THEORY

TIME-VARYING DISCHARGE

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TVDI contains models for calculating the continuous time-varying discharge from a vessel with / without an attached pipe. Three types of failure / release scenarios may be simulated: (a) Leaks from the main process vessel; (b) Full bore rupture of connected pipe; (c) Discharge from pressure relieving devices (e.g. bursting discs or pressure relief valve).

The model handles multi-component fluid mixtures by splitting liquid and vapour phases and tracking the transient compositions as the release progresses.

TVDI is capable of simulating the simultaneous effects of production inflow and outflows (e.g. from connected pipework), blowdown, and isolation on the overall discharge process.

No.	Date	Reason for Issue	Prepared by	Verified by	Approved by
1	March 2009	Phast 6.6	Ade Oke	Witlox and Stene	
2	April 2009	Add gas theory	Witlox	Oke and Stene	
3	June 2009	General updates, added user guidance	Stene		
4	July 2010	Revised theory. Literature review addded to appendix.	Stene	Witlox	
5	May 2012	Revised TVDI for Safeti Offshore	Stene		
6	October 2012	Updates for Safety System Modelling	Stene		
7	October 2014	MC theory added, change of template	Stene		
8	May 2015	Update for Safeti Offshore 7.2	Stene		
9	October 2017	Update for Phast/Safeti 8.0	Stene		
10	March 2018	Update for Phast/Safeti 8.1	Stene		
11	May 2019	Update for Safeti Offshore 7.7	Stene		
12	April 2020	Update for Phast/Safeti 8.4	Stene		
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ABSTRACT

This report describes the revised time-varying discharge model (TVDI), which replaces the old TVDI model present in Phast and Safeti versions up to and including 7.21. The revised TVDI model is also present in all versions of Safeti Offshore. TVDI determines the transient variation of release, fluid inventory and vessel (thermo-physical) conditions following a loss of containment event. The vessel may contain single (pure gas), or multi-phase (i.e. vapour-liquid) fluids. For multi-phase containment, the release could either occur from the vessel's vapour or liquid space and may involve single or two-phase flow.

Three types of release scenarios can be simulated. These are:

- Leaks from the main process vessel.
- Full bore rupture of connected pipe.
- Discharge from pressure relieving devices (e.g. bursting discs or pressure relief valve).

TVDI employs the DISC suite of discharge models, described in the DISC modelling manual, in simulating fluid flow due to expansion from storage conditions to a vessel orifice or short pipe exit. The modelling of subsequent expansion to atmospheric conditions for each source-term is carried out by the ATEX model (described in the ATEX modelling manual). The underlying theory for modelling release from a vapour or a multi-phase vessel is presented, together with a brief indication of how that theory is applied to obtain a solution.

An important extension in the revised TVDI model compared to the old TVDI model is the ability to account for the effects of production inflow and outflows as well as safety systems in the form of isolation and blowdown. Another crucial improvement is the addition of rigorous multi-component treatment of fluid mixtures which allows tracking of the time-varying vapour and liquid compositions.

Table of contents

1 INTRODUCTION

1.1 Model overview

Hazardous chemicals are frequently stored in vessels. Following a loss of containment event, the hazardous chemical will be discharged to the atmosphere. The **t**ime-**v**arying **di**scharge model TVDI determines the transient variation of release and containment (fluid – vessel physical and thermo-physical) conditions following such a loss of containment event. The vessel storage conditions may be categorized as follows:

- Homogeneously mixed vessel contents:
  - Initially pure gas vessel, may undergo condensation during release
  - Initially at two-phase conditions with liquid and vapour homogeneously mixed in the tank
- Stratified liquid-vapour vessel contents with liquid phase at the bottom of the vessel and vapour phase above the liquid:
  - Two-phase liquid and vapour
  - Pressurized liquid padded by inert gas (nitrogen)

For a homogeneously mixed fluid containment, the release phase will be either pure vapour or two-phase, whereas for a stratified two-phase containment, the release could either occur from the vapour or liquid space, but not from both vapour and liquid space simultaneously (i.e. only single phase fluid approaching the orifice at any given moment in time[i]). The hole or pipe entry may be present in initially any of the two phases, and the discharged fluid phase may change from liquid to vapour as a function of time. Finally, for a padded liquid containment, only liquid release is considered.

A schematic illustration of the release scenarios is given in Figure 1. Note that there is currently no support for multiple leaks/line ruptures from the same vessel – the model is limited to release from one single source. Three types of accident scenarios can currently be simulated[ii], and these are

- leaks from an orifice in the main process vessel,
- full bore rupture of connected pipework, and
- discharge from pressure relieving devices (e.g. bursting discs or pressure relief valve).

For the above release scenarios, TVDI employs the DISC suite of discharge models, described in the DISC model theory document, in simulating fluid flow due to expansion from upstream conditions to a vessel orifice or short pipe exit. The modelling of the subsequent expansion to atmospheric conditions is carried out by the ATEX model. The ATEX model theory document describes this final stage of expansion for all discharge models. The transient vessel response is calculated by TVDI itself, and key model assumptions include:

- No heat transfer between fluid and vessel or between vessel and the external surroundings[iii]. Heat gain/losses due to mass inflow/outflows are taken into account.
- Liquid phase, vapour phase and vessel walls are in thermal equilibrium at all times (homogeneous equilibrium).
- The following mass flows are considered: production inflow into the vessel, production liquid and vapour outflows out of the vessel, accident outflow and outflow through a blowdown valve.
- For a homogeneously mixed containment the accident release phase is either vapour or two-phase, whereas for stratified liquid-vapour vessels the accident release phase is either vapour or liquid.
- Liquid swell is ignored (i.e. no vapour entrained in the liquid)
- Impact of safety systems is taken into account: isolation and blowdown occurs at times as specified by the user.
- Multi-component treatment of fluid mixtures: for two-phase mixtures the liquid and vapour space compositions will be different and these will be tracked dynamically as the release progresses

The model input includes material type and mass, storage conditions of material and composition in case of mixtures, the geometry and dimensions of the vessel/pipe, accident data (scenario type, orifice size etc), safety system data and ambient conditions. Mass flow rate, velocity, temperature, droplet size and liquid fraction of the discharged material are among the key output results from the model.

[i] FUTURE. This is based on an assumption of zero vapour entrainment in the liquid.

[ii] Venting of vapour from a tank during a filling operation is only supported in DISC as a steady state discharge model

[iii] FUTURE. Heat transfer processes are currently ignored in the first version of the model but may be included in future versions.

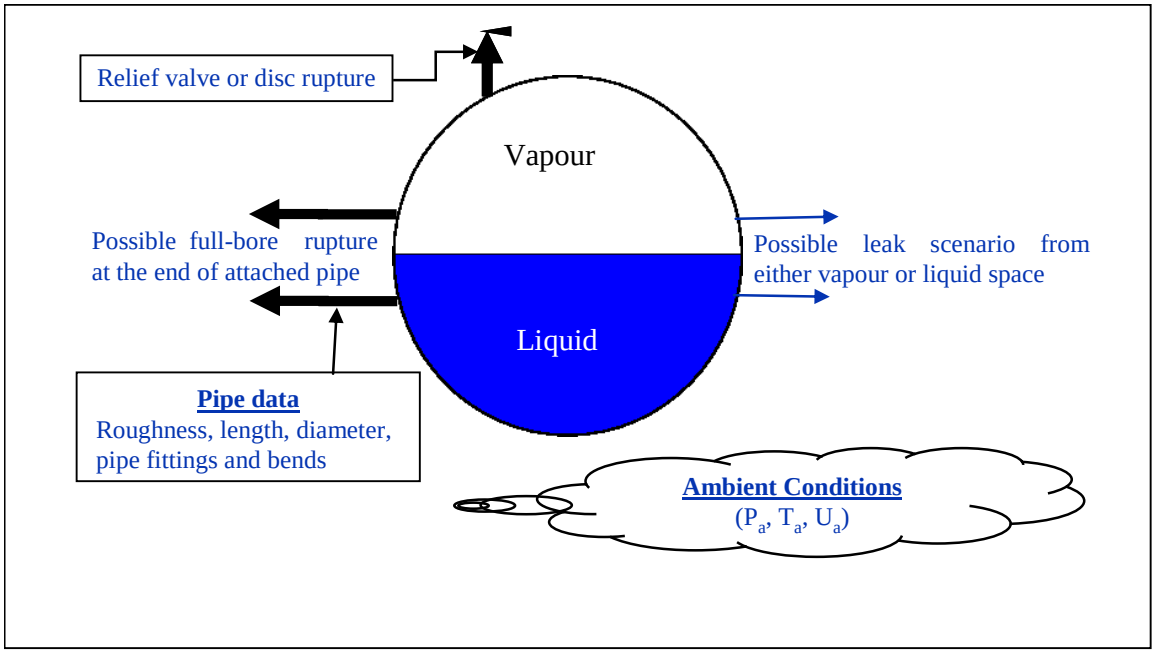


Figure 1: Schematic illustration of TVDI release scenarios

Release scenarios include vessel leak (liquid or vapour part of vessel), release from end of pipe attached to vessel (liquid or vapour part), relief valve or disc rupture (vapour or two-phase)

Note that TVDI is applicable only for the scenarios as indicated above. Separate discharge models exist in Phast for other discharge scenarios, e.g. time-dependent vapour or two-phase discharge from long pipelines (GASPIPE or PIPEBREAK).

1.2 TVDI in Phast and Safeti 8.4

This document describes the TVDI model with all its general functionality. Most of this functionality is available in Phast and Safeti 8.4 with one important exception:

- No multi-component modelling, i.e. the traditional pseudo-component approach is used for mixtures.

The intention is to make the multi-component modelling available in future versions of Phast and Safeti, aligning with the version of TVDI found in the Safeti Offshore product.

1.3 Contents and organization

The old TVDI model (present in versions prior to Phast and Safeti 8.0), suffers from numerical instability for certain scenarios. Before extending the functionality of the old TVDI model, it was crucial to first establish a robust model that is fully understood. To achieve this it has been decided to revise some of the theory of the old TVDI model as it appears unnecessarily complex. It is the revised theory and associated solution algorithm that is presented in this document with the resulting model referred to as the “new” or “revised” TVDI model. Chapter 2 describes mathematical models for simulating loss of containment for the relevant scenarios, while Chapter 3 covers details on the safety system modelling. Chapter 4 includes multi-component modelling, while Chapter 5 deals with specific issues near the critical point. Chapter 6 summarises future developments, while detailed model input and output can be found in Appendix A. A literature review of liquid swell modelling is included in Appendix B, and a more general top-level overview of blowdown models is presented in Appendix C. Potential extensions to heat transfer modelling are given in Appendix D.

1.4 Publications

Two publications on the TVDI model may be of interest:

- The first paper presents the model and focusses on production flow and safety system modelling[1].
- The second paper presents a multi-component extension of the model and studies how a rigorous treatment of mixtures impacts on the results[2].

2. TVDI THEORY

2.1 Top-level theory

The main extensions compared to the previous TVDI model are the modelling safety systems (including production flows) and rigorous multi-component treatment of mixtures. Furthermore, the revised model has a unified theory encompassing vessels with both pure gas and two-phase fluid, which contrasts the old model where two completely different sub-models were used.

For modelling purposes, the definition of the system consists only of the fluid contained in the vessel, excluding vessel/pipe walls[iv] and also excluding any fluid in any attached pipe. The contained fluid, which may be single phase (i.e. pure gas) or two-phase (liquid-vapour), is assumed to be in homogeneous equilibrium throughout the release.

