two-phase can be determined from Equation (56)⁴⁸:

$$\begin{aligned} s > s_V(P, T_{sat}) & \quad \text{Vapour } (\eta_L = 0) \\ s_L(P, T_{sat}) < s < s_V(P, T_{sat}) & \quad \text{Two-phase } (0 < \eta_L < 1) \\ s < s_L(P, T_{sat}) & \quad \text{Liquid } (\eta_L = 1) \end{aligned} \quad (56)$$

If two-phase, then Equation (55) can be re-arranged to solve for η_L , and T is the saturated temperature T_f . Otherwise, $\eta_L = 0$ or 1 and temperature is iterated.

Method of solution

1. If the expansion is forced (see above)

1.1. set η_{Lf} to zero or one, and iterate on T_f to satisfy Equation (55).

2. Else

⁴⁸ If $P > P_{crit}$ then T_{sat} cannot be evaluated. However the expanded state must be pure vapour ($T > T_{crit}$) or pure liquid ($T < T_{crit}$). It is possible to determine which by comparing entropy with vapour entropy at the critical point. Similar logic applies to isenthalpic and isoenergetic flashes.

- 2.1. If improved multi-components is being used,
 - 2.1.1. A standard fixed entropy flash is performed
- 2.2. Else
 - 2.2.1. Determine final phase from Equation (56).
 - 2.2.2. If two-phase, set T_f to T_{sat} and solve Equation (55) for to find η_f
 - 2.2.3. If single-phase, set η_f to 0 or 1 and iterate on T_f to solve Equation (55)
- 2.3. End if
3. End if

A.2 Fixed energy

Inputs and Outputs

The isoenergetic expansion requires as input:

- energy, E (J kg⁻¹)
- mass flux, G (kg m⁻² s⁻¹)
- pressure, P (Pa)

It returns as output:

- temperature, T (K)
- liquid fraction, η_L (-)

Description

In terms of vapour and liquid enthalpies, conservation of energy requires:

$$E = \eta_L h_L + \eta_V h_V + \frac{u^2}{2} \quad (57)$$

where the speed u is given by:

$$u = Gv = G(\eta_L v_L + \eta_V v_V) \quad (58)$$

By expressing vapour fraction $\eta_V = 1 - \eta_L$ and combining Equations (57) and (58) we get:

$$0 = \eta_L^2 \left[\frac{G^2}{2} (v_L - v_V)^2 \right] + \eta_L \left[(h_L - h_V) + G^2 v_V (v_L - v_V) \right] + \left[h_V + \frac{G^2 v_V^2}{2} - E \right] \quad (59)$$

As described for the fixed entropy flash (Section A.1), some scenarios require that initial pure vapour or liquid discharges remain so after expansion. In these cases the final vapour or liquid fraction is set to 1. Otherwise, as we know that liquid energy is less than vapour energy, whether the final state is single phase or two-phase can be determined:

$$\begin{array}{ll} E > E_V(P, T_{sat}) & \text{Vapour } (\eta_L = 0) \\ E_L(P, T_{sat}) < E < E_V(P, T_{sat}) & \text{Two-phase } (0 < \eta_L < 1) \\ E < E_L(P, T_{sat}) & \text{Liquid } (\eta_L = 1) \end{array} \quad (60)$$

If two-phase, then the quadratic Equation (59) can be solved for η_L and T set to the saturated temperature, T_{sat} . Otherwise, η_L is set to 0 or 1 and T iterated.

Method of solution

1. If the expansion is forced (see above)
 - 1.1. Set η_L to zero or one, and iterate on T to satisfy Equation (59)⁴⁹.
2. Else
 - 2.1. If improved multi-component modelling is being used
 - 2.1.1. A standard isoenergetic flash is performed.
 - 2.2. Else
 - 2.2.1. Determine final phase from Equation (60).
 - 2.2.2. If two-phase, set T to T_{sat} and solve Equation (59) for η_L .
 - 2.2.3. If single-phase, set $\eta_L = 0$ or 1 and iterate on T to solve Equation (59).
 - 2.3. End if
3. End if

⁴⁹ Currently, forced isoenergetic expansions are not used in the models. However, the design adopted for the revised SAFETI 6.5 models allows this flexibility.

Appendix B. Discharge coefficient

The theory below is based on old PHAST documentation, itself derived from the work of Bragg (1960)⁶. It has not been reviewed or its implementation verified.

The discharge coefficient of an orifice, C , is defined as the ratio of the actual mass flow to that which could be passed through the full area of the orifice, A_o . Assuming that at the *vena contracta* a full expansion to ambient pressure has occurred, it follows that:

$$C = \frac{A_v}{A_o} = G \frac{v_v}{u_v} \quad (61)$$

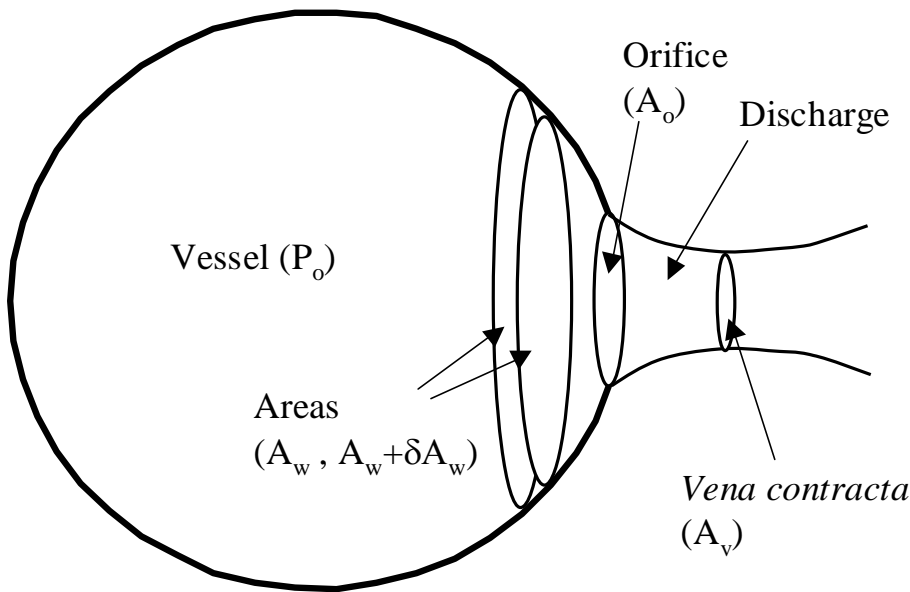


Figure 11. Discharge from an orifice and *vena contracta*.

A_v , v_v and u_v are respectively the area, specific volume and velocity at the *vena contracta*. G is the mass flow per unit area through the orifice.

For liquids the discharge coefficient is taken to be an assumed value for incompressible fluids, $C_i = 0.6^{50}$. For compressible fluids, the coefficient is calculated according to a generalised method based on the work of Bragg (1960). A brief summary of this method as applied is included here. The principle behind the method is to derive an expression for discharge coefficient in terms of an estimated orifice pressure, P_o , which is refined until a convergence is achieved.

The equation of motion of the fluid within a control surface that includes the reservoir and the flow up to the *vena contracta* is:

$$F + A_o P_{st} - (A_o - A_v) P_a = A_v P_v + A_o G u_v \quad (62)$$

Where F is the force defect, and is defined as the net force resulting from the reduction in pressure on the vessel walls due to the fluid being in motion near the orifice. The pressure P_v at the *vena contracta* is assumed to be equal to the supplied choke pressure, P_c^{51} . Both energy and entropy are conserved between the vessel and *vena contracta*:

$$h_i = h_v + \frac{u_v^2}{2} \quad (63)$$

$$s_i = s_v \quad (64)$$

⁵⁰ DOC. In Lees [15/7], the average experimental C for a sharp-edged orifice is given as 0.62.

⁵¹ DOC. Or ambient pressure if not choked flow.

From Equation (61), the mass flow rate can be expressed in terms of the discharge coefficient. An expression can also be derived for the force defect: consider a position, W , to the left of the orifice where the fluid is in motion and the pressure is reduced to P_w . The element of surface over which pressure acts subtends an area δA_w parallel to the plane of the orifice (Figure 11). The force defect is then:

$$F = \int_{A_o}^{\infty} (P_{st} - P_w) dA_w \quad (65)$$

Integrating by parts, and recognising that as $A_w \rightarrow \infty$, $P_w \rightarrow P_{st}$, and when $A_w = A_o$, $P_w = P_o$, gives:

$$F = -(P_{st} - P_o)A_o + \int_{P_o}^{P_{st}} A_w dP_w \quad (66)$$

Now the mass flux is at the walls is assumed to be proportional to the mean flux through area A_w :

$$\frac{u_w}{v_w} = k \frac{GA_o}{A_w} \quad 0 < k < 1 \quad (67)$$

The proportionality constant, k , is the same at all points in a particular orifice configuration regardless of operating conditions - although there is no theoretical justification for this assumption (Bragg, 1960)⁵². Substituting for A_w allows the integral in Equation (66) to be written as:

$$\int_{P_o}^{P_{st}} A_w dP_w = kGA_o \int_{P_o}^{P_{st}} \frac{v_w}{u_w} dP_w \quad (68)$$

For an adiabatic expansion:

$$dh = v dP \quad (69)$$

And by conservation of energy:

$$dh = -u du \quad (70)$$

Combining these enables Equation (68) to be evaluated:

$$\int_{P_o}^{P_{st}} A_w dP_w = -kGA_o \int_{P_o}^{P_{st}} du_w = kGA_o u_o \quad (71)$$

if the storage velocity is zero. The force defect, Equation (66) becomes:

$$F = -(P_{st} - P_o)A_o + kGA_o u_o \quad (72)$$

Consider now the incompressible case. The force defect according to Equation (65) can be rewritten using Bernoulli's Equation as:

$$F = \int_{A_o}^{\infty} \left(\frac{\rho_w u_w^2}{2g} \right) dA_w \quad (73)$$

⁵² JUSTIFY. How well justified are these k values? Are they used apart from in this paper? Are they tabulated for orifices in standard reference works?

But the local velocity, u_w , is proportional to the mass flow GA_o . Consequently it is useful to define a dimensionless 'force defect coefficient', f , which is independent of flow rate for a given orifice⁵³:

$$f = \frac{F}{G^2 A_o v_{st}} \quad (74)$$

A similar quantity is defined for the compressible case, and Equation (72) can be written:

$$F = fG^2 A_o v_{st} = -(P_{st} - P_o)A_o + kGA_o u_o \quad (75)$$

Equation (67) allows the expression of G in terms of local velocity and specific volume at the orifice, so:

$$\frac{f u_o^2 v_{st}}{k^2 v_o^2} = -(P_{st} - P_o) + \frac{u_o^2}{v_o} \quad (76)$$

The constant k is calculated from the coefficient of discharge for incompressible fluids, C_i ⁵⁴:

$$\frac{k^2}{2} = f_i = \frac{1}{C_i} - \frac{1}{2C_i^2} \quad (77)$$

Substituting in f_i and pressure ratio for density ratio gives:

$$f = f_i \frac{v_o}{v_{st}} \left[-\frac{2v_o(P_{st} - P_o)}{u_o^2} + 2 \right] \quad (78)$$

By conservation of energy this becomes:

$$f = f_i \frac{v_o}{v_{st}} \left[\frac{v_o(P_{st} - P_o)}{H_o - H_{st}} + 2 \right] \quad (79)$$

Conservation of entropy is assumed to hold between storage and orifice conditions:

$$s(P_{st}, T_{st}, \eta_{Lst}) = s(P_o, T_o, \eta_{Lo}) \quad (80)$$

Going back to the equation of motion, Equation (62), and substituting in for F (74) and G (61) gives a quadratic in C :

$$\left[\frac{f u_v^2 v_{st}}{v_v^2} \right] C^2 - \left[P_v - P_a + \frac{u_v^2}{v_v} \right] C + P_{st} - P_a = 0 \quad (81)$$

Appendix C. Guidance on using the DISC model

C.1 Orifice model input and output data

A list of the orifice model inputs and outputs (taken from the model's MDE Generic Spreadsheet) is illustrated in Figure 12 and Figure 13, respectively. For each input parameter a brief description of the meaning of the parameter is given, its unit, and its lower and upper limits. Column N contains a complete list of input data corresponding to a leak from a

⁵³ Not actually dimensionless - has units of acceleration.

⁵⁴ This looks odd. The k value is predicted from the f_i value for incompressible flow, which in turn is calculated from C_i , which is the same for all orifices. Hence k is the same for all orifice types (≈ 0.745).

refrigerated ammonia tank containing liquid at small overpressure. Columns to the right indicate those values that need to be changed to invoke (column O) a pressurised methane vapour leak; and (column P) a liquid leak of propane stored at saturation conditions.

Input Data:

1. Material name. The user specifies the name for the material stored in the vessel.
2. Storage state. The vessel stagnation data used to define the state of the stored material. This is taken as the state at the top of any liquid in the vessel. This can be specified in a number of ways, as described below.
 - 2.1. Specification flag. A material at equilibrium can be specified using any 2 of pressure, temperature, or liquid fraction. A material not at equilibrium must have all 3 specified. This input flag tells the model how determine the state:
 - -1 – Fixed temperature T and prescribed fixed flow rate.
 - 0 – Not at equilibrium.
 - 1 – fixed P_{st} & T_{st} . f_L is ignored. All 3 of P,T and f_L are specified
 - 2 – bubble point at T_{st} . P_{st} and f_L are ignored
 - 3 – bubble point at P_{st} . T_{st} and f_L are ignored
 - 4 – dew point at T_{st} . P_{st} and f_L are ignored
 - 5 – dew point at P_{st} . T_{st} and f_L are ignored
 - 6 – fixed P_{st} and f_L . T_{st} is ignored.
 - 7 – fixed T_{st} and f_L . P_{st} is ignored.
 - 2.2. Pressure (P_{st}). Storage pressure, excluding liquid head.
 - 2.3. Temperature (T_{st}). Storage temperature.
 - 2.4. Liquid fraction (f_L). Storage liquid mole fraction.
3. Vessel data.
 - 3.1. Total inventory. The mass contained in the vessel. Note that even for vapour releases the entire inventory is discharged.
 - 3.2. Orifice diameter (not applicable for fixed-duration scenario).
 - 3.3. Liquid head (applicable for liquid and not fixed-flow rate scenario). The vertical distance height above the orifice of the liquid surface in the vessel. Liquid head is ignored for all vapour releases.
 - 3.4. Pump head (applicable for liquid and not fixed-flow rate scenario). The orifice scenario is sometimes used to simulate small leaks from pipes with an upstream pump
4. Atmospheric expansion data. Atmospheric pressure, temperature, humidity and wind speed at the discharge height. Note that the wind speed is only used for the Melhem droplet correlation.
5. Scenario data.
 - 5.1. Scenario flag. Value = 4 corresponds to standard orifice leak and value = 5 corresponds to fixed duration scenario. In the latter scenario the model is forced to release of the entire inventory in a specified time (input by user, see below) by varying the orifice diameter.
 - 5.2. Phase to release for 2-phase storage. For a 2-phase vessel, the user can choose to release either liquid (3; orifice below the liquid level), vapour (1; orifice above the liquid level) or as a homogeneous 2-phase mixture (otherwise). For liquids, any liquid head is added in.
 - 5.3. Fixed duration (only applicable to fixed-duration scenario). The time in which the entire inventory will be evacuated - see Equation (9).
 - 5.4. Fixed flow rate. Only used when the specification flag = -1. The model then uses input stagnation temperature T_{st} and iterates on stagnation pressure P_{st} to obtain the prescribed fixed flow rate.

Parameters (to be changed only by expert users):

1. Multi-component modelling flag (not allowed for fixed-flow rate scenario). A value = 0 enables multi-component modelling for mixtures, rather than the pseudo-component approach (= 1) in PHAST 6.5 and earlier releases.
2. Phase change upstream of orifice? If set to 0, pure liquid or vapour leaks will not be allowed to change phase before or in the orifice. If set to 1, phase change is always allowed. If set to 2 (default), then phase change is disallowed for liquid only (meta-stable liquid assumption). When liquid phase change is disallowed then the orifice pressure will be set equal to the ambient pressure.
3. Use Bernoulli model for metastable liquid releases? If this is TRUE and flashing is not allowed to the orifice, then the incompressible Bernoulli equation will be used to calculate the flow rate for liquid discharge. The default value of this parameter is FALSE.
4. Is discharge coefficient specified? If this is TRUE, then the user must specify a discharge coefficient in a subsequent parameter. The default value of this parameter is FALSE, i.e. the model itself calculates the value of the discharge coefficient.
5. Orifice L/D ratio. Used for the new JIP droplet size correlation, this is the ratio of orifice length to diameter. The model uses minimum and maximum cut-offs of 2 and 50, and values outside this range will have no effect. See ATEX model documentation for further details.