2.1.1 Mass balance

The adopted model assumptions are as follows:

- Production flows. The model can account for fluid entering the vessel as a single production inflow with a user-specified, constant flow rate. In addition there is fluid leaving the vessel as a liquid production outflow and a vapour production outflow (one or two production outflows are present depending on the vessel type).
- Accidental outflow. The accident is modelled as fluid leaving the system through one single orifice / pipe entrance[v]. The multiple leak locations shown in Figure 1 are only for illustration purposes.
- Isolation. As a safety system measure, production inflow and outflows may be shut off at a user-specified isolation time.
- Blowdown. As a safety system measure to reduce the pressure driving the accidental release, fluid may be evacuated through a blowdown valve of a given size. This evacuation occurs from the vapour space and commences at a user-specified blowdown time
- Air ingestion through release plane[vi]. If the stagnation pressure drops below ambient pressure then air from the outside will be sucked into the vessel – a phenomenon often referred to as air ingestion or 'gulping'. This is taken into account in the present TVDI model for padded liquid vessels[vii], but not for other two-phase vessels.
- Vacuum relief valve. To avoid sub-atmospheric pressure in the vapour space of a closed vessel, a vacuum relief valve may be present. Such a valve is taken into account in the present TVDI model for padded liquid vessels[viii], but not for other two-phase vessels.
- No other inflow or outflow out of vessel

The mass balance equation presented below is valid for a pure single component fluid – for the more complex case of multi-component mixtures see Chapter 4. The mass balance for a single component fluid with assumptions as given above may be expressed as

$$\frac{dM(t)}{dt} = \dot{m}_{in} - \dot{m}_{acc} - \left(1 - x_{V,N_2}\right)\dot{m}_{BD} - \dot{m}_{out}^{vap} - \dot{m}_{out}^{liq}\,, \qquad (1)$$

where $M(t)$ is the total mass of hazardous material in the system at time t. The production inflow rate is denoted $\dot{m}_{in}$, while $\dot{m}_{out}^{vap}$ and $\dot{m}_{out}^{liq}$ is the production vapour and liquid outflow, respectively. Both the accidental flow rate $\dot{m}_{acc}$ and blowdown flow rate $\dot{m}_{BD}$ are calculated by utilizing the steady-state DISC sub-model at each time step. Note that the mass fraction of nitrogen in the vapour space, x_{V,N_2}, is only non-zero for pressurized liquid vessels. Details about all of the terms in Equation (1) can be found in subsequent sections.

[iv] CHANGE: The system in the old multi-phase model is the liquid and the vessel/pipe walls.

[v] FUTURE: This could be relaxed to allow accidental outflow from several locations

[vi] CHANGE: 'Gulping' was taken into account in the old TVDI, though in a very crude manner.

[vii] As an approximation, the model ingests pure nitrogen as opposed to actual air

[viii] CHANGE: In the old version, vacuum relief valve was supported also for two-phase vessels

For padded liquid vessels, where nitrogen is present in the vapour space, we have an additional mass balance equation for nitrogen mass in the vapour space M_{N_2}:

$$\frac{dM_{N_2}(t)}{dt} = -x_{V,N_2}\,\dot{m}_{BD}\,. \qquad (2)$$

Note that there is no term for air ingestion in the differential equation for the mass balance as the air ingestion is assumed to happen instantaneously – see Section 2.2.3 for further details.

2.1.2 Energy balance

The adopted top-level model assumptions are as follows:

- Negligible potential energy
- No external work is added to the system by e.g. pumps
- No heat transfer between fluid and vessel wall.
- The vessel is assumed to be adiabatic, i.e. no heat transfer between the vessel walls and the surroundings[ix].
- No heat transfer due to potentially ingested air
- Heat loss due to loss of fluid:
  - Production vapour and liquid outflows
  - Accidental outflow
  - Blowdown outflow
- Heat gain due to fluid inflow:
  - Production inflow

The old TVDI model has some additional assumptions applied:

- Negligible kinetic energy
- Negligible work by fluid expansion (enthalpy equal internal energy)

The energy balance of the system may then be expressed in terms of the internal energy U, namely[x]

$$\begin{aligned}\frac{dU}{dt} = {} & \dot{m}_{in}\left[h\left(P(t=0),T(t=0);\eta_{in}^{liq}\right)+\frac{1}{2}u_{in}^2\right] \\ & -\dot{m}_{acc}\left[h\left(P_{acc},T_{acc};\eta_{acc}\right)+\frac{1}{2}u_{acc}^2\right] \\ & -\dot{m}_{BD}\left[h\left(P_{BD},T_{BD};\eta_{BD}\right)+\frac{1}{2}u_{BD}^2\right] \\ & -\dot{m}_{out}^{vap}\left[h\left(P,T;\eta_{out}^{vap}\right)+\frac{1}{2}\left(u_{out}^{vap}\right)^2\right] \\ & -\dot{m}_{out}^{liq}\left[h\left(P_{out}^{liq},T;\eta_{out}^{liq}=1\right)+\frac{1}{2}\left(u_{out}^{liq}\right)^2\right].\end{aligned} \qquad (3)$$

[ix] CHANGE: The old TVDI multi-phase model takes into account heat transfer between surroundings and the liquid-vessel system, though all coefficients are hard-coded.

[x] Kinetic energy was ignored in the old TVDI model but is included as a parameter option in the new model. This is consistent with the DISC model, both for orifice and pipe scenarios.

where h is the specific enthalpy[xi], η is the liquid mass fraction and u is the velocity; all quantities relate to fluid entering/leaving the vessel. Further details can be found in Chapter 3.

In addition to tracking the internal energy, the work carried out by the expanding gas is taken into account[xii] through the use of the total system enthalpy H,

$$\begin{aligned} H(P,T) &= U(P,T) \quad \text{(Old TVDI)} \\ H(P,T) &= U(P,T) + \iiint_{System} P dV \quad \text{(New TVDI)} \end{aligned} \tag{4}$$

where P is the pressure in the system. If we assume that the pressure is constant equal to the vapour space pressure P throughout the vessel, then the energy associated with *PV* work simplifies:

$$H(P,T) = U(P,T) + PV\,. \tag{5}$$

However, in reality the pressure will only be constant in the vapour space, while in the liquid space (if present) the pressure will vary with the liquid height and we may re-express the total system enthalpy as

$$H(P,T) = U(P,T) + \int_0^{Z_{\text{tank}}} A(z)\,P(z)\,dz\,, \tag{6}$$

where $A(z)$ is the horizontal cross-sectional area of the storage vessel at height z. For tanks with constant cross-sectional area this simplifies to

$$H(P,T) = U(P,T) + PV + \frac{1}{2} M_L g Z_L\,. \tag{7}$$

See Section 2.3.6 for derivation of the above expression and for tanks with variable cross-sectional areas.

The constant system volume (vessel volume) is denoted by V and relates to the system mass M through

$$M(t)\,v(t) = V\,, \tag{8}$$

where v is the average specific volume of the fluid in the vessel. Note that the three Equations (1), (3) and (5) constitute the three main equations for the three primary variables mass M, internal energy U and pressure P.

2.2 Different vessel types: Detailed theory and algorithm

The TVDI model considers four different vessel types depending on the initial storage conditions:

- **Pure gas or homogeneous two-phase vessel**: Initial storage conditions (P,T) correspond to either
  - the gas phase of the stored material or
  - two-phase fluid with liquid assumed to be homogeneously mixed in the vapour space
- **Stratified two-phase vessel**: Initial storage conditions (P,T) give two-phase fluid with liquid assumed at the bottom and vapour on top of the liquid (saturated conditions for pure components)
- **Pressurized liquid vessel**: The initial storage conditions (P,T) correspond to the liquid phase of the stored material

[xi] Like in the old model, the specific enthalpy is evaluated at stagnation conditions – this is strictly speaking not accurate as the discharged material is leaving the orifice/pipe exit and the specific enthalpy should accordingly be evaluated at the correct pressure and temperature.

[xii] CHANGE: The old TVDI model ignores this expansion energy for multi-phase vessels but includes it for pure gas vessels, which assumes isentropic expansion.

- **Atmospheric storage tank**: The pressure P is assumed to be ambient while the temperature T is given by the user. The input temperature must be below the boiling point temperature at ambient pressure, so we have pure liquid storage.

Each of first three vessel types are all governed by the same system of differential-algebraic equations, namely (1), (3) and (5). The atmospheric storage tank is simpler and governed by the mass balance only (1). There are still significant differences in the modelling of the transient vessel response during the discharge process depending on the initial storage phase, and more detailed theory for each of the vessel types are provided below.

2.2.1 Pure gas or homogenous two-phase vessel (PG-H2PH)

The hazardous material in the system may initially be stored as a pressurized pure gas. Condensation may occur during the discharge process, resulting in two-phase conditions in the vessel. In this case it is assumed that the liquid is uniformly dispersed in the vessel, as opposed to a liquid pool forming at the bottom of the vessel. Therefore the fluid approaching the orifice/pipe entry is homogenous two-phase when condensation occurs inside the vessel.

Primary and secondary variables
The primary and secondary variables for the pure gas vessel are as for the stratified two-phase vessel described in 2.2.2 with the following exceptions for secondary variables:

- Additional secondary variable specific enthalpy:
  - $h = \frac{H}{M}$
- The temperature will be obtained from a fixed enthalpy/fixed pressure flash calculation:
  - $(T, \eta, \rho) = f(h, P)$

  For the special case of a pure component two-phase fluid, the temperature is simply the saturation temperature at the given pressure.
- For pipe releases, some of the secondary variables will be evaluated differently – in particular some quantities will have the same value at the pipe entrance as in the vessel since the pipe is not part of the system:
  - $P_O = P$
  - $\eta_O = \eta$
  - $\rho_O = \rho$
- There will be no separate liquid phase – in case of condensation the liquid is assumed to remain uniformly dispersed in the vapour space. The following secondary variables that are used for stratified two-phase vessels are therefore irrelevant in this case:
  - P_{st}, ΔZ_L, Z_L, V_L, ρ_L

2.2.2 Stratified two-phase vessel (S2PH)

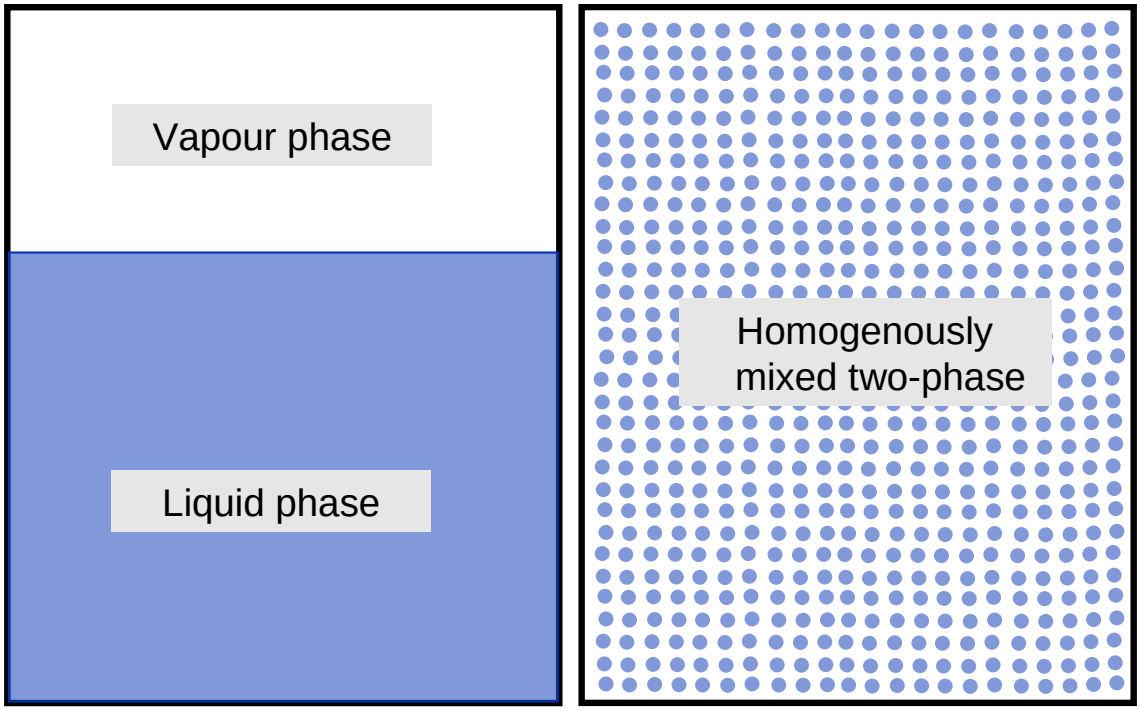
The multi-phase thermodynamic model considers all fluid phases within the vessel to be in thermal equilibrium at all times[xiii] (known as the homogenous equilibrium assumption). The following considerations are based on assumptions of pure-component two-phase storage, and the depressurization process follows the saturation curve.