6. Input discharge coefficient. This user-specified value of the discharge coefficient will be used only if the earlier 'Is discharge coefficient specified?' parameter is TRUE.
7. ATEX expansion method. Sets the method to be used by the ATmospheric EXpansion model. Option 0 is 'minimum thermodynamic change'. The other methods are isentropic (=1); conservation of momentum (=2); and DNV recommended (=4, default). See ATEX model theory for a fuller discussion.
8. Droplet-related parameters:
 - 8.1. Droplet correlation method (-). Sets which one of eight correlation methods is used for calculating droplet size in ATEX. See `droplet_size_theory_validation.doc` for further details.
 - 8.1.1. 0 – the original CCPS (Phast 6.4) method – default in Phast 6.6 and earlier versions.
 - 8.1.2. 1 – the JIP method uses the correlation proposed by the Flashing Liquid Jets Phase II project.
 - 8.1.3. 2 – the TNO Yellow Book correlation
 - 8.1.4. 3 – the droplet size correlation developed by Tilton and Farley
 - 8.1.5. 4 – the Melhem correlation.
 - 8.1.6. 5 – the correlation proposed in the JIP Phase III
 - 8.1.7. 6 – the Modified CCPS correlation – new default in Phast 6.7
 - 8.1.8. 7 – the Modified CCPS correlation but not for two-phase pipes
 - 8.2. Of these only the Original CCPS, Modified CCPS, Melhem and JIP phase III correlations are available in Phast, with the Modified CCPS correlation as the default
9. Force mechanical or flashing break-up. If > 0 , and where applicable, this forces the use of the flashing (= 2) or mechanical (= 1) break-up correlation used by a particular method (PHAST 6.4, JIP or TNO as described above).
 - 9.1. PHAST 6.4. Can force either flashing or mechanical break-up.
 - 9.2. JIP. Can force mechanical break-up only
 - 9.3. TNO. Purely a mechanical break-up correlation, so this parameter has no effect.
10. Atmospheric molecular weight.
11. Maximum velocity capping method. This parameter is used to limit the post-expansion velocity in cases where the model predicts values that may be too large. There are two capping options available:
 - 11.1. (=0): Fixed value - the post-expansion velocity is capped at a specified user-defined value. The default is uncapped (1.0e8 m/s).
 - 11.2. (=1): Sonic capping - the post-expansion velocity is capped at the sonic velocity.
12. Maximum velocity and duration or release.
13. Critical Weber number. Used for the PHAST 6.4 mechanical droplet size correlation. See ATEX model documentation for further details.
14. Minimum and maximum droplet diameter.
15. Relative tolerance for optimisation and root finding calculations.

	D	E	F	L	M	N	O	P	
1									
2	Inputs	MDE_Test_DISC_Orifice: Orifice discharge model testbed							
3	Input Index	Description	Units	Limits		OrificeA	OrificeB	OrificeC	
4				Lower	Upper				
5		Material							
9	2	Specification flag (0 = P&T&LF, 1 = P&T, 2 = Tsub, 3 = Psub, 4 = Tdew, 5 = Pdew, 6 = P&LF, 7 = T&LF)	-	0	7	1	1	6	
10	3	Gauge pressure	Pa	0		8675	898675	398675	
11	4	Temperature	K	10	1000	230	160		
12	5	Liquid fraction (MOLE basis)	mol/mol	0	1	1		0.95	
13		Vessel data							
14	6	Total inventory	kg	10		5.00E+03	500	1000	
15	7	Orifice diameter	m	0.001	50	0.025	0.05	0.1	
16	8	Liquid head	m	0		3	0	0	
17		Atmospheric expansion data							
18	9	Atmospheric pressure	Pa	50000	120000	101325			
19	10	Atmospheric temperature	K	10		293.15			
20	11	Atmospheric humidity	-	0	1	0.7			
21	12	Wind speed	m/s	0		0			
22		Scenario data							
23	13	Scenario flag (4 = leak, 5 = fixed duration)	-	4	5	4			
24	14	Phase to release for 2-phase storage (1 = vapour, 2 = 2-phase, 3 = liquid)	-	1	3	3		3	
25	15	Fixed duration	s	0	10000	600			
26		PARAMETERS (values to be changed by expert users only)							
27	16	Multi-component modelling flag (1 = MC, 0 = PC)	-	0	1	0			
28	17	Phase change upstream of orifice? (0=disallow phase change, 1=allow phase change, 2=disallow liquid phase change only)	-	0	2	2			
29	18	Use Bernoulli model for metastable liquid releases?				FALSE			
30	19	Is discharge coefficient specified? TRUE = Specified	-			FALSE			
31	20	Orifice L/D ratio	-	0	1000	1			
32	21	Input discharge coefficient	-	0	1	1			
33	22	ATEX expansion method (0 = min change, 1 = isentropic, 2 = cons moment, 4 = DNV GL recommended)	-	0	4	2			
34	23	Droplet correlation (0=original CCPS, 1= JIPII, 2=TNO, 3=Tilton, 4= Melhem, 5=JIPIII, 6=modified CCPS, 7=modified CCPS excl. 2PH pipe)	-	0	7	6			
35	24	Force mechanical or flashing breakup (0 = No, 1 = force mechanical, 2 = force flashing)	-	0	2	0			
36	25	Atmospheric molecular weight	kg/kmol	10	100	28.966			
37	26	Maximum velocity capping method (0 = user input, 1 = sonic velocity)	-	0	1	0			
38	26	Maximum velocity	m/s	10		1.00E+08			
39	27	Maximum duration	s	1		3600			
40	28	Critical Weber number	m	1	50	12.5			
41	29	Minimum droplet size	m	0	0.01	1.00E-08			
42	30	Maximum droplet size	m	0	1	0.01			
43	31	Relative tolerance	-	1.00E-06	0.1	0.001			

Figure 12. Orifice model input data.

Output Data:

1. Release state. The initial material state prior to release, including liquid head. The model returns all 3 of P_i , T_i and f_{Li} . Also returned in an array containing the mole fractions of all components in the released stream.
2. Orifice state. The material state at the orifice, prior to atmospheric expansion conditions. The model returns all 3 of P_o , T_o and f_{Lo} . It also returns orifice velocity u_o and the orifice or vena contracta diameter.

3. Final (post-expansion) state. The material state after the expansion to ambient conditions. The model returns T_f and f_{Lf} . The final pressure $P_f = P_a$. The model also returns final velocity u_f .
4. ATEX outputs. Please see ATEX documentation for further details.
 - 4.1. Droplet diameter.
 - 4.2. Rossin-Rammler 'b' coefficient (b_{RR}). Used in determining the droplet size distribution.
 - 4.3. Flashing (=1) or mechanical (=2) droplet size correlations used. For the JIP correlation, a value of 3 is possible, indicating the droplets are in the transitional zone between flashing and mechanical break-up.
 - 4.4. ATEX expansion method used. If the 'minimum thermodynamic change' or 'DNV recommended' method has been chosen, this output will indicate which of the two expansion methods was actually used.
 - 4.5. Expanded diameter.
 - 4.6. Partial expansion energy used as the basis of the PHAST 6.4/ CCPS flashing droplet size correlation. This output variable also doubles up as the Rossin-Ramler A_{rr} value in case of JIP droplet correlations.
5. Other data
 - 5.1. Discharge coefficient.
 - 5.2. Mass release rate.
 - 5.3. Release duration.

	D	E	F	L	M	N	O	P
	MDE_Test_DISC_Orifice: Orifice discharge							
2	Inputs	model testbed						
3	Input	Description	Units	Limits		OrificeA	OrificeB	OrificeC
4	Index			Lower	Upper			
5		Material						
45	Output	Description						
46	Index							
47		ERROR STATUS				OK	OK	WARN
48		Release state						
49	1	Pressure	Pa			130412.7	1000000	500000
50	2	Temperature	K			230	160	282.676
51	3	Liquid fraction (MASS basis)	kg/kg			1	0	1
52	4	Array of composition mole fractions	mol/mol					
53		Orifice state						
54	5	Pressure	Pa			101325	580707.6	101325
55	6	Temperature	kg/kg			229.996	138.12	282.4711
56	7	Liquid fraction (MASS basis)	-			1.00E+00	8.90E-04	1
57	8	Velocity	m/s			10.27129	270.7404	24.42802
58	9	Vena contracta diameter	m			1.94E-02	4.65E-02	7.75E-02
59		Final (post-expansion) state						
60	10	Temperature	K			229.996	111.666	239.1593
61	11	Liquid fraction (MASS basis)	kg/kg			1	6.35E-02	0.860293
62	12	Velocity	m/s			10.27129	463.9079	24.42802
63		ATEX outputs						
64	13	Droplet diameter	m			3.64E-03	6.45E-07	4.69E-04
65	14	Rossin-Rammler 'b' coefficient	-			Undefined	Undefined	Undefined
66	15	Flashing or mechanical (1 = mechanical, 2 = flash, 3 = transition)	-			1	1	1
67	16	ATEX expansion method (1 = isentropic, 2 = cons momentum)	-			2	2	2
68	17	Expanded diameter	m			1.94E-02	7.73E-02	5.76E-01
69	18	Expansion energy	J/kg			Undefined	Undefined	Undefined
70	19	Partial expansion energy	J/kg			Undefined	6456.948	-276.8955
71		Other data						
72	20	Discharge coefficient	-			0.6	0.863254	0.6
73	21	Mass release rate	kg/s			2.10E+00	4.206457	165.8102
74	22	Release duration	s			2382.175	118.8649	6.030992

Figure 13. Orifice model output data.

C.2 Pipe Model Input and Output Data

A list of the pipe model inputs and outputs (taken from the model's MDE Generic Spreadsheet) is illustrated in Figure 14 and Figure 15 (inputs) and Figure 16 (outputs). For each input parameter a brief description of the meaning of the parameter is given, its unit, and its lower and upper limits. Columns N through contain a complete list of input data corresponding to a line ruptures from a refrigerated ammonia tank containing liquid at small overpressure; a pressurised methane vapour vessel; and saturated liquid propane.

Input Data

Many input data are the same as described for the orifice model above.

1. Material name. The user specifies the name for the material stored in the vessel.
2. Storage state. The vessel stagnation data used to define the state of the stored material, as described for the orifice model above.
3. Vessel data. Fluid inventory excludes fluid mass in the pipe (fluid mass in pipe is calculated by the model and added to the total system inventory). The orifice diameter refers to the diameter of the join between the pipe and vessel, but is ignored in all but the relief valve scenario which explicitly models this constriction. Liquid head: adding to initial pressure for liquid releases, and ignored otherwise.
4. Pipe and valve data
 - 4.1. Basic pipe data. Diameter, length, (interior) surface roughness.
 - 4.2. Bend and fitting frequencies (number per metre). These contribute a fixed amount to pipe friction, reducing mass flow through the pipe.
 - 4.3. Valve type head loss. The velocity head losses for one of each of the three types of valve.
 - 4.4. Frequencies (number per metre) of valve types
5. Atmospheric expansion data. Atmospheric pressure, temperature, humidity and wind speed at the discharge height. Note that the wind speed is only used for the Melhem droplet correlation.
6. Scenario data.
 - 6.1. Release scenario. Line rupture, relief valve, and disk rupture are the 3 scenarios, and are described in Section 3.2.1.
 - 6.2. Line rupture: phase to release for 2-phase storage. For a line rupture from a 2-phase vessel, the user can choose to release either liquid (3; pipe below the liquid level), vapour (1; pipe above the liquid level) or as a homogeneous 2-phase mixture (otherwise). For liquids, any liquid or pump head is added in.
 - 6.3. Relief valve or disk rupture: phase to release for 2-phase storage. For a relief valve or disk rupture scenario, a 2-phase vessel may release vapour (i.e. from a large vapour space vessel) or 2-phase (i.e. from a small vapour space vessel). Liquid releases are not allowed for these scenarios.
7. Flow control options (only applicable to Line Rupture scenario). These options allow the user to model a pre-defined accidental flow rate ('fixed-rate scenario'). The following flow control options are available:
 - 7.1. (=0) None – standard line rupture scenario
 - 7.2. (=1) Compressor (Vapour phase; temperature and fixed flow rate required)
 - 7.3. (=2) Pump (Liquid phase)
 - 7.3.1. Fixed rate: temperature and fixed flow rate required
 - 7.3.2. Pump head: temperature, pressure and pump head required
 - 7.4. (=3) Control valve (vapour or liquid phase; temperature, pressure and fixed rate required)

Parameters (to be changed only by expert users):

These are mainly as described for the orifice model. The exceptions are:

1. Maximum number of output steps for results along the pipe. Not intended to be changed by the user.
2. Disk rupture scenario: 2nd phase critical pressure. Even if a 2-phase release is chosen for this scenario, it will be released as a vapour if the initial gauge pressure is less than this parameter.
3. Ratio of non-equilibrium to equilibrium flow rates. The constricted valve orifice (area A_o) for the relief valve scenario is assumed to be 'over-drilled' by this ratio (i.e. for the leftmost case in Figure 15 $A_o = 1.2 \times A_o$). See Equation (27). Thus the orifice will be less constricted than suggested by the ratio of orifice and pipe diameters.
4. Capping method for flow rate. Permissible values are (0 – uncapped, 1 – capped with flashing allowed, 2 – capped with flashing disallowed). Capping the pipe model will prevent mass flow rates from exceeding those through a similarly sized orifice. The different flashing options will control whether during this orifice calculation flashing is suppressed (as with a normal leak), or enabled.

Output Data

Part of the output data are very similar to the orifice scenario, but there are some additional outputs relating to presence of the pipe that are highlighted below.

1. Control valve data. This is relevant only for line rupture scenarios with a control valve specified.
 - 1.1. Control valve data under normal operation. An isothermal expansion is assumed and so only the pressure and velocity immediately downstream of the control valve is reported.
 - 1.2. Control valve data after rupture. The fluid state immediately downstream of the control valve after rupture is given in terms of pressure, temperature, liquid fraction and velocity.
2. Data along the pipe. For all short pipe scenarios, the fluid state generally varies along the pipe as a function of distance from the upstream end of the pipe. In this section several fluid properties along the pipe are reported as arrays. The 'accumulated mass along pipe' is the fluid mass in the pipe between the upstream end and the given distance along the pipe.
3. 'Fluid mass in pipe' is the total mass in the pipe. This is of interest as it is added to the input inventory to obtain the total inventory released.
4. 'Dimensionless pipe friction'. An additional output used mainly for verification.

	D	E	F	L	M	N	O	P
		MDE_Test_DISC_Pipe: Pipe discharge model						
2	Inputs	testbed						
3	Input	Description	Units	Limits		PipeA	PipeB	PipeC
4	Index			Lower	Upper			
9		Material						
10	N	Stream name	-			Ammonia	Methane	Chlorine
12		Storage state						
13	A	Specification flag (0 = P&T&LF, 1 = P&T, 2 = T bub, 3 = P bub, 4 = T dew, 5 = P dew, 6 = P&LF, 7 = T&LF)	-	0	7	1	1	6
14	A	Gauge pressure	Pa	0		8675	898675	398675
15	A	Temperature	K	10	1000	230	160	
16	A	Liquid fraction (MOLE basis)	mol/mol	0	1	1		0.95
17		Vessel data						
18	A	Total inventory (excluding fluid in pipe)	kg	1		5.00E+03	500	1000
19	A	Orifice diameter	m	0.001	50	0.025	0.05	0.1
20	A	Liquid head	m	0		3	0	0
21		Pipe and valve data						
22	A	Pipe diameter	m	0.001	50	0.1	0.05	0.2
23	A	Pipe length	m	0.01	1.00E+06	10	4	20
24	A	Pipe roughness	m			0.000045		
25	A	Frequency of couplings	/m		10	0		
26	A	Frequency of junctions	/m		10	0		
27	A	Frequency of bends	/m		10	0		
28	6	Valve data						
29	A	Valve type 1 (excess flow) velocity head loss	-			1		
30	A	Valve type 2 (no return) velocity head loss	-			2		
31	A	Valve type 3 (shut-off) velocity head loss	-			3		
32	A	Frequency of valve type 1	/m		10	0		
33	A	Frequency of valve type 2	/m		10	0		
34	A	Frequency of valve type 3	/m		10	0		
35		Atmospheric expansion data						
36	7	Atmospheric expansion data						
37	A	Atmospheric pressure	Pa	50000	120000	101325		
38	A	Atmospheric temperature	K	200	350	293.15		
39	A	Atmospheric humidity	-	0	1	0.7		
40	A	Wind speed	m/s	0		5		

Figure 14. Pipe model input data (Part 1)

	D	E	F	L	M	N	O	P
2	MDE_Test_DISC_Pipe: Pipe discharge model testbed							
3	Input	Description	Units	Limits		PipeA	PipeB	PipeC
4	Index			Lower	Upper			
41	Scenario data							
42	A	Release scenario (1 - line rupture, 2 - disk rupture, 6 - relief valve)	-	1	6	1		
43	A	Line rupture: phase to release for 2-phase storage (1 = vapour, 2 = 2-phase, 3 = liquid)	-	1	3	3	1	
44	A	Relief valve / Disk rupture: phase to release for 2-phase storage (1 = vapour, 2 = 2-phase)	-	1	2	2		
45	Flow control options (Line Rupture only)							
46	A	Flow controller (0=None, 1=Compressor(T, fixed rate), 2=Pump(T, fixed rate)/(P,T,pump head), 3=Control valve(P,T, fixed rate)	-	0	3	0		
47	A	Specification option (0 = Not applicable, 1 = Fixed flow rate, 2 = Pump head)	-	0	2	0		
48	A	Fixed flow rate	kg/s	0		0		
49	A	Pump Head	m	0		0		
51	PARAMETERS (values to be changed by expert users only)							
52	8	Maximum nr. of steps along the pipe	-	2	10000	1000		
53	A	Disk rupture: Second phase critical pressure	Pa			3.45E+04	3.45E+04	
54	A	Multi-component modelling flag (1 = MC, 0 = PC)	-	0	1	0	0	
55	A	Ratio of non-equilibrium to equilibrium flow rate (overdrilling of constricted orifice)	-			1.2	1.2	
56	A	Capping method for flow rate (0 - no cap, 1 - orifice cap, allow flashing, 2- orifice cap, disallow flashing)	-	0		0	0	
57	A	ATEX expansion method (0 = min change, 1 = isentropic, 2 = cons moment, 4 = DNV GL recommended)	-	0	4	2	2	
58	A	Droplet correlation (0=original CCPS, 1= JIPII, 2=TNO, 3=Tilton, 4= Melhem, 5=JIPIII, 6=modified CCPS, 7=modified CCPS excl. 2PH pipe)	-	0	7	6	6	
59	A	Force mechanical or flashing breakup (0 = No, 1 = force mechanical, 2 = force flashing)	-	0	2	0	0	
60	A	Atmospheric molecular weight	kg/kmol	10	100	28.966	28.966	
61	A	Maximum velocity capping method (0 = user input, 1 = sonic velocity)	-	0	1	0	0	
62	A	Maximum velocity	m/s	10		1.00E+08	1.00E+08	
63	A	Maximum duration	s	1		3600	3600	
64	A	Critical Weber number	m	1	50	12.5	12.5	
65	A	Minimum droplet size	m	0	0.01	1.00E-08	1.00E-08	
66	A	Maximum droplet size	m	0	1	0.01	0.01	
67	A	Relative tolerance	-	1.00E-06	0.1	1.00E-04	1.00E-04	