For two-phase storage, the liquid is assumed to be at the bottom of the vessel with the vapour filling the space above the liquid – see Figure 2 (a) for an illustration. Thus no vapour is entrained in the liquid, nor is there any liquid dispersed in the vapour space. Thus the fluid approaching the orifice is either 100% liquid or 100% vapour depending on the orifice location. During the release, there may be a transition from liquid to vapour release if the liquid level drops below the orifice. However, for the purpose of thermodynamic equilibrium calculations carried out by the model, it is assumed that the fluid is homogeneously mixed as illustrated in Figure 2 (b). The

[xiii] The submodel DISC allows use of the meta-stable liquid assumption which entails non-equilibrium in the orifice, though equilibrium still prevails inside the vessel itself.

mass fraction of liquid in the vessel, η_L, is the same in both Figure 2 (a) and (b). The assumption that vessels (a) and (b) are thermodynamically equivalent is a simplification:

In vessel (a), the top layer of the liquid is in thermodynamic equilibrium with the vapour and therefore at saturated conditions. However, the liquid below the top layer is sub-cooled since the pressure $P_L > P = P_{sat}$ due to liquid head. This contrasts the situation in vessel (b) where all the liquid is assumed to be at saturated conditions in a homogeneous mixture. The question is then how similar are vessel (a) and (b) thermodynamically?



(a) Separated phases (b) Homogeneously mixed phases

Figure 2: Two different interpretations of the same vessel: (a) for discharge purposes, and (b) for the purpose of thermodynamic calculations

Primary variables and their initial calculation

- M - total system mass, Equation (1)
- U - total system internal energy, Equation (3)
- P - vapour space pressure, Equation (5)

Assuming saturated storage conditions, the user supplies either pressure $P(0)$ or temperature $T(0)$ and two out of vessel dimensions, material mass $M(0)$ and liquid fill fraction by volume $\eta_{fill}(0)$. We then have the relations

$$V = V_L + V_V \quad (9)$$

and

$$M = \rho_L(P,T)\,V_L + \rho_V(P,T)\,V_V\,, \tag{10}$$

where subscripts L and V refer to liquid and vapour phases, respectively. One may calculate the liquid volume V_L from

$$V_L = \frac{M - V\rho_V(P,T)}{\rho_L(P,T) - \rho_V(P,T)}. \tag{11}$$

For the case when *M* and *V* is specified, the liquid fill fraction by volume is then simply

$$\boldsymbol{\eta_{\text{fill}} = \frac{V_L}{V}} \tag{12}$$

When the mass and liquid fill fraction is supplied then we can obtain the required vessel volume from

$$\boldsymbol{V = \frac{\eta_{\text{fill}} M}{\rho_L} + \frac{(1-\eta_{\text{fill}})M}{\rho_V}} \tag{13}$$

Similarly, the mass inventory can be calculated when the volume and liquid fill fraction is input:

$$\boldsymbol{M = \frac{\rho_V \rho_L V}{(1-\eta_{\text{fill}})\rho_L + \eta_{\text{fill}}\rho_V}} \tag{14}$$

The total specific enthalpy for the system h can then be calculated from

$$h(P,T) = \eta_L h_L(P,T) + (1-\eta_L)\,h_V(P,T)\,, \tag{15}$$

where the liquid and vapour specific enthalpies h_L and h_V are obtained from the property system, and η_L is the liquid mass fraction. One may then obtain total system enthalpy $H(P,T) = M\,h(P,T)$ and total internal energy $U(P,T) = H(P,T) - PV$.

Secondary variables and their calculation

- Total system enthalpy $H = U + PV$
- Orifice / pipe entry data:
  - Common for orifice and pipe releases:
    - $\dot{m}_{DISC}$ (from DISC)
  - Unique to orifice releases:
    - T_O, P_O, η_O, u_O (all from DISC)
  - Unique to pipe releases:
    - $T_O = T$, $P_O = P_{st}$, $\eta_O = \eta_{st}$, $u_O = \dfrac{\dot{m}_{DISC}}{A\rho_O}$,
    - $\eta_{st} = \begin{cases} 1 & \text{if } \Delta Z_L > 0 \\ 0 & \text{otherwise} \end{cases}$, $\rho_O = \begin{cases} \rho_L & \text{if } \Delta Z_L > 0 \\ \rho_V & \text{otherwise} \end{cases}$.
- From the property system:
  - $T = T_{sat}(P)$

- $\rho_L = \rho(P,T,\eta=1)$
- $\rho_V = \rho(P,T,\eta=0)$
- $h_O = f(P_o,T_o;\eta_o)$

- Hydrostatic and liquid head:
  - $P_{st} = P + \rho_L(P,T)\, g\, \Delta Z_L$
  - $\Delta Z_L = Z_L - Z_O$
  - $Z_L = f(V_L, \text{geometry})$
  - $V_L = \dfrac{M - V\rho_V(P,T)}{\rho_L(P,T) - \rho_V(P,T)}$

2.2.3 Pressurized liquid vessel (PL)

The stored hazardous material may be a pressurized liquid. In this case there would be a pressurizing gas in the vessel above the liquid – an inert padding gas like nitrogen stored at high pressure. There will also be a certain amount of the stored hazardous material in the vapour space, so in practice there would be a multi-component vapour space mixture – see Figure 3 for a schematic illustration. This vessel type only allows for accidental outflow from the liquid space of the vessel.

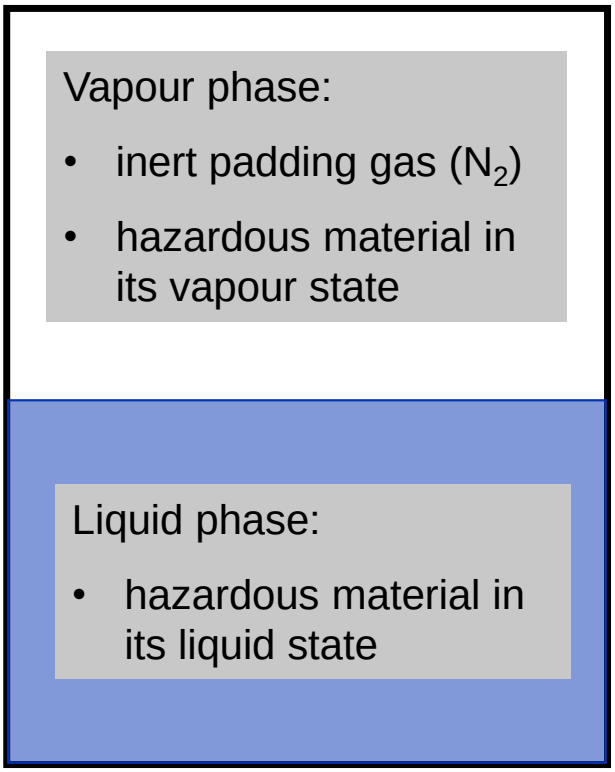


Figure 3: Schematic illustration of a pressurized liquid vessel.

Primary variables and their initial calculation

The primary variables remain the same as for the two-phase vessel and the pure gas vessel, through their initial calculation differ. Knowing the mole vapour fraction of the hazardous material *k* as given by Equation (32) we may also calculate the mass vapour fraction $x_{V,k}$ of material *k*. The user supplies storage conditions (P,T), and from the property system one may then obtain liquid and vapour density ρ_L and ρ_V, respectively. Further user input is two out of mass of hazardous material *k*, M_k, vessel dimensions (and thereby vessel volume) and liquid fill fraction η_{fill}. Assuming the case with mass M and volume V input, remaining unknowns still include volume of liquid and vapour space V_L and V_V, liquid mass $M_{L,k}$, mass of material *k* in the vapour space $M_{V,k}$, total vapour space mass M_{vap} and mass of nitrogen M_{N_2}. These six unknowns can be found from the following six Equations:

$$V = V_V + V_L, \quad (16)$$

$$x_{V,k} = \frac{M_{V,k}}{M_V}, \quad (17)$$

$$M_V = \rho_V V_V, \quad (18)$$

$$M_k = M_{V,k} + M_{L,k}, \quad (19)$$

$$M_{L,k} = \rho_L V_L, \quad (20)$$

$$M_{N_2} = M_V - M_{V,k}. \quad (21)$$

One may then solve for the unknowns – in particular one can obtain

$$V_L = \frac{M_k - x_{V,k}\rho_V V}{\rho_L - x_{V,k}\rho_V} \quad (22)$$

$$M_{N_2} = \rho_V (V - V_L)(1 - x_{V,k}), \quad (23)$$

and thus the total system mass M

$$M = M_k + M_{N_2}. \quad (24)$$

The liquid fill fraction by volume is then simply

$$\boldsymbol{\eta_{\text{fill}} = \frac{V_L}{V}} \quad (25)$$

When the mass and liquid fill fraction is supplied then we can obtain the required vessel volume from

$$\boldsymbol{V = \frac{M}{(\eta_{\text{fill}}\,\rho_L + x_V \rho_V (1 - \eta_{\text{fill}}))}} \quad (26)$$

Similarly, the mass inventory can be calculated when the volume and liquid fill fraction is input:

$$\boldsymbol{M = V\,(\eta_{\text{fill}}\,\rho_L + x_V \rho_V (1 - \eta_{\text{fill}}))} \quad (27)$$

The total system enthalpy H may be calculated as

$$H = M_{N_2} h_{N_2}(P,T) + M_{V,k} h_{V,k}(P,T) + M_{L,k} h_L(P,T). \quad (28)$$

Finally, the initial calculation of the total system energy can be done through $U(P,T) = H(P,T) - PV$.

Secondary variables and their calculation
The secondary variables used for the two-phase vessel (S2PH) are still used though some are calculated in a different manner:

- The temperature T : For a saturated vessel the temperature is simply obtained from the saturated vapour curve, while the temperature for the pure gas vessel is obtained from a fixed enthalpy, fixed pressure flash. Neither of these two approaches is suitable for the pressurized liquid scenario due to the presence of an inert padding gas in the vapour space. As such the temperature T will be obtained through iteration until Eq. (28) is satisfied.
- It is assumed that the discharge calculations terminate when the liquid head ΔZ_L reaches zero. Thus, for pipe releases we will always have:
  - $\eta_O = 1$
  - $\rho_O = \rho_L$

Furthermore, there are some additional secondary variables applicable to the pressurized liquid scenario – mainly related to the presence of the inert padding gas in the vapour space:

- Mole fraction of haz. material in vapour space $y_{V,k}$
- Mass fraction of haz. material in vapour space $x_{V,k}$
- Vapour mass of haz. material $M_{V,k}$
- Liquid mass of haz. material $M_{L,k}$
- Liquid specific enthalpy h_L
- Vapour specific enthalpy h_V

The calculation of these variables is mainly given above, but we here provide details on how to find the mole fraction of hazardous material in the vapour space. Without loss of generality we may assume that the inert padding gas is nitrogen. Assuming Raoult's law is valid we have

$$P_{pp,k}(T) = P_{V,k}^{sat}(T) y_{L,k}. \quad (29)$$

Here $P_{pp,k}$ is the partial pressure of component *k*, $P_{V,k}^{sat}$ is the saturated vapour pressure of component *k* and $y_{L,k}$ is the liquid mole fraction of component *k* in the liquid. If in this case of a pressurized liquid we assume that the pressurizing gas is non-condensable and that the stored material is a pseudo-component liquid, then $y_{L,k} = 1$ and Equation (29) simplifies to

$$P_{pp,k}(T) = P_{V,k}^{sat}(T). \quad (30)$$

Further assuming an ideal gas mixture in the vapour space, Dalton's law yields the mole fraction of the hazardous material in the vapour space

$$P_{pp,k} = P\, y_{V,k}\,. \qquad (31)$$

Combining Raoult's and Dalton's law through Equation (30) and Equation (31) we then get

$$y_{V,k} = \frac{P_{V,k}^{sat}(T)}{P}\,. \qquad (32)$$

Vacuum relief valve and gulping
The vapour space pressure may drop below ambient pressure as the vapour space expands during liquid discharge. The TVDI model for pressurized liquids handles this in a certain manner depending on whether a vacuum relief valve is present or not:

- The presence of a vacuum valve is model input
- When a vacuum valve is present:
  - the vacuum valve opens when the vapour pressure falls below a user-specified set pressure
  - default valve opening pressure equals the ambient pressure
  - subsequent discharge modelling after vacuum valve opening is carried out based on these assumptions:
    - Transition to "atmospheric liquid" vessel:
      - Redefine system to include only the liquid mass, thereby ignoring potential evaporation/condensation
      - Keep pressure on top of liquid constant equal to the valve set pressure
      - Keep temperature constant
      - See Section 2.2.4 for details.
- When a vacuum valve is not present:
  - The vapour space pressure may drop below ambient pressure ('vacuum')
  - When the stagnation pressure (vapour pressure plus liquid head) drops below the ambient pressure, air will be ingested into the vessel through the release orifice – a phenomenon sometimes called 'gulping'.
  - The ingested air is approximated by nitrogen for simplicity as the vapour space of a pressurized liquid vessel already contains this component
  - The mass of nitrogen ingested is such that the vapour space pressure immediately after ingestion equals the ambient pressure.
  - The ingestion is assumed to happen instantaneously and there is therefore no air ingestion term in the mass balance ODE (1).
  - Any heat transfer related to gulping is ignored.

2.2.4 Atmospheric storage tank (AST)

When the storage tank contains liquid at ambient pressure vented to the atmosphere, we apply the "atmospheric storage tank" (AST) sub-model. This is a particularly simple case where the pressure remains ambient and all energy transfer is ignored, so the system has a constant temperature. The system can in this case be described by the mass balance equation (1), and the driving force for the release is the liquid head.

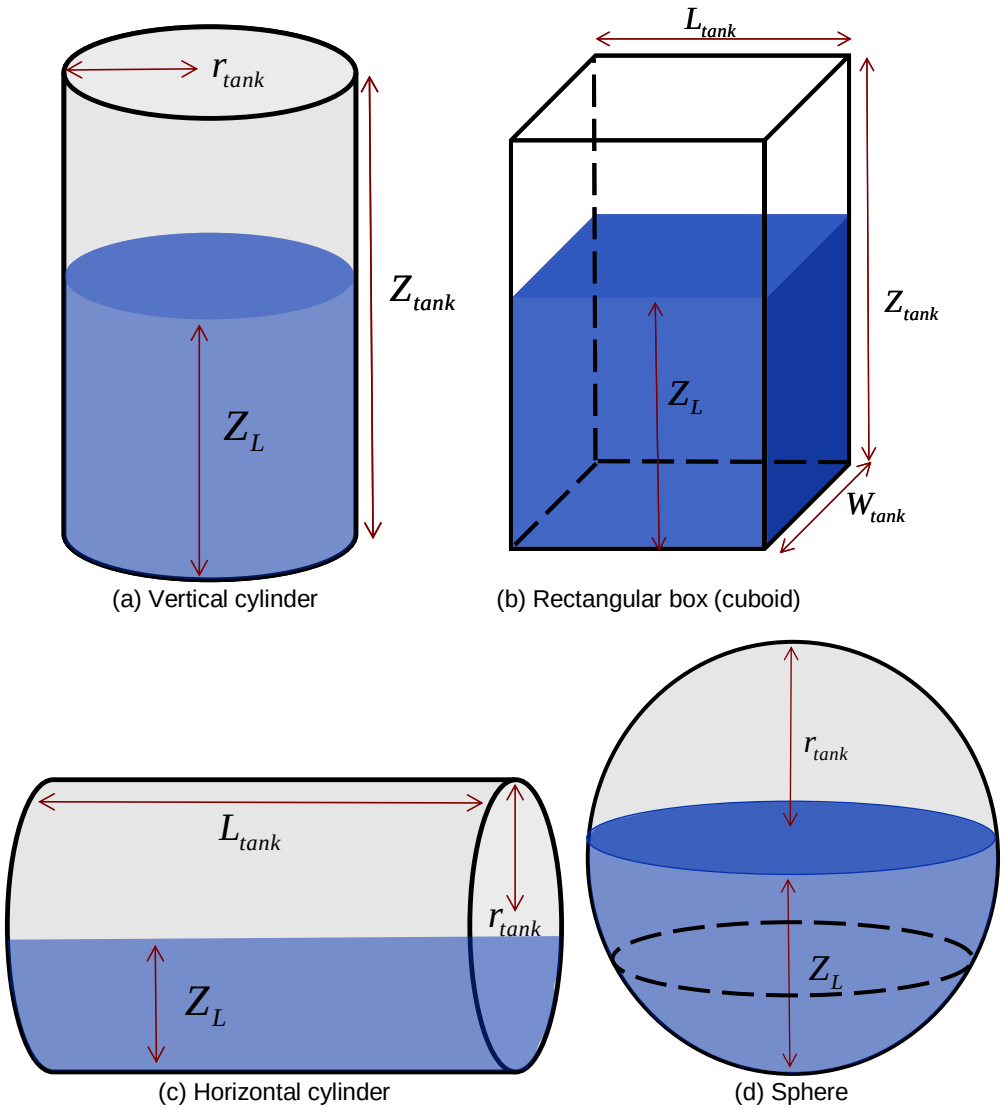
As mentioned in Section 2.2.3, a pressurized liquid vessel can transition to an atmospheric storage tank situation when a vacuum valve is open and the pressure drops to the set pressure of the valve.

2.3 Other modelling aspects: detailed theory

2.3.1 Geometry modelling

The geometry modelling in TVDI is employed in determining the vessel and time-varying liquid inventory volumetric characteristics. TVDI can be configured to model releases from any of the following four containment types:

- Vertical cylindrical tanks
- Rectangular tanks (cuboids)
- Horizontal cylindrical tanks
- Spherical tanks



(a) Vertical cylinder (b) Rectangular box (cuboid)

(c) Horizontal cylinder (d) Sphere

Figure 4: The various tank types supported by TVDI

The tank shapes and associated physical dimensions are given in Figure 4. For a given mass inventory[xiv], vessel type and dimensions, the following data are derived from the geometrical model for use in the time-varying mass, heat and discharge modelling:

- Total vessel volume (V)
- Total storage volume ($V_{storage}$) – including pipe if present

[xiv] CHANGE: TVDI in Phast 7.21 and earlier assumes that the user specified inventory corresponds to the liquid and not the total vessel inventory. This has been recitified in the new TVDI model whereby the specified inventory is the total fluid mass in the system (excluding mass of padding gas for pressurized liquid vessels).

- Volume of liquid ($V_{L)}$ for a given liquid height (Z_L)
- Height of liquid (Z_L) for a given liquid volume (V_L)
- For a horizontal cylinder, the fractional wetted area (f_w) at the ends of the vessel
- Total wetted wall area ($S_{wet\text{-}wall}$) (for wall-to-fluid heat transfer calculations)

Total vessel volume (V)
The total vessel volume (V) is determined as:

For cuboidal tanks:

$$V = L_{tank} Z_{tank} W_{tank} \quad (33)$$

For spherical tanks:

$$V = 4\pi r_{tank}^3 / 3 \quad (34)$$

For horizontal cylindrical tanks:

$$V = \pi r_{tank}^2 L_{tank} \quad (35)$$

For vertical cylindrical tanks:

$$V = \pi r_{tank}^2 Z_{tank} \quad (36)$$

Where: L_{tank}, W_{tank}, Z_{tank} and r_{tank} correspond to the tank length, breadth, height and radius respectively.

Total storage volume ($V_{storage}$)
The total storage volume ($V_{storage}$) is determined as:

$$V_{storage} = V + \frac{\pi}{4} L_{pipe} D_{pipe}^2 \quad (37)$$

Volume of liquid ($V_{L)}$ for a given liquid height ($Z_{L)}$ or vice-versa
For cuboidal and vertical cylindrical tanks, the volume of liquid, given a liquid height (and vice-versa) is determined from the solution of equations (33) and (36) respectively, where, V_{tank} and Z_{tank} are replaced with V_L and Z_L respectively.

For horizontal cylindrical tanks, liquid volume is related to liquid height analytically as:

$$V_L = L_{tank}\left(\left(Z_L - r_{tank}\right)\sqrt{Z_L\left(2r_{tank} - Z_L\right)} + r_{tank}^2 \left(\sin^{-1}\left(\frac{Z_L}{r_{tank}} - 1 \right) + \frac{\pi}{2} \right) \right) \quad (38)$$

For spheres, liquid volume is related to liquid height analytically as:

$$V_L = \frac{1}{3}\pi Z_L^2 \left(3r_{tank} - Z_L\right) \quad (39)$$

Thus, for horizontal cylindrical and spherical tanks, the volume of liquid, given a liquid height (and vice-versa) is determined from the solution of equations (38) and (39), respectively.[xv,xvi]

Fractional area (f_w) of ends of horizontal cylinder covered by liquid
The fractional area (f_w) of the ends of a horizontal cylinder covered by liquid (for wall – liquid heat transfer calculations) is determined as:

[xv] CHANGE: In TVDI 7.21 and earlier the liquid height in a sphere for given liquid volume was found iteratively; in the new TVDI model an exact analytical expression is used.

[xvi] IMPROVE: Horizontal (and vertical) tanks commonly possess domed ends, the geometry modelling in TVDI may be extended to handle these vessel shapes and others (e.g. octagonal membrane tanks).

$$f_w = \left(\left(Z_L - r_{tank}\right)\sqrt{Z_L\left(2r_{tank} - Z_L\right)} + r_{tank}^2 \left(\sin^{-1}\left(\frac{Z_L}{r_{tank}} - 1 \right) + \frac{\pi}{2} \right) \right) \Big/ \left(\pi r_{tank}^2\right) \quad (40)$$

Total wetted wall area ($S_{wet\text{-}wall,i}$)

The total wetted wall area ($S_{wet\text{-}wall}$) covered by liquid (for wall – liquid heat transfer calculations) is determined as:

For cuboidal tanks[xvii]:

$$S_{wet-wall} = 2Z_L\left(L_{tank} + W_{tank}\right) \quad (41)$$

For spherical tanks:

$$S_{wet-wall} = 2\pi r_{tank} Z_L \quad (42)$$

For horizontal cylindrical tanks [xviii]:

$$S_{wet-wall} = 2\pi r_{tank}\left(f_w r_{tank} + L_{tank} \cos^{-1}\left(-\left(\frac{Z_L}{r_{tank}} - 1 \right) \right) \right) \quad (43)$$

For vertical cylindrical tanks[xvii]:

$$S_{wet-wall} = 2\pi r_{tank} Z_L \quad (44)$$

2.3.2 Liquid swell modelling

Liquid swell modelling is not included in the first version of the new TVDI model. Nevertheless, a literature review of swell modelling and the swell modelling in Phast 7.21 is given in Appendix B.

2.3.3 Discharge modelling

Flow rate calculations are carried out using appropriate methods (based on multi-component thermodynamic logic) in DISC. For liquid leaks, a meta-stable expansion process is assumed to prevail at the orifice, while homogeneous equilibrium flow is assumed for all other release scenarios.

The conditions upstream of the release plane are assumed to correspond to fluid conditions (total pressure, temperature, entropy, phase etc.) at the hole height. Thus, the hole inlet pressure (P_{st}) upstream of the orifice / pipe is calculated as:

$$P_{st} = P + P_{hyd}\,. \quad (45)$$

Here, P_{hyd} is the hydrostatic pressure due to liquid given by

$$P_{hyd} = \begin{cases} \rho_L(P,T)\, g\, \Delta Z_L & \text{if} \quad \Delta Z_L > 0, \\ 0 \quad \text{otherwise.} \end{cases} \quad (46)$$

Furthermore, ρ_L is the liquid density on top of the liquid[xix], g the gravitational acceleration and ΔZ_L the tank head (height of liquid above the hole/pipe entrance).