Figure 15: Pipe model input data (Part 2)

MDE_Test_DISC_Pipe: Pipe discharge model testbed						
Output Index	Description Description	Units	Limits	PipeA	PipeB	PipeC
	ERROR STATUS			OK	OK	OK
	Release state					
1	Pressure	Pa		130412.7	1000000	500000
2	Temperature	K		230	160	282.676
3	Liquid fraction (MASS basis)	kg/kg		1	0	1
4	Array of composition mole fractions	mol/mol				
	Control valve data normal operation					
5	Pressure	Pa		Undefined	Undefined	Undefined
6	Velocity	m/s		Undefined	Undefined	Undefined
	Control valve data after rupture					
7	Control valve constriction after rupture	m		Undefined	Undefined	Undefined
8	Pressure	Pa		Undefined	Undefined	Undefined
9	Temperature	K		Undefined	Undefined	Undefined
10	Liquid fraction	kg/kg		Undefined	Undefined	Undefined
11	Velocity	m/s		Undefined	Undefined	Undefined
	Data along the pipe					
12	Number of steps along pipe	-		14	10	11
13	Distance along pipe	m				
14	Pressure along pipe	Pa				
15	Temperature along pipe	K				
16	Liquid fraction along pipe	kg/kg				
17	Velocity along the pipe	m/s				
18	Density along pipe	kg/m ³				
19	Accumulated mass along pipe	kg				
	Pipe exit state					
20	Pressure	Pa		101325	420192.6	375306.7
21	Temperature	kg/kg		230.0074	136.8205	273.5976
22	Liquid fraction (MASS basis)	-		1.00E+00	0	0.96823
23	Velocity	m/s		4.989422	288.7311	19.40559
	Final (post-expansion) state					
24	Temperature	K		230.0074	111.666	239.1593
25	Liquid fraction (MASS basis)	kg/kg		1	4.27E-02	0.866638
26	Velocity	m/s		4.989422	4.60E+02	64.92692
	ATEX outputs					
27	Droplet diameter	m		1.00E-02	6.57E-07	2.90E-04
28	Rossin-Rammler 'b' coefficient	-		Undefined	Undefined	Undefined
29	Flashing or mechanical (1 = mechanical, 2 = flash, 3 = transition)	-		1	1	2
30	ATEX expansion method (1 = isentropic, 2 = cons momentum)	-		Undefined	2	2
31	Expanded diameter	m		1.00E-01	7.33E-02	0.368911
32	Expansion energy	J/kg		0	Undefined	Undefined
33	Partial expansion energy	J/kg		Undefined	-489.0906	1642.569
	Other data					
34	Fluid mass in pipe	kg		Undefined	Undefined	Undefined
35	Mass release rate	kg/s		27.18826	3.66065	189.0847
36	Release duration	s		183.9029	136.5878	5.288634
37	Dimensionless pipe friction	-		3.368319	1.836364	1.457505

Figure 16. Pipe model output data

C.3 Rupture Model (instantaneous release)

A list of the orifice model inputs and outputs (taken from the model's MDE Generic Spreadsheet) is illustrated in Figure 17. The inputs and outputs are exactly as described for the orifice and pipe models. No atmospheric expansion method input is specified, as all instantaneous cases use the same method. See ATEX for further details.

	D	E	F	L	M	N	O	P
2	Inputs	MDE_Test_DISC_Instantaneous: Instantaneous discharge model testbed						
3	Input Index	Description	Units	Limits		RuptA	RuptB	RuptC
4				Lower	Upper			
5		Material						
6	N	Stream name	-			Ammonia	Methane	Chlorine
8		Storage state						
9	2	Specification flag (0 = P&T&LF, 1 = P&T, 2 = Tsub, 3 = Psub, 4 = Tdew, 5 = Pdew, 6 = P&LF, 7 = T&LF)	-	1	9	1	1	6
10	3	Gauge pressure	Pa	0		8.68E+03	8.99E+05	3.99E+05
11	4	Temperature	K			230	160	
12	5	Liquid fraction	-			1		0.95
13	6	Liquid head	m			3	0	0
14		Atmospheric expansion data						
15	7	Atmospheric pressure	Pa			101325		
16	8	Atmospheric temperature	K			293.15		
17	9	Atmospheric humidity	-			0.7		
18	10	Wind speed	m/s	0		5		
19		Scenario data						
20	11	Phase to release for 2-phase storage (1 = vapour, 2 = 2-phase, 3 = liquid)	-	1	3	3		
21		PARAMETERS (values to be changed by expert users only)						
22	12	Multi-component modelling flag (1 = MC, 0 = PC)	-	0	1	0		
23	13	Droplet correlation (0=original CCPS, 1= JIPII, 2=TNO, 3=Tilton, 4= Melhem, 5=JIPIII, 6=modified CCPS, 7=modified CCPS excl. 2PH pipe)	-	0	7	6		
24	14	Force mechanical or flashing breakup (0 = No, 1 = force mechanical, 2 = force flashing)	-	0	2	0		
25	15	Atmospheric molecular weight	kg/kmol			28.966		
26	16	Maximum velocity capping method (0 = user input, 1 = sonic velocity)	-	0	1	0		
27	17	Maximum velocity	m/s			500		
28	18	Critical Weber number	-			12.5		
29	19	Minimum droplet size	m			1.00E-08		
30	20	Maximum droplet size	m			0.01		
31		Outputs						
32	Output Index	Description						
33								
34		ERROR STATUS				OK	OK	OK
35		Release state						
36	1	Pressure	Pa			120206.34	1000000	500000
37	2	Temperature	K			230	160	282.67601
38	3	Liquid fraction	-			1	0	1
39	4	Array of composition mole fractions	mol/mol					
40		Final (post-expansion) state						
41	5	Temperature	K			229.99746	111.66603	239.15932
42	6	Liquid fraction	-			1	0.115409	0.8720691
43	7	Velocity	m/s			3.6832711	375.14447	82.016791
44		ATEX outputs						
45	8	Droplet diameter	m			5.91E-04	9.87E-07	4.16E-05
46	9	Flashing or mechanical (1 = mechanical, 2 = flash)	-			2	1	1
47	10	Expansion energy	J/kg			6.7832429	70366.689	3363.377
48	11	Partial expansion energy	J/kg			27.213588	70366.689	3363.377
49	12	UNUSED	-			Undefined	Undefined	Undefined

Figure 17. Rupture model input and output data.

C.4 Vent from Vapour Space Model

A list of the orifice model inputs and outputs (taken from the model's MDE Generic Spreadsheet) is illustrated in Figure 18. The inputs and outputs are exactly as described for the orifice and pipe models.

MDE_Test_DISC_Vapourvent: Vent from vapour space discharge model testbed						
Input Index	Description	Units	Limits		Vent1	Vent2
			Lower	Upper		
Material						
N	Stream name	-			Ammonia	Propane
Storage and vessel data						
2	Temperature	K			220	230
3	Total inventory (incorrectly used)	kg			1.00E+03	1.00E+03
4	Liquid volumetric flow rate	m3/s			2	1
5	Outflow diameter	m			0.25	0.1
Atmospheric data						
6	Atmospheric pressure	Pa			101325	
7	Atmospheric humidity	-			0.7	
PARAMETERS (values to be changed by expert users only)						
8	Multi-component modelling flag (1 = MC, 0 = PC)	-	0	1	0	
9	Atmospheric molecular weight	kg/kmol			28.966	
10	Maximum velocity	m/s			500	
11	Maximum duration	s			3600	
Outputs						
Output Index	Description	Units	Lower	Upper	Vent1	Vent2
ERROR STATUS					OK	OK
1	Humid air mass release rate	kg/s			2.1303038	7.19E-02
2	Material mass release rate	kg/s			0.6462728	2.3019395
3	Temperature	K			220	230
4	Duration	s			1547.3341	434.41628
5	Velocity	m/s			40.743665	127.32395
6	Array of vapour phase mole fractions	kmol/kmol				

Figure 18. Vent from vapour space input and output data.

Most inputs are as described for the orifice and pipe models. The liquid volumetric flow rate is that of the liquid inflow to the vessel during the filling operation. The outflow diameter is the orifice diameter through which the vapour exits the vessel.

For the outputs, the air and material mass release rates are the Q_a and Q_c respectively (49) and (50).

C.5 Model warnings and errors

Below are descriptions of the possible DISC model error and warning messages.