The discharge modelling is designed to handle scenarios involving phase change/transition at the orifice inlet where the liquid level drops below the orifice inlet. The discharge process is assumed to terminate when certain

[xvii] NOTE: This equation ignores the base of the tank in contact with the fluid. The heat transfer term for the base of the cylinder will differ (i.e. horizontal plate) from that employed for its vertical/curved sides

[xviii] CORRECT/IMPROVE: Equation (40) includes the area of the fluid in contact with the ends of the cylinder. The heat transfer correlation employed for this portion of the tank should be for a vertical plate, while another correlation is to be applied for the curved/horizontal portion of the tank.

[xix] In reality the liquid density will vary with liquid height. However the variation is minor and the assumption of constant liquid density when calculating liquid head is consistent with assumptions in the DISC model.

conditions are satisfied – these conditions may vary depending on the vessel type. For example, discharge from a pressurized liquid vessel terminates if the liquid head is zero even if the vapour space is still pressurized, while for a pure gas vessel or stratified two-phase vessel discharge may continue until the vapour space is completely depressurized.

2.3.4 Liquid and vapour space mass conservation equations

In case of a vessel containing both liquid and vapour, the two phases are assumed to be in equilibrium. A pressure-enthalpy flash is used at each time step to determine the phase split. For multi-component mixtures (See Chapter 4), each component in a mixture will have a liquid fraction. Thus knowing the total mass of a component one can also easily deduce the liquid mass and vapour mass of the component.

The amount of evaporation/condensation at each time step can also be computed through these mass balances.

2.3.5 Energy balances and heat transfer effects

One of the decisions to make is which heat transfer effects to include in the model. The simplest approach is to assume no heat transfer at all between the fluid and the vessel walls – an approach that was investigated by Cumber[3]. This is indeed also the approach taken in the first version of the new TVDI model. Possible refinement and extensions to this simple approach is given in Appendix D.

2.3.6 Calculating the total system enthalpy

In Section 2.1 we gave an expression for the total system enthalpy, and we will here show its derivation. The general equation is given by

$$H(P,T) = U(P,T) + \iiint_{System} P\,dV\,. \qquad (47)$$

In reality the pressure will only be constant in the vapour space, while in the liquid space (if liquid is present) the pressure is a function of the height z above the vessel bottom:

$$P(z) = \begin{cases} P + \rho_L(P,T)\, g\, (Z_L - z) & \text{if} \quad 0 \le z \le Z_L \\ P & \text{if} \quad Z_L < z \le Z_{\text{tank}} \end{cases}. \qquad (48)$$

We may then re-express the total system enthalpy as

$$H(P,T) = U(P,T) + \int_0^{Z_{\text{tank}}} A(z)\, P(z)\, dz\,, \qquad (49)$$

where $A(z)$ is the horizontal cross-sectional area of the storage vessel at height z. Considering this integral more closely we get

$$\int_0^{Z_{\text{tank}}} A(z)\, P(z)\, dz = \int_0^{Z_L} A(z)\, P(z)\, dz + \int_{Z_L}^{Z_{\text{tank}}} A(z)\, P(z)\, dz = \int_0^{Z_L} A(z)\, P(z)\, dz + PV_V\,. \qquad (50)$$

Looking in detail at the remaining integral on the right-hand-side yields

$$\int_0^{Z_L} A(z)\,P(z)dz = \int_0^{Z_L} A(z)\left[P + \rho_L\, g\,(Z_L - z)\right]dz \qquad (51)$$

$$= \left(P + \rho_L g Z_L\right)\int_0^{Z_L} A(z)\,dz - \rho_L g \int_0^{Z_L} z\,A(z)\,dz$$

$$= PV_L + M_L g Z_L - \rho_L g \int_0^{Z_L} z\,A(z)\,dz$$

The total system enthalpy may thus be expressed as

$$H(P,T) = U(P,T) + PV_V + PV_L + M_L g Z_L - \rho_L g \int_0^{Z_L} z\,A(z)\,dz \qquad (52)$$

$$= U(P,T) + PV + M_L g Z_L - \rho_L g \int_0^{Z_L} z\,A(z)\,dz.$$

For a storage tank with constant horizontal cross-sectional area $A(z) = A$, e.g. a vertical cylinder or a cuboid, we get $\int_0^{Z_L} z\,A(z)\,dz = A\int_0^{Z_L} z\,dz = \frac{1}{2}AZ_L^2$, and the above expression simplifies to

$$H(P,T) = U(P,T) + PV + M_L g Z_L - \rho_L g \frac{1}{2} A Z_L^2 \qquad (53)$$

$$= U(P,T) + PV + \frac{1}{2} M_L g Z_L$$

In the current model we consider two tanks where the horizontal cross-sectional area A varies with the liquid height z, namely spherical and horizontal cylinder tanks. For a sphere it can be shown that $A(z) = \pi\left(2r_{\text{tank}} z - z^2\right)$, and we can evaluate the integral

$$\int_0^{Z_L} z\,A(z)dz = \int_0^{Z_L} z\,\pi\left(2r_{\text{tank}} z - z^2\right)dz = \pi\int_0^{Z_L}\left(2r_{\text{tank}} z^2 - z^3\right)dz \qquad (54)$$

$$= \pi\left(\frac{2}{3} R Z_L^3 - \frac{1}{4} Z_L^4\right) = \frac{2}{3} V_L Z_L - \frac{1}{36}\pi Z_L^4$$

Using this expression we can find an analytical expression for the total enthalpy of a sphere with liquid height Z_L:

$$H(P,T) = U(P,T) + PV + \frac{1}{3} M_L g Z_L + \frac{1}{36}\pi\,\rho_L\, g\, Z_L^4. \qquad (55)$$

For a horizontal cylinder, the cross-sectional area is given by $A(z) = 2L_{\text{tank}}\sqrt{2Rz - z^2}$ and we can evaluate the integral

$$\int_0^{z_L} z\, A(z)dz = 2L_{\text{tank}} \int_0^{z_L} z\sqrt{2R\, z - z^2}\; dz\,. \qquad \textbf{(56)}$$

The above integral can be evaluated analytically according to the online Wolfram Integrator – it's rather complicated and we will leave the details out at this stage.

2.3.7 Termination criteria

There are various control mechanisms and modelling aspects that determine when the TVDI model stops calculations for a specific release case, and this will be discussed further in this section.

Maximum release duration

The maximum release duration is an input into the TVDI model, and all releases will terminate if and when the maximum release duration is reached.

Minimum release rate[xx]

There is an option to supply a minimum release rate threshold to the TVDI model. Calculations terminate if and when the flow rate falls below the supplied minimum value.

Pressure reduction threshold[xx]

The user can supply a cut-off pressure such that calculations stop when the vapour space pressure in the vessel falls below the threshold. This is done by inputting a fraction, where a value of 1 means depressurize to ambient pressure and a value of 0.5 would depressurize to half of the initial gauge pressure.

Default termination

In absence of any of the above-mentioned termination mechanisms, the termination of the TVDI calculations happens when no more fluid can come out of the vessel:

- Pure gas vessel, homogeneous two-phase vessel and stratified two-phase vessel: terminates when the vapour space pressure has reduced to the ambient pressure
- Pressurized liquid vessel and atmospheric storage tank: terminates when the liquid level falls below the hole height (note that the hole height might be adjusted if the user has requested for a certain amount of liquid to be trapped, i.e. unavailable to be released).

2.3.8 Use of steady-state results

There can be situations when the time-varying discharge model runs into calculation difficulties. In such cases the model will only be able to give a partial transient description of the release and there will still be hazardous material left in the vessel at the time the time-varying calculations stop. A pragmatic approach is then taken

[xx] This option is not available in Phast and Safeti Onshore.

where the model reports time-varying release results already obtained up until the time calculation difficulties occur, say at t_{ERR}. However, at this time there is still hazardous material left in the vessel. To avoid under-estimating the hazards of the release, the model therefore assumes that the hazardous material continues to be released at a constant rate subsequent to the calculation difficulty. The steady-state release rate applied is the same as the flow rate predicted by the model at time t_{ERR}. The duration of the steady-state period of the release depends on the amount of remaining material that can be released – this is determined as follows:

- For pressurized liquid vessels, the duration is set so that all remaining liquid at time t_{ERR} is discharged.
- For a vapour release from a stratified two-phase vessel, the duration is set so that all remaining vapour at time t_{ERR} is discharged.
- For all other releases, the duration is set so that all remaining mass at time t_{ERR} is discharged.

2.4 Differences with the Phast 7.21 TVDI model

The revised model currently differs from the TVDI model as per Phast 7.21 and earlier – in particular:

- Liquid swell is ignored in the revised model:
  The swell modelling in 7.21 is questionable – see 6.Appendix B for details. Swell modelling is therefore ignored in the first version of the revised TVDI model but may very well be incorporated in future versions.

- No air ingestion for stratified two-phase vessels (no 'gulping' through orifice, no vacuum relief valve):
  The 7.21 model can take into account air ingestion through the release orifice (gulping), though the modelling is done in a very crude fashion. As such, in the 7.21 model it is recommended to use a vacuum relief valve to avoid sub-atmospheric conditions in the vapour space. For stratified two-phase vessels, neither air ingestion through the release orifice nor through a vacuum relief valve is supported in the first version of the revised TVDI. However, vacuum relief valve and gulping is modelled in the revised modelled for pressurized liquid vessels.

- No heat transfer between fluid-vessel wall and the surroundings:
  The 7.21 model considered heat transfer with the surroundings by lumping the vessel and fluid together as one single thermodynamic entity that was heated by the surroundings. Thus the fluid and wall was always assumed to be in thermodynamic equilibrium. This model may not be reasonable as experiments show that the fluid cools more and quicker than the wall. The revised TVDI model does currently not model any heat transfer between fluid-wall-surroundings, but some theory has been developed in Appendix D and may be included in a future version of the model.

- Support for one single liquid only. The old model had some logic for two immiscible liquids (oil based + water based) though this was not "activated" in the code. As such the revised model, which supports one single liquid, is in practice consistent with the 7.21 model.

- Vapour expansion energy IS taken into account in the new model but was ignored in the old multi-phase model. This must be viewed as a significant improvement as ignoring PV work by the expanding gas is the same as assuming that the gas remains at constant pressure.

3. SAFETY SYSTEM MODELLING

3.1 Background and overview

The Safeti Offshore software package required a time-varying discharge model with safety system functionality. The original TVDI model in Phast 7.21 and the first version of the revised model as described in Section 2 did not include such safety system functionality. Numerous discussions within DNV therefore took place with regards to the development of such a time-varying discharge model satisfying Offshore QRA needs. The modelling approach and assumptions set out in Section 3 in this document are the result of such discussions.

Note that in general the model assumptions described in Section 2 are still valid for the TVDI model with safety systems as described in this section as the safety system modelling is an extension of the model as described in Section 2. In case of conflicting information, then the information in this section supersedes the one from Section 2.

3.1.1 The original TVDI model without safety systems

The original TVDI model did not allow any production inflows or outflows, which effectively is equivalent to assuming instantaneous isolation. Emergency evacuation of the vapour space to reduce pressure, known as blowdown, was also not supported. A schematic overview of the mass inflows and outflows to and from the vessel is shown[xxi] in Figure 5.

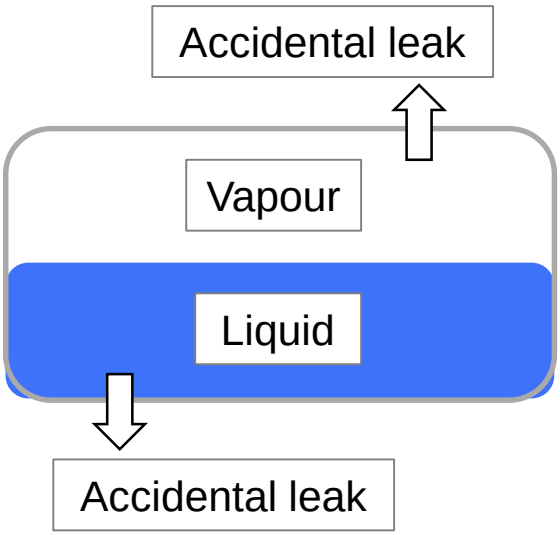


Figure 5: Schematic overview of inflows and outflows of original TVDI model without safety systems.