Errors:

- 1 "Scenario flag %1%integer% invalid the model"
- 2 "Orifice diameter %1%Length% is out of range"
- 3 "Inventory %1%Mass% is out of range"
- 4 "Liquid head %1%Length% is out of range"
- 5 "Pipe roughness %1%real% is out of range"
- 6 "Pipe bend or fitting frequency %1%PerUnitLength% is out of range"
- 7 "Pipe valve frequency or head loss of valve type %1%integer% is out of range"
- 8 "Pipe diameter %1%Length% is out of range"
- 9 "Pipe length %1%Length% is out of range"
- 10 "Vent from vapour space model: vapour pressure %1%Pressure% exceeds atmospheric: initially vapour"

The vent from vapour space model must have a material initially in the liquid state.

11 "Vent from vapour space model: unable to determine the initial amount of air"

The MC vent from vapour space model must iterate using a dew point flash to find the initial composition of the air/component mixture. This error indicates it has failed to bracket a solution even using the extreme cases of pure material and pure air. Vent from vapour space model must have a material initially in the liquid state.

12 "Unpressurised releases must be liquid"

Generated by instantaneous unpressurised releases, which must be liquid.

13 "Volume flow rate, %1%Volume%, out of range"
 15 "Ambient humidity, %1%Real%, out of range"
 16 "Atmospheric mol wt, %1%MolarMass%, out of range"
 17 "Maximum velocity, %1%Velocity%, out of range"
 18 "Storage temperature, %1%Temperature%, out of range"
 19 "Maximum duration, %1%Time%, out of range"
 20 "Liquid release not allowed from relief valve scenario"
 21 "Liquid release not allowed from disk rupture scenario"

Liquids cannot be released using these scenarios, but saturated liquids (bubble point) are permissible.

22 "No release possible if initial pressure, %1%Pressure%, less than ambient pressure"
 23 "Atmospheric pressure, %1%Pressure%, out of range"
 24 "Coefficient of velocity, %1%Real%, out of range"
 25 "Relative tolerance, %1%Real%, out of range"
 26 "Can't have instantaneous releases using JIP droplet correlation"
 27 "Conservation of energy predicts square of exit velocity is negative. Unable to solve case"

Orifice enthalpy exceeds initial enthalpy so conservation of energy predicts a negative square for orifice velocity. The model cannot be solved.

29 "Vent from vapour space not allowed for mixtures containing air"

The vent from vapour space cannot handle mixtures including air. However as a requirement of the model is that unpressurised the fluid must be liquid, this is unlikely to be a problem.

30 "Bracketing routine fails to find a suitable pair of pipe fluxes to bracket desired root"

The pipe model is unable to find a value of the mass flow rate for which the thermodynamically calculated friction along the pipe agrees with the empirical value. The model cannot therefore solve.

31 "Invalid flow rate capping method specified for pipe model"

32 "Entropy not conserved in calculation of choked flow by orifice model"

This error was previously warning 1005 and was upgraded to an error in Phast 6.7. The error indicates that for some reason expansion to the orifice has failed to conserve entropy. This is often caused by liquid forced to remain so at the orifice when the equation of state has no liquid solution.

33 "User-specified fixed flow rate smaller than the allowed minimum, %1%MassFlow%"

Requested flow rate must be greater than minimum value $1.0e10^{-9}$ kg/s for fixed flow rate scenarios (pumps and compressors)

34 "Cannot find suitable storage pressure for fixed flow rate scenario"

This error happens when the model cannot find a storage pressure that would give the requested flow rate. This could happen if a very large flow rate is requested; attempting a lower fixed flow rate may overcome the error..

35 "User-specified fixed flow rate smaller than accidental flow rate at atmospheric pressure, %1%MassFlow%"

The requested fixed flow rate is smaller than the accidental flow rate you would get from the line rupture scenario if you have atmospheric pressure in the upstream tank; an error is given. Increase the fixed rate or change other relevant data to overcome the error.

```
36 "User-specified fixed flow rate larger than accidental flow rate at max
pressure, %1%MassFlow%"
```

The requested fixed flow rate is larger than the accidental flow rate you would get from the line rupture scenario if you have 300 bar pressure in the upstream tank; an error is given. Decrease the fixed rate or change other relevant data to overcome the error.

```
37 "Inconsistent input for control valve scenario; sub-atmospheric pressure, %1%Pressure%,
at pipe end during normal flow"
```

The error is given for control valve scenarios where the pressure at the pipe end during normal flow is sub-atmospheric. The user should adjust the storage pressure and/or the fixed flow rate if encountering this error.

```
38 "User-specified fixed flow rate for control valve scenario exceeds orifice leak flow
rate %1%MassFlow%"
```

Reduce the requested fixed flow rate to a value below the one given in the error message (which is the flow rate you would get from a corresponding orifice leak scenario).

```
39 "Too many steps (%1%integer%) required for integration from pipe upstream to downstream
of control valve"
```

The model cannot solve the expansion from upstream of the control valve to downstream of the control valve during normal flow. Tweaking the fixed flow rate or some of the pipe characteristics may help overcome the issue.

```
40 "Pressure downstream of control valve after rupture, %1%Pressure%, higher than pipe
inlet pressure - too high fixed flow rate specified"
```

The specified fixed flow rate for control valve scenario is too high as it would require a pressure increase across the control valve. Increase the storage pressure and/or reduce the fixed flow rate to obtain a consistent set of inputs.

```
41 "Phase change along pipe not allowed during normal flow for control valve scenario"
```

Liquid has changed to two-phase along the pipe during normal flow for the control valve scenario. This is not allowed. Consider changing conditions like the storage pressure or fixed flow rate to avoid this error.

```
42 "Invalid value %1%integer% for choice of flow controller"
```

```
43 "User-specified fixed flow rate must be larger than %1%MassFlow% for fluid to be
liquid at given temperature"
```

A pump has been chosen, but the requested fixed rate is smaller than what can be achieved in the liquid phase. Either change to vapour storage and compressor or increase the fixed rate to get consistent inputs for a liquid release with a pump.

```
44 "User-specified fixed flow rate must be smaller than %1%MassFlow% for fluid to be
vapour at given temperature"
```

A compressor has been chosen, but the requested fixed rate is larger than what can be achieved in the vapour phase. Either change to liquid storage and pump or decrease the fixed rate to get consistent inputs for a vapour release with compressor.

Warnings:

```
1010 "Flow rate capped to that predicted by the orifice model"
```



The flow rate predicted by the pipe model exceeds that predicted using the leak model using an orifice of the same diameter. In line with the user's wishes (see parameter "Capping method for flow rate") the flow rate is capped to the latter value.

1014 "Flow rate cap based on no flashing failed; cap therefore based on allowing flashing instead."

1015 "Flow rate cap based on allowing flashing failed; cap therefore based on disallowing flashing instead."

The two above warnings are issued for short pipe scenarios if the requested flow rate capping method fails; an alternative flow rate cap method is then used instead.

Appendix D. Short Pipe Model – pressure along the pipe

Section 3.3 contains a description of the method of solution⁵⁵ for the short pipe model. This includes a pressure integral as given in Equation (28). We here include explicit expressions for calculating the pressure as a function of distance along the pipe.

Equation (28) can be solved numerically to give P_n ($P_e \leq P_n < P_i$; $n = 1, 2, \dots$) and solution I_n . Assuming constant friction f along the pipe, Equation (17) can also be solved numerically to give an expression for the distance along the pipe L_n ($L_i=0 \leq L_n \leq L_p$; $n = 1, 2, \dots$):

$$L_n = \frac{D}{2f} \left(\ln \left(\frac{\rho_i}{\rho_n} \right) - \frac{I_n}{G^2} \right). \quad (82)$$

Since I is a function of P , we now effectively have an expression for the length along the pipe as a function of pressure P .

The mass M_n in a pipe segment $[0, L_n]$ can be obtained by integrating Equation (30) using the trapezoidal rule to obtain

$$M_n = M_{n-1} + \frac{\pi D^2}{4} \left(\frac{\rho_n + \rho_{n-1}}{2} \right) (L_n - L_{n-1}). \quad (83)$$

In case of uniform temperature T_i and pressure P_i along the pipe, Equation (83) simplifies to give the total mass in the pipe M_p as

$$M_p = \frac{1}{4} \pi D^2 \rho(T_i, P_i) L_p. \quad (84)$$

⁵⁵ An alternative solution algorithm based on the SUNDIALS numerical solver is proposed in the DISC algorithm document.

Appendix E. Pipe entry friction

The modelling of short pipe scenarios described in Section 3 includes several potential friction terms. One of these terms is due to sudden contraction of the fluid flow as the fluid flows from storage conditions within the vessel into the pipe – hereafter referred to as the pipe entry friction term. It has been identified that the current pipe entry friction term in DISC does not seem to be directly aligned with the literature, and an investigation into this pipe entry friction term has therefore been carried out and is documented in this section. We first present some formulations identified following a brief literature review before recapping how the pipe entry friction term is currently modelled in DISC. Next some validation cases are studied to see if modifying the pipe entry friction improves model predictions compared to experimental data. Finally a test study is carried out to investigate how changing the pipe entry friction term impacts on the mass release rate for a range of line rupture cases.

E.1 A brief literature review

In trying to assess the current pipe entry losses in DISC, a brief look to the literature has been made.