3.1.2 TVDI with safety system support

The safety systems of relevant to model is those of emergency shutdown (ESD), sometimes also called isolation, and blowdown. A revised schematic overview of the mass inflows and outflows to and from the vessel with safety systems is shown[xxi] in Figure 6.

[xxi] Note that only one single accidental leak can be modelled and that the two leaks shown in the figure is only to illustrate that the leak may occur from either the liquid or vapour space.

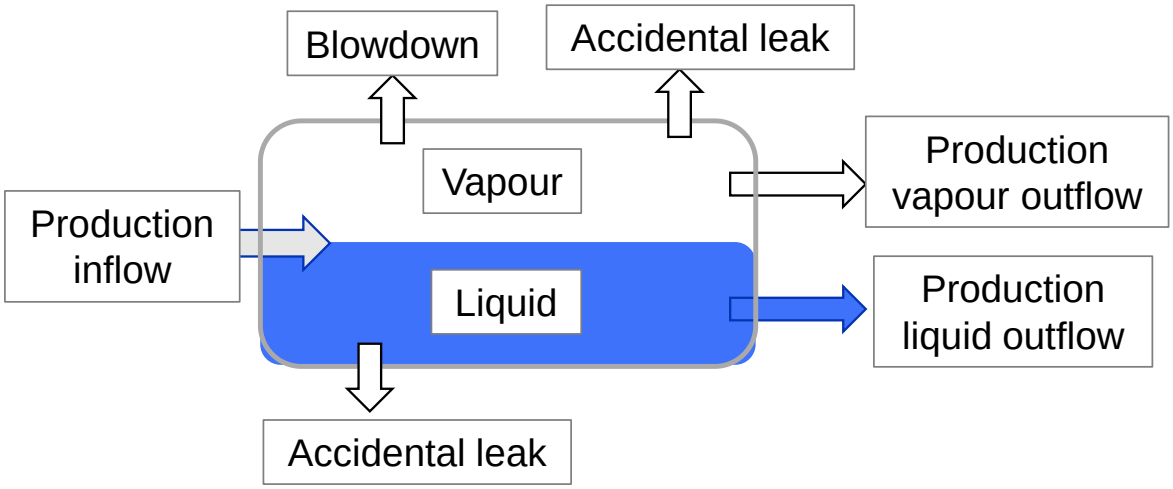


Figure 6: Schematic overview of inflows and outflows of the revised TVDI model with safety system support.

3.2 Emergency shutdown: detailed theory

We first start this section with the top-level modelling assumptions and then follow on with a more detailed discussion and explanation of these assumptions. Note that two approaches have been implemented for modelling the time period prior to shutdown time: a detailed approach described in Sections 3.2.2 to 3.2.4 and a more simplistic approach given in Section 3.2.5.

3.2.1 What is ESD?

In a process facility, a vessel may be connected to one or more other process units. When an accidental leak is detected in a vessel, the emergency shutdown works successfully if all valves connecting the vessel to other units shut down – the vessel has then been successfully isolated, reducing the amount of hazardous material that can potentially be released.

3.2.2 Summary of modelling assumptions for isolation

Although certain considerations specific to a two-phase vessel/separator is included below, the following ESD assumptions should be valid for all the relevant storage types: pure gas, two-phase and pressurized liquid.

- The successful operation of the isolation process is a model input
- A key input is the time delay to ESD, t_{ESD}.
- If ESD failure is modelled, then:
  - only one single ESD valve fails, namely the production inflow valve
  - the outflow production valves close successfully at time t_{ESD}.
- Normal production inflow and outflow will be modelled from the time of the accidental leak t=0 until the time to isolation $t=t_{ESD}$ (at which time ESD may be successful or may fail):
  - The production inflow is assumed constant for $0<t<t_{ESD}$
  - The production outflows are assumed to decrease in proportion to the pressure difference between vessel pressure and downstream pressure
    i. The downstream pressure is assumed constant, further details in Section 3.2.4.
- If ESD is successful at t_{ESD} then there is subsequently no mass flow into the vessel and the only outflow is through the accidental leak and through a potential blowdown valve.
- If ESD fails at t_{ESD}, then the isolatable section in question will be merged with the neighbouring isolatable section whose isolation valve has failed:
  - Mass from the neighbouring isolatable section will be added to the isolatable section under consideration, assuming instantaneous mixture of the contents. The isolatable section under consideration will have its volume expanded accordingly.

- Continuity: The merged isolatable section will have the same storage pressure and temperature as before the merging, and for liquid releases the hole height will be set to ensure continuity in liquid head (if possible).
- Composition of vapour and liquid space is the same in both sections, though the overall liquid fraction may differ.
- After merging at time $t=t_{ESD}$, there is no mass flow into the merged section and the only outflow is through the accidental leak and through a potential blowdown valve.

3.2.3 Normal operation before accidental leak

The normal operation before the accidental leak will determine the initial state of the vessel when the accidental leak occurs and will in turn affect what happens upon emergency shutdown. In particular we are interested in the production inflows and outflows to and from the vessel, which will depend on the vessel type in question. We will in turn look at a stratified two-phase vessel, homogeneous vessel (pure gas or two-phase) and pressurized liquid vessel, but let us first introduce some notation:

- M_{US}: mass in neighbouring upstream vessel
- $\dot{m}_{in}$: production inflow from upstream vessel
- η^{liq}: liquid fraction of production inflow
- P_{DS}^{vap} / P_{DS}^{liq}: fixed downstream pressure for production vapour and liquid outflow
- $\dot{m}_{out}^{vap}$ / $\dot{m}_{out}^{liq}$: transient flow rates for vapour and liquid production outflows
- ΔP^{vap} / ΔP^{liq}: initial difference between vessel pressure and downstream pressure for vapour / liquid production outflows during normal operation

Stratified two-phase vessel

A stratified two-phase vessel with liquid at the bottom and vapour at the top may be part of a two-phase separator: there is a two-phase inflow into the vessel on one side, and on the other side of the vessel there are two outflows: we assume one liquid outflow at the bottom of the vessel and one vapour outflow at the top as seen in Figure 7. During normal operation we assume that the net inflow equals the net outflow, and indeed that the liquid/vapour inflow equals the liquid/vapour outflow such that the liquid level in the vessel is constant. The inflow is the same material as in the vessel at the same pressure and temperature, and the user specifies the inflow rate and liquid fraction. One may then calculate the liquid and vapour outflow, respectively, under normal operation.

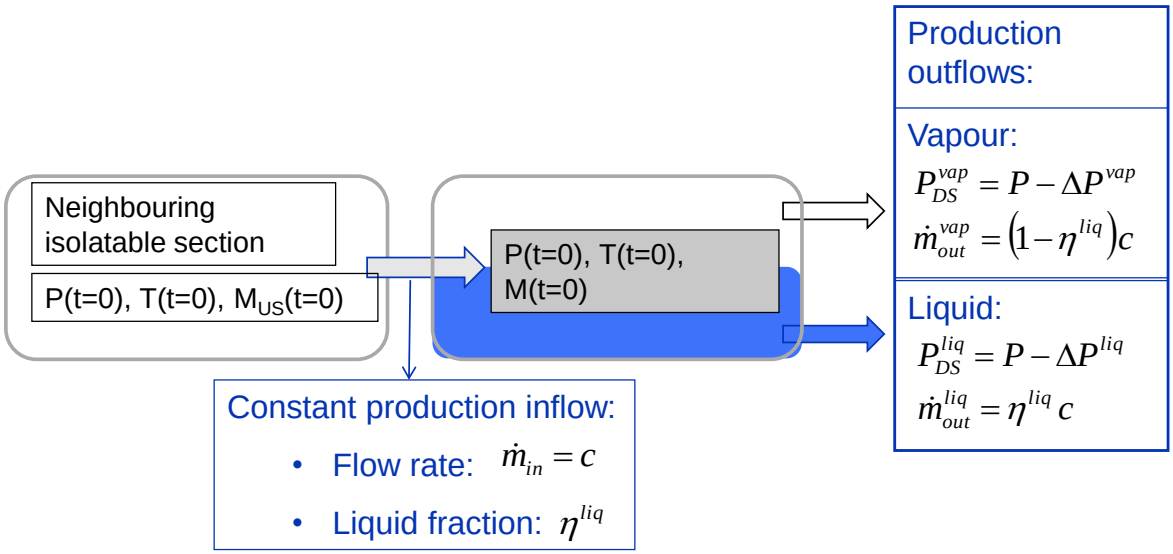


Figure 7: Illustration of production inflows and outflows during normal operation of a two-phase vessel, no accidental leak.

Homogeneous vessel

When it comes to the production inflows and outflows, the homogeneous vessel model can be considered as a special case of the two-phase vessel model as seen in Figure 8. The production inflow is vapour with liquid fraction = 0, while there is only one production outflow of vapour (no pure liquid outflow present).

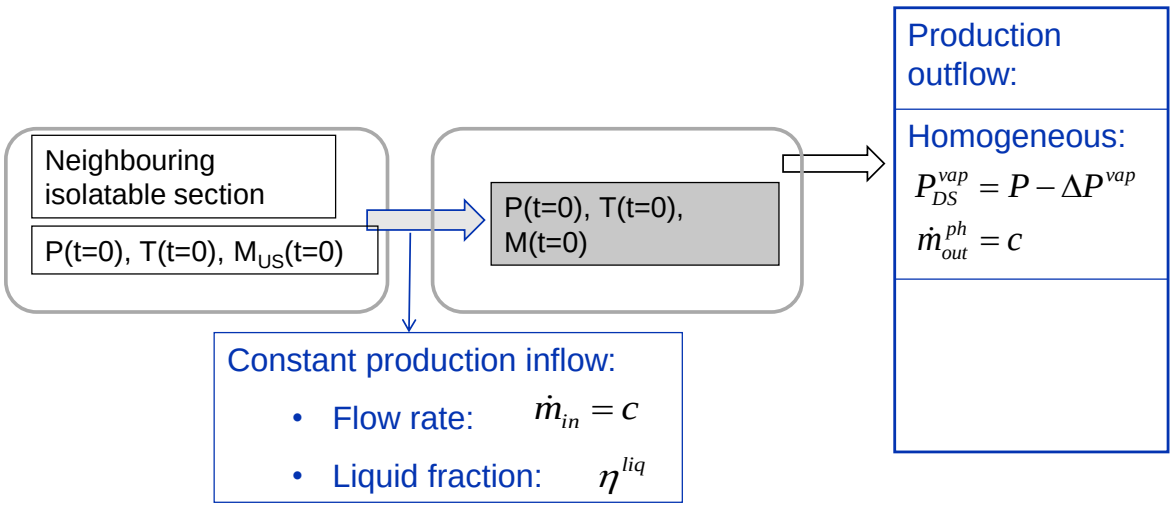


Figure 8: Illustration of production inflow and outflow during normal operation of a homogeneous vessel (pure gas or two-phase), no accidental leak.

Pressurized liquid vessel

Just like the pure gas vessel, the pressurized liquid vessel can be viewed as a special case of the two-phase vessel when it comes to production inflows and outflows under normal operation. The production inflow is pure liquid, i.e. liquid fraction = 1, while there is only one production outflow of pure liquid vapour (no vapour outflow present).

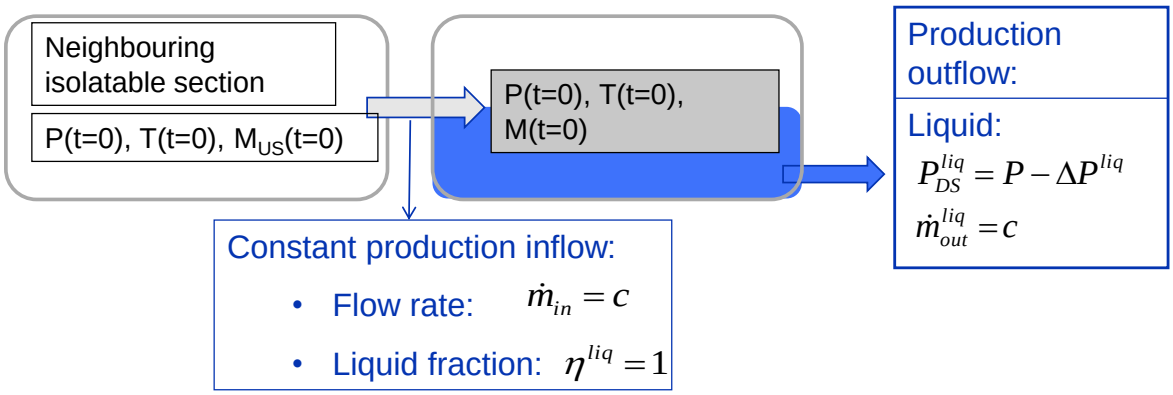


Figure 9: Illustration of production inflow and outflow during normal operation of a pressurized liquid vessel, no accidental leak.