A common way of expressing frictional losses in a pipe is in terms of velocity head losses K:

$$F_{\text{entry}} = K \cdot \frac{1}{2} u^2 \quad (85)$$

Here F_{entry} is the entry loss, K the associated velocity head loss and u is the fluid velocity at the start of the pipe. Based on this formulation a brief comparison of pipe entry friction terms from the literature has been made and is summarised in the table below. The values below are based on the case without a constricted pipe entry.

Reference	K value	Comments
DISC implementation	$K=1/(C_d \cdot C_d) - 1$	For liquids $C_d=0.6 \rightarrow K=1.78$ For vapour may have $C_d=0.85 \rightarrow K=0.38$
Vennard and Street ¹²	$K=1/(C_v \cdot C_v) - 1 = 0.5625$	Based on $C_v=0.8$. Page 536.
McCabe et al. ⁷	$K=0.4$	Page 106/107, Eq. 5.66. ($C_v=0.8452$)
Crane ⁸	$K=0.5$	Page 2-11, Eq. 2-10. ($C_v=0.8165$)
Lees ⁹	$K=0.4$	Ch. 15, page 6. Refers to McCabe.

Table 2. Frictional loss constant due to sudden contraction.

The value of the pipe entry loss coefficient depends on the geometry of the vessel-pipe connection. This is further discussed in Munson et al¹⁰, pages 417 and 418.

The above is generally applicable to incompressible fluid flow (liquids). For friction losses in gas pipes one must consider compressible flow. References for compressible gas pipe friction losses seem sparse, though one potentially relevant source by Turner and Yoos¹¹ has been identified. A closer look to this reference would be required to see if it covers pipe entry friction losses for gas flows.

E.2 Current implementation in DISC

The number of velocity heads lost through entrance to the pipe is taken from Vennard and Street (1982)¹², page 536:

$$F_{entry} = \frac{1}{(kC_v)^2} - 1 \quad (86)$$

C_v is the 'coefficient of velocity', which in the reference by Vennard and Street is given a constant value of 0.8 subject to the following assumptions:

- The flow is from a vessel into an attached short pipe, as opposed to a sharp-edged or rounded orifice
- Fairly high Reynolds number for C_v to be constant:
 - Pipe diameter larger than 25 mm
 - Liquid head larger than 1.2 m

The current implementation in DISC, however, does not apply a constant value of $C_v=0.8$. Instead, C_v is set equal to the discharge coefficient C_d for the equivalent orifice scenario with flashing allowed (orifice diameter = pipe diameter). This means that C_v can range from 0.6 (liquid releases) up to values towards 1 for vapour releases. Validation results in Section E.3 shows that the DISC implementation gives more accurate flow rates than the alternative formulations found in the literature.

Furthermore, the factor k is used to model the increase in frictional losses on entering the pipe through a constricted pipe entry where the diameter of the pipe entry D_o is smaller than the pipe diameter D_p . No such factor k appears in the reference by Vennard and Street, and as such this factor is of unknown origin. In DISC it is defined as

$$k = \min \left[R_{neq} \left(\frac{D_o}{D_p} \right)^2, 1 \right] \quad (87)$$

The smaller this ratio of diameters (*i.e.* the more constricting the pipe entry), the greater the frictional losses. R_{neq} is a safety factor to allow for possible under-estimation of the constricting pipe entry (used to allow for over-drilling in the relief valve scenario). For most short pipe scenarios there is no constriction at the pipe entry and so $k=1$. However, for the relief valve and control valve scenarios one may generally have $k<1$.

E.3 Modified pipe entry friction: selected validation

We here redo validation for two sets of experimental data for the full-bore rupture of subcooled liquid pipes, namely the Uchida and Nariai set and the Propane Shell set. The Sozzi and Sutherland experiments were excluded as flashing were reported along the pipe for these cases, which would invalidate the assumption of incompressible flow (Vennard and Street assumption when using $C_v=0.8$). These experiments are detailed in the DISC validation document – here we simply present the results of the revalidation exercise which is extended to include a modified pipe entry friction term based on Vennard and Street ($C_v=0.8$).

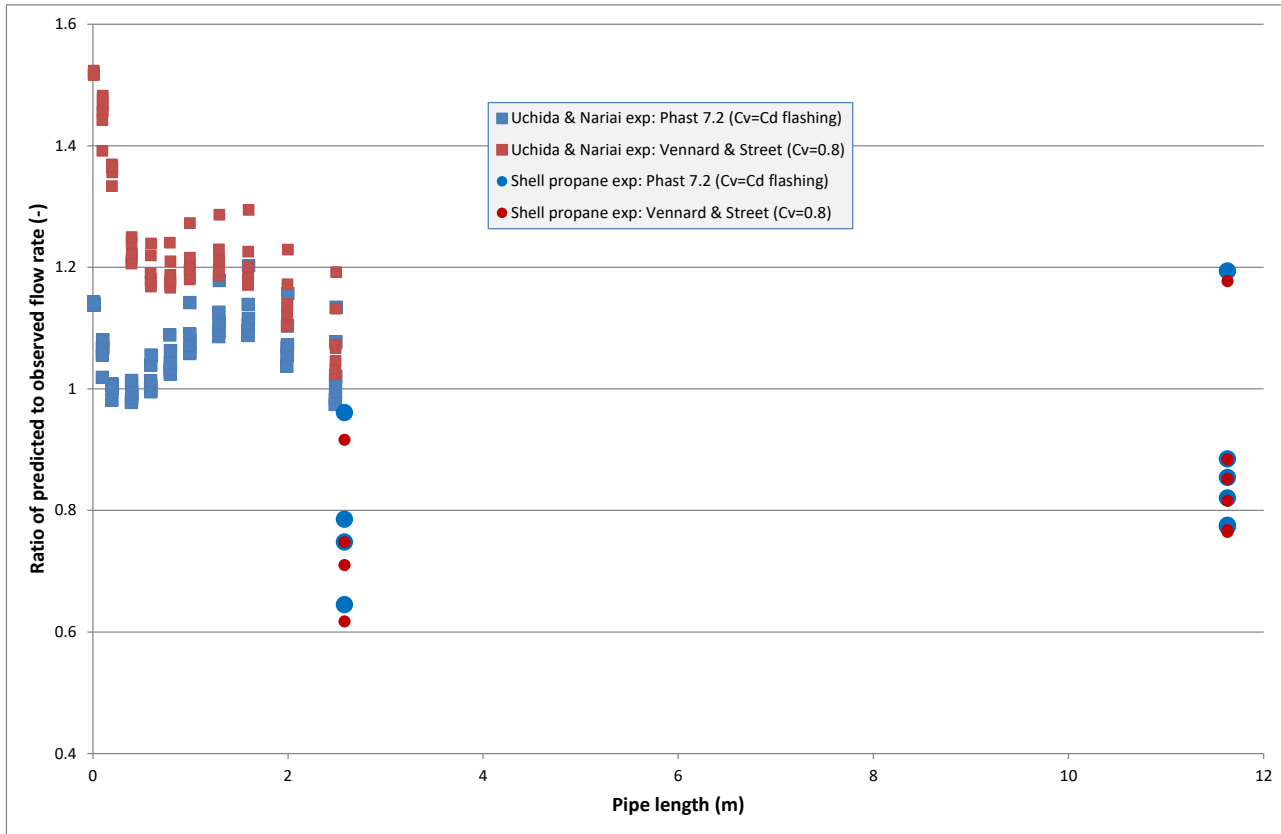


Figure 19: Ratio of predicted to experimental flow rates for two sets of subcooled line rupture cases (Uchida and Nariai (water) and Shell Propane).

shows the ratio of predicted to experimental flow rates for the Uchida and Nariai subcooled water line ruptures (square markers) and the Shell Propane subcooled line rupture (circular markers). Two sets of model predictions are compared with the experimental data: The default line rupture predictions in Phast 7.2 (blue markers) and the results when using a modified pipe entry friction term as given by Vennard and Street (red markers). It is clear that the default DISC implementation gives more accurate flow rates than the modified Vennard and Street approach for almost all the data considered.

Note that the Vennard and Street formulation gives higher flow rates than DISC default for the Uchida and Nariai cases. This is because Vennard and Street uses a fixed $C_v=0.8$, while the DISC default in these cases uses $C_v=0.6$. The latter gives higher pipe entry friction and thus smaller flow rates. Interestingly the opposite trend is observed for the Shell Propane cases where Vennard and Street actually gives lower flow rates than the default Phast approach. The explanation for this is that the calculated discharge coefficient used as C_v by DISC defaults ranges from 0.806 to 0.965 for these experiments.