3.2.4 Time period after accidental leak before ESD

Now assume that an accidental leak occurs at time t=0, either from the vapour or liquid space of the vessel. Further let there be an ESD at time t_{ESD} after the accident.

The pressure in the vessel starts dropping due to the accidental leak, and this will affect the production inflow and outflow rates in some dynamic manner. How do we model this? We here make a conscious decision to focus the modelling efforts on the vessel in question and not try to model the vessels upstream and downstream in detail. The latter would be considerably more complex and computationally expensive and would be more like process simulator functionality.

To focus the modelling efforts on the vessel in question, there is a need for well-defined and fairly simple boundary condition towards the upstream and downstream vessels.

Boundary condition for upstream vessel

A constant mass inflow rate c is assumed with a constant liquid fraction η^{liq}, both specified by the user[xxii]. The justification for assuming constant inflow is that since this is prior to ESD, material is still flowing into the upstream vessel, contributing to maintaining its pressure.

Boundary condition for downstream vessel

First consider the production outflows from a two-phase vessel in which case we model two production outflows – one from the vapour space and one from the liquid space. To model this we assume constant downstream pressures as boundary condition: P_{DS}^{vap} for the downstream vapour pressure and P_{DS}^{liq} for the downstream liquid pressure. The user will specify the downstream pressure boundary conditions in terms of pressure differentials under normal operating conditions: $P_{DS}^{vap} = P_0 - \Delta P_{DS}^{vap}$ and $P_{DS}^{liq} = P_0^{liq} - \Delta P_{DS}^{liq}$, where P_0^{liq} is the initial pressure at liquid outflow height including hydrostatic pressure and $P_0 = P(t=0)$. Note that the production liquid and vapour outflow is assumed to be at the bottom and top of the vessel, respectively.

For a pure gas vessel there will only be a vapour outflow and thus the user will only need to specify the pressure differential ΔP_{DS}^{vap}, while only the pressure differential ΔP_{DS}^{liq} needs to be specified for a pressurized liquid vessel.

Transient production outflow rates after accidental leak ($0<t<t_{ESD}$)

First we discuss the case of a two-phase vessel. During normal production before the accidental release we assume that the liquid and vapour inflow equals the vapour and liquid outflows, i.e. the vapour outflow rate $\dot{m}_{out}^{vap} = \left(1-\eta^{liq}\right)c$ and the liquid outflow rate $\dot{m}_{out}^{liq} = \eta^{liq} c$. However, upon the accidental release the pressure in the vessel decreases and consequently the production outflow rates will also decrease. Note that during normal production, the downstream pressures must be lower than the actual vessel pressure P_0.

After the accidental leak, t>0, the pressure $P(t)$ starts dropping and the production outflows will also drop. Let us first consider the vapour outflow: When at some stage the vessel pressure $P(t) = P_{DS}^{vap}$, there will no longer be any production vapour outflow, i.e. $\dot{m}_{out}^{vap}\left(P_{DS}^{vap}\right) = 0$. We already know that $\dot{m}_{out}^{vap}\left(P_0\right) = \left(1-\eta^{liq}\right)c$, and assuming that the flow rate is linearly proportional to the pressure drop, we get that

$$\dot{m}_{out}^{vap}(P) = \left(1-\eta^{liq}\right)c\left(1-\frac{P_0-P}{\Delta P_{DS}^{vap}}\right) \qquad (57)$$

for $P_{DS}^{vap} \le P \le P_0$. If we further assume the presence of a non-return valve, i.e. vapour will not flow back into the vessel when $P < P_{DS}^{vap}$, then we get that

$$\dot{m}_{out}^{vap}(P) = \max\left\{\left(1-\eta^{liq}\right)c\left(1-\frac{P_0-P}{\Delta P_{DS}^{vap}}\right),\ 0\right\} \qquad (58)$$

for $P_{amb} \le P \le P_0$. Using similar assumptions for the liquid production outflow we get

[xxii] For a pure gas and pressurized liquid vessel the liquid fraction of the inflow will be set to 0 and 1, respectively.

$$\dot{m}_{out}^{liq}(P) = \max\left\{\eta^{liq} c\left(1 - \frac{P_{st,0} - P_{st}}{\Delta P_{DS}^{liq}}\right), 0\right\} \quad (59)$$

for $P_{amb} \le P \le P_0$.

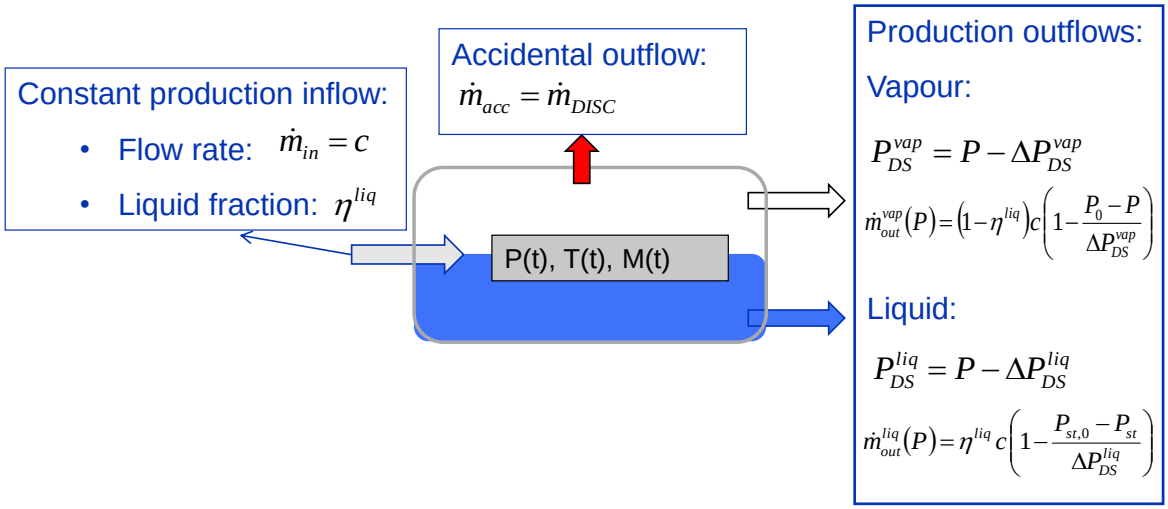


Figure 10: Illustration of system after accidental leak, before ESD ($0<t<t_{ESD}$)

In terms of production inflow and outflows, the cases of pure gas and pressurized liquid vessels are merely special cases of the two-phase vessel as explained earlier.

3.2.5 ESD: A simpler alternative

A simpler modelling approach to ESD than the one described in Sections 3.2.2 to 3.2.4 is also included as a model option. This alternative approach is based on the following assumptions:

- After the onset of the accidental leak, the production inflows and outflows are assumed to behave in such a way as to keep a steady-state situation in the tank until the ESD time.
- This means that for $0<t<t_{ESD}$ then all variables like flow rate, pressure, temperature etc remain constant.
- The alternative approach has different modelling only for $0<t<t_{ESD}$, i.e. for $t>t_{ESD}$, the modelling is exactly as described in Section 3.2.6.

With this alternative approach, there is no need for the user to provide any inputs related to the production flow modelling. The approach is generally more conservative than the detailed approach as the initial flow rate is assumed to prevail until the time of isolation.

3.2.6 Time period after ESD, $t > t_{ESD}$:

After the ESD, it is assumed that both the production outflows are always closed off. In the event that the inflow isolation valve does close successfully, the vessel is fully isolated with exception of accidental outflow as well as possibly blowdown – see Figure 11 for an illustration of this. The modelling of this situation is fairly well understood and as described in Chapter 2. However, modelling the scenario when the ESD fails is more challenging – the following approach has been adopted:

If ESD fails at t_{ESD}, then the vessel in question will be merged with the neighbouring vessel whose isolation valve has failed, and subsequent outflow for $t>t_{ESD}$ will then occur from this merged vessel with increased inventory – see Figure 12 for an illustration. There are several issues to consider related to the merging of vessels at time $t=t_{ESD}$ as discussed in the following.

Mass immediately after merging

Denote the inventory in the vessel undergoing a leak by M and the inventory of the neighbouring upstream vessel whose isolation valve failed by M_{US}. Further let t_{ESD}^- and t_{ESD}^+ denote time immediately before and after merging, respectively. Note that the inventory in the section undergoing a leak changes with time, so generally $M_(t=0) \neq M(t=t_{ESD}^-)$. However, prior to ESD we assume that the inventory in the neighbouring vessel remains constant, i.e. $M_{US}(t=0)=M_{US}(t=t_{ESD}^-)$. Letting M(t) be the inventory of the merged vessel, then assuming[xxiii] all the inventory in the neighbour contributes to the release due to the isolation failure, we get $M(t_{ESD}^+) = M(t_{ESD}^-) + M_{US}(t=0)$. The liquid fraction η_{US} of the added mass M_{US} is determined as follows depending on the vessel type:

- Pure gas vessel: $\eta_{US} = 0$
- Homogeneous and stratified two-phase vessel[xxiv]: $\eta_{US} = \eta\left(t = t_{ESD}^-\right)$
- Padded liquid vessel: $\eta_{US} = 1$

Continuity of some key variables

The merging of the sections at time $t=t_{ESD}$ leads to an instantaneous change in variables like mass and volume of the section. For the model to produce reasonable results in the case of isolation failure, it is important that as many key variables as possible remain continuous before and after merging. In particular let the pressure and temperature be continuous, i.e. . $P(t_{ESD}^+)= P(t_{ESD}^-)$ and $T(t_{ESD}^+)= T(t_{ESD}^-)$.

Shape and physical dimension after merging

Increasing the inventory of the section when isolation fails while retaining the pressure and temperature, can only be possible if the volume of the section is increased upon merging. We let the section retain its original shape while increasing the volume by expanding each dimension (e.g. height, diameter) such that $s=s_2*(V/V_2)^{(1/3)}$, where s_2 and V_2 is dimension and volume before merging, s and V dimension and volume after merging. The new volume V will be determined based on the new mass $M(t=t_{ESD}^+)$ and new liquid fraction $\eta\left(t = t_{ESD}^+\right)$.

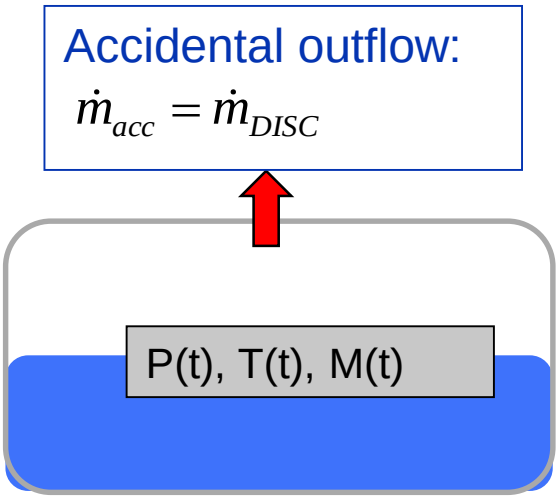


Figure 11: The system after successful ESD.

[xxiii] NOTE: It was considered to allow only a user-specified fraction of the liquid mass upstream to be added upon merging. However, we generally have very limited information about the upstream vessel and do not know the transient liquid mass in this vessel – only the total fluid mass is known (user input, assumed constant before merging).

[xxiv] NOTE: The liquid fraction of the added upstream mass for a two-phase vessel could alternatively be set equal to the liquid fraction of the production inflow.

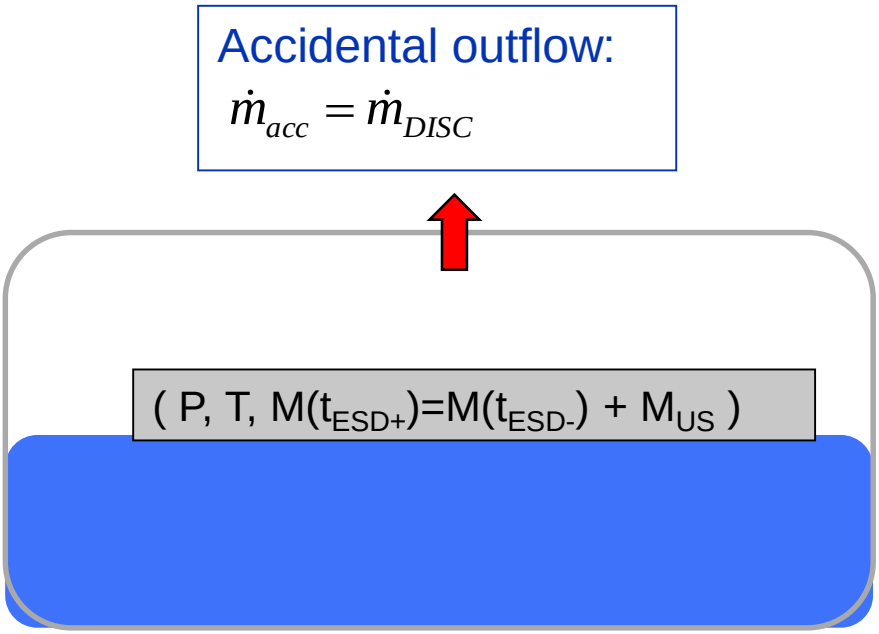


Figure 12: The system after unsuccessful ESD: The inventory and volume of the vessel is increased while continuity is enforced for pressure, temperature and liquid head.

Issues related to the "merging" approach

The relatively simplistic approach of merging vessels at time of an isolation failure is motivated by the fact that we in general have very little knowledge about the conditions in the upstream vessel – the focus here is on the vessel undergoing the accidental leak and detailed modelling of the upstream vessel is beyond the current scope. There are certain potential issues to be aware of related to the current approach:

- The upstream mass flowing into the vessel prior to isolation is assumed to be at conditions (P(t=0), T(t=0)), but when the upstream mass is added to the merged vessel after isolation failure then this mass is assumed to be at current vessel conditions (P(t=t_{ESD}), T(t=t_{ESD})).
    - The above assumption is made to ensure continuity of temperature in the vessel before and after merging
- The merging of contents in case of isolation failure means that the tank size is increased to fit the increased inventory. A side effect of this is that the liquid head may potentially be discontinuous, which could lead to a jump in the accidental flow rate.
- An alternative to the merging method could be to continue the constant inflow after isolation failure until the upstream mass is depleted. This approach was not taken due to the uncertainty of the pressure evolution in the upstream vessel after isolation failure.

3.3 Blowdown: detailed theory

In addition to the emergency shutdown measure described in 3.2, blowdown is also a common safety system - designed to reduce pressure with the aim of reducing the amount of hazardous material released. We first highlight the main assumptions taken for blowdown modelling in TVDI in Section 3.3.1 and discuss blowdown valve size and its calculation in Section 3.3.2 and 3.3.3, respectively.

3.3.1 Assumptions for blowdown modelling

The following assumptions are made for modelling of blowdown:

- The successful operation of the blowdown process is a model input
- If the blowdown operates successfully, blowdown commences after a user-specified input time t_{BD}. In principle blowdown can commence at any given time, e.g. t_{BD}=0, t_{BD}<t_{ESD}, t_{BD}>t_{ESD}, regardless of whether isolation is successful or fails. Note though that in Safeti Offshore it is enforced that $t_{BD} \geq t_{ESD}$.
- The blowdown valve is assumed to be a circular orifice with diameter d_{BD}, given in one of two ways:

    - a user-specified value
    - calculated in such a way that the initial system pressure P_0 is reduced to a certain pressure P^* after time t^*, with P_0, P^* and t^* all specified by the user[xxv, xxvi]. See Section 3.3.3 for details.
- The backpressure of the blowdown valve is assumed to be equal to the ambient pressure
- If blowdown is requested, the blowdown is assumed to be located at the top of (roof) the vessel so that vapour is evacuated (i.e. no liquid is blown down)
- Blowdown is only taken into account for the vessel undergoing an accidental leak, not for any of its neighbouring vessels.

Why blowdown valve assumed to be a circular orifice?

- In reality there might be a tail pipe connected to the vessel through which the blowdown is carried out. Nevertheless we have used the orifice scenario. Partly this is because it is more computationally efficient than using a pipe scenario, and partly because for short tail pipes it will often give the same results. However for longer tail pipes this assumption may be inaccurate as it will overpredict blowdown flow rates[xxvii].

3.3.2 Choosing an appropriate valve size for blowdown modelling

The actual diameter of a blowdown valve on a containment may be known and provided by the operator. However, use of this actual valve size when modelling blowdown may give misleading results. The reason for this is that the backpressure of the blowdown valve will typically be unknown and vary throughout the blowdown process, making it almost impossible to obtain accurate predictions for the flow rate through the blowdown valve. In some cases the operator may be able to provide an equivalent blowdown valve diameter assuming atmospheric back pressure. If this is not supplied, an equivalent blowdown valve diameter may be obtained using the following alternative approach:

> *Assuming a constant valve backpressure equal to the atmospheric pressure, choose a valve diameter such that the blowdown process satisfies a certain pressure/time requirement, e.g. reducing the initial pressure to 6.9 barg or half of the initial pressure, whichever is smaller, in 15 minutes.*

The above example of time-pressure requirement is very common and based on the assumption that the system and blowdown valve is designed to satisfy API 521 requirements. In general terms these requirements may be formulated as reducing initial system pressure P_0 to a certain pressure P^* after time t^*.

3.3.3 Calculation method for sizing of blowdown valve

In case the blowdown valve size is not specified by the user, it will be calculated in order to satisfy a certain pressure reduction as described in Section 3.3.2. Further details of this calculation are given in the following:

- The valve sizing calculations will be based on depressurizing an isolated vessel with its only outflow through the blowdown valve.
- The actual calculation procedure for the valve size is as follows:
    - The TVDI model is run once with an initial guess/default value for the valve size.
        - The initial guess may be based on some simple ideal gas formulas
    - The TVDI model is subsequently run iteratively, adjusting the valve size until the requested pressure reduction is satisfied.

3.4 Revised governing equations

3.4.1 Mass balance

The general ODE for the mass balance when safety systems are included may thus be expressed as

[xxv] Note that if there is an accidental leak and blowdown commences immediately, then the initial pressure P_0 will be reduced to P^* sooner than time t^* due to the additional loss of mass from the accidental release.

[xxvi] The producer of the blowdown valve will in general have used modelling techniques for valve sizing that differ from the modelling in TVDI.

[xxvii] This could be worked around by specifying a reduced C_d

$$\frac{dM(t)}{dt} = \dot{m}_{in} - \dot{m}_{acc} - \dot{m}_{BD} - \dot{m}_{out}^{vap} - \dot{m}_{out}^{liq}, \qquad (60)$$

where the terms on the RHS is given by:

- $\dot{m}_{in} = \begin{cases} 0 \text{ if } (t \geq t_{ESD}) \\ c \text{ otherwise} \end{cases}$
- $\dot{m}_{acc} = \dot{m}_{acc}^{DISC}$
- $\dot{m}_{BD} = \begin{cases} 0 & \text{if } t < t_{BD} \text{ or } F_{BD} = 0 \\ \dot{m}_{BD}^{DISC} & \text{otherwise} \end{cases}$
- $\dot{m}_{out}^{vap} = \begin{cases} 0 & \text{if } t \geq t_{ESD} \text{ or } P \leq P_{DS}^{vap} \\ (1-\eta_{in}^{liq}) c \left(1 - \dfrac{P_0 - P}{\Delta P_{DS}^{vap}}\right) & \text{otherwise} \end{cases}$
- $\dot{m}_{out}^{liq} = \begin{cases} 0 & \text{if } t \geq t_{ESD} \text{ or } P_{st} \leq P_{DS}^{liq} \\ \eta_{in}^{liq} c \left(1 - \dfrac{P_{st,0} - P_{st}}{\Delta P_{DS}^{liq}}\right) & \text{otherwise.} \end{cases}$

Note that in the above F_{ESD} and F_{BD} are flags indicating whether the shutdown and blowdown works successfully, respectively. (Value of 1 means that the safety system is working, value of 0 the safety system is not working.)

3.4.2 Energy balance

The general ODE for the energy balance when safety systems are included may thus be expressed as

$$\begin{aligned} \frac{dU}{dt} = {} & \dot{m}_{in}\left[h\left(P(t=0), T(t=0); \eta_{in}^{liq}\right) + \frac{1}{2}u_{in}^2\right] \\ & - \dot{m}_{acc}\left[h\left(P_{acc}, T_{acc}; \eta_{acc}\right) + \frac{1}{2}u_{acc}^2\right] \\ & - \dot{m}_{BD}\left[h\left(P_{BD}, T_{BD}; \eta_{BD}\right) + \frac{1}{2}u_{BD}^2\right] \\ & - \dot{m}_{out}^{vap}\left[h\left(P, T; \eta_{out}^{vap}\right) + \frac{1}{2}\left(u_{out}^{vap}\right)^2\right] \\ & - \dot{m}_{out}^{liq}\left[h\left(P_{st}, T; \eta_{out}^{liq} = 1\right) + \frac{1}{2}\left(u_{out}^{liq}\right)^2\right]. \end{aligned} \qquad (61)$$

It can be seen that each of the inflows and outflows yield a term in the energy Equation (61), each term consisting of energy due to added/removed mass and kinetic energy due to entry/exit fluid velocity:

- Production inflow:
  - Specific enthalpy evaluated at initial pressure and temperature, liquid fraction constant as specified by the user
  - Fluid velocity not known unless inflow diameter is specified. Assumed to be relatively small velocity and may therefore be reasonable to set $u_{in} = 0$.
- Accidental outflow:
  - Enthalpy and velocity evaluated at the orifice state as calculated by the DISC model
- Blowdown outflow:
  - Enthalpy and velocity evaluated at the orifice state as calculated by the DISC model
- Production vapour outflow:
  - Specific enthalpy evaluated at prevailing vapour pressure and system temperature with liquid fraction normally set to 0 – a non-zero liquid fraction will be used for a homogeneously mixed two-phase vessel (initial pure gas vessel in which condensation has occurred).
  - Fluid velocity not known unless production vapour outflow diameter is specified. Assumed to be relatively small velocity (?) and may therefore be reasonable to set $u_{out}^{vap} = 0$.
- Production liquid outflow:
  - Specific enthalpy evaluated at prevailing stagnation pressure and system temperature with liquid fraction always equal 1.
  - Fluid velocity not known unless production liquid outflow diameter is specified. Assumed to be relatively small velocity and may therefore be reasonable to set $u_{out}^{liq} = 0$.

4. MULTI-COMPONENT EXTENSION

The multi-component (MC) extension described in this chapter is not relevant for the TVDI model present in Phast and Safeti 8.4 as these versions are running the pseudo-component (PC) version of the model. However, this MC extension has been included in the TVDI model present in Safeti Offshore 7.2 and subsequent Safeti Offshore releases.

4.1 Background

The original TVDI model as featured in Phast 7.21 and earlier versions was a pseudo-component (PC) model. This means that the model strictly speaking was developed for the release of single-component materials only. However, materials made up of several components could still be used as the model treated the mixture as a pseudo-component material – an imaginary single-component material with averaged properties meant to represent the mixture. There are several weaknesses when using this PC approach for multi-component mixtures. In particular, for a two-phase vessel with a multi-component mixture, the PC approach will maintain equal composition on the vapour and liquid space throughout the release. However, in reality the lighter components will dominate the vapour space while the heavier components will dominate