E.4 Pipe entry friction test cases

It was shown in Section E.1 and Section E.2 that the current pipe entry friction term in DISC does not appear to be aligned with the literature. To gain an understanding of how this deviation impacts on results, two test spreadsheets were set up and run:

- Scenario: line rupture
- Fluid state:

- Vapour - ethane at 10 bara and 293.15 K
- Liquid - propane at 50 bara and 293.15 K
- Pipe diameter = 0.154 m
- Pipe roughness: 4.57e-5 m
- Pipe lengths: 1 m, 10 m, 100 m and 1000 m.
- Pipe entry friction:
 - Current DISC implementation ($C_v=C_d$), Vennard ($C_v=0.8$), Crane ($C_v=0.8165$) and McCabe ($C_v=0.8452$).
- Flow rate capping:
 - The default option of capping based on non-flashing orifice scenario
 - No capping
- Other inputs: defaults

The pipe entry friction term is expected to become less important the longer the pipe is due to increasing surface roughness friction along the pipe. When studying the impact of the pipe entry friction term it was therefore decided to run cases for a range of pipe lengths. It was also decided to run one liquid case and one vapour case as the calculated C_d used by DISC for pipe entry friction varies significantly depending on fluid state. The impact of removing the flow rate capping was also investigated. Results for the flow rates generated can be seen in **Table 3**. The following can be observed:

- The deviation increases for shorter pipes as the pipe entry friction term becomes more important as compared to the pipe surface friction.
- The deviation is larger for liquid than for vapour because the calculated discharge coefficient depends on the fluid state. The discharge coefficient for the liquid case was 0.6044 while for the vapour case it was 0.8704.
- The flow rate is capped by the orifice flow rate for all liquid cases with pipe lengths 1 m and 10 m. When capping occurs, the uncapped flow rate and uncapped deviation is given in brackets in **Table 3**.
- Note that the capped flow rate varies for different pipe entry friction formulations. This is because the discharge coefficient C_d used when running the orifice scenario to obtain the maximum flow rate is given by

$$C_d = \sqrt{\frac{1}{F_{entry} + 1}}$$

- Note that in current DISC implementation then $F_{entry} = \frac{1}{(kC_d)^2} - 1$. So if $k=1$ (no additional constriction nor overdrilling safety factor), then the C_d you send in to the orifice model to obtain a max flow rate is the same as the originally calculated C_d for the pipe entry friction. The question then is on what basis was this C_d originally calculated? Flashing/no flashing? What orifice diameter? Constricted or not? And could it be that the C_d used for calculating the max flow rate by orifice model need to take into account overdrilling/additional constriction and therefore is back-calculated from

$$C_d = \sqrt{\frac{1}{F_{entry} + 1}} ?$$



- Current DISC release rates are under-predicted for liquid. The under-prediction is significant for short pipes, and removing the capping makes the under-prediction even more significant.
- Current DISC release rates are slightly over-predicted for the vapour release cases.

Pipe length [m]	C_v [-]	Vapour ethane release		Liquid propane release	
		Release rate [kg/s] (Uncapped)	% deviation (Uncapped)	Release rate [kg/s] (Uncapped)	% deviation (Uncapped)
1	C_d	38.2 (47.7)	0	814.0 (1160.6)	0
	0.8	35.1 (43.5)	-8.1 (-8.8)	1085.3 (1915.5)	33.3 (65.0)
	0.8165	35.8 (44.4)	-6.2 (-6.8)	1107.7 (2035.5)	36.1 (75.4)
	0.8452	37.1 (46.1)	-2.9 (-3.3)	1146.6 (2274.9)	40.9 (96.0)
10	C_d	37.3	0	814.0 (907.6)	0
	0.8	35.1 (35.5)	-5.8 (-4.6)	1085.3 (1241.7)	33.3 (36.8)
	0.8165	35.8 (35.9)	-3.8 (-3.5)	1107.7 (1275.5)	36.1 (40.5)
	0.8452	36.7	-1.6	1146.6 (1334.9)	40.9 (47.1)
100	C_d	18.8	0	378.1	0
	0.8	18.6	-1.0	402.9	6.6
	0.8165	18.7	-0.7	404.4	7.0
	0.8452	18.7	-0.3	406.7	7.6
1000	C_d	6.8	0	122.8	0
	0.8	6.8	-0.1	123.6	0.6
	0.8165	6.8	-0.1	123.6	0.6
	0.8452	6.8	-0.04	123.7	0.7

Table 3. Release rates for different pipe entry friction formulations.

E.5 Conclusions and recommendations

We have shown that the DISC model applies a pipe entry friction force which is slightly different from those found in the literature. To understand the significance of this difference several test cases were studied and selected validation carried out. It turns out that the predictions by the default DISC model are more accurate than when using the Vennard and Street pipe entry friction based on the two experimental data sets considered. On this basis it can therefore not be recommended to adopt Vennard and Street's $C_v=0.8$ value above the current DISC default behaviour ($C_v=C_d$). Nevertheless a number of observations have been made for potential further investigation and improvement:

- Add the pipe entry friction loss as a model input
 - All friction losses except the entry friction loss can be specified by the user in the DISC pipe model. The amount of loss is also strongly dependent on the geometry of the vessel-pipe connection. As such it

would make sense to promote the pipe friction entry loss to a model input – either in terms of C_v input or velocity head loss input (K losses).

- The current pipe entry loss for an additional constriction has no known literature reference and could as such be considered further. This entry loss applies to relief valve scenarios where an additional constriction is specified and also to line rupture scenarios with fixed flow rate imposed by a control valve with opening diameter less than the pipe diameter.

NOMENCLATURE

A	Area (m ²)
C _D	Coefficient of discharge (-)
C _v	Coefficient of velocity (-)
D _p	pipe diameter (m)
E	Energy (J kg ⁻¹)
E _{exp}	Expansion energy (J kg ⁻¹)
f	Fanning friction factor (-), or force defect coefficient (-)
G	Mass flux (kg m ⁻² s ⁻¹)
g	Gravitational constant (m s ⁻²)
h	Specific enthalpy (J/kg)
K	Number of velocity head losses (-)
L	Length (m)
M	Mass (kg)
P	Pressure (Pa)
P _{st} [*]	Initial storage pressure (excluding head; corresponding to top of liquid) (Pa)
P _{st}	Initial storage pressure (including head; corresponding to orifice height) (Pa)
Q	Mass flow (kg s ⁻¹)
s	Specific entropy (J K ⁻¹ kg ⁻¹)
T	Temperature (K)
t _{rel}	Release duration (s)
u	Velocity (m s ⁻¹)
v	Specific volume (m ³ kg ⁻¹)
z ₀	Surface roughness (m)

Greek letters

ΔH	Head (m)
Δh	Specific enthalpy change (J kg ⁻¹)
ρ	Density (kg m ⁻³)
τ _o	Shear stress (N m ⁻²)
η	Liquid mass fraction (-)

Subscripts

X_a	Ambient
X_o	Orifice (pre atmospheric expansion)
X_i	Initial
X_f	Final (post atmospheric expansion)
X_{st}	Storage
X_c	Choke
X_L	Liquid
X_V	Vapour
X_e	Pipe exit



About DNV

We are the independent expert in risk management and quality assurance. Driven by our purpose, to safeguard life, property and the environment, we empower our customers and their stakeholders with facts and reliable insights so that critical decisions can be made with confidence. As a trusted voice for many of the world's most successful organizations, we use our knowledge to advance safety and performance, set industry benchmarks, and inspire and invent solutions to tackle global transformations.

Digital Solutions

DNV is a world-leading provider of digital solutions and software applications with focus on the energy, maritime and healthcare markets. Our solutions are used worldwide to manage risk and performance for wind turbines, electric grids, pipelines, processing plants, offshore structures, ships, and more. Supported by our domain knowledge and Veracity assurance platform, we enable companies to digitize and manage business critical activities in a sustainable, cost-efficient, safe and secure way.

REFERENCES

- ¹ Oke, A., and Witlox, H.W.M., "DISC validation document", March 2009, Phast Technical Reference (2009)
- ² Coulson, J.M., Richardson, J.F., "Chemical Engineering." Volume 1, 2nd Edition, Pergamon, Oxford, (1977).
- ³ Vennard, J.K. and Street, R.L., "Elementary Fluid Mechanics" 6th Edition, Wiley & Sons, New York (1982).
- ⁴ Webber, D., Witlox, H.W.M., and Stene, J., "Gaspipe theory documentation", Phast Technical Reference (2011)
- ⁵ Waller, A., "Realistic dispersion modelling of chlorine release incident." Process Industry Incidents Conference, Florida (2000)
- ⁶ Bragg, S.L. "Effect of Compressibility on the Discharge Coefficient of Orifices and Convergent Nozzles", Journals of Mechanical Engineering Science, Vol. 2, pp. 35-44 (1960).
- ⁷ McCabe, W.L., Smith, J.C., and Harriott, P., "Unit Operations of Chemical Engineering", (1993)
- ⁸ Crane, "Flow of Fluids Through Valves, Fittings and Pipe", Technical Paper No. 410 M, (1982)
- ⁹ Lees, Frank, "Loss Prevention in the Process Industries", (2004)
- ¹⁰ Munson, Young, Okiishi, and Huebsch, "Fundamentals of Fluid Mechanics", 6th Edition, Wiley & Sons, (2009)
- ¹¹ Turner, J.R. and Yoos, T.R., "Pressure loss calculation procedures for high speed gas flow in ducts", Dynatech Corp report submitted to U. S. Navy Bureau of Ships, (1961)
- ¹² Vennard, J.K. and Street, R.L., "Elementary Fluid Mechanics" 6th Edition, Wiley & Sons, New York (1982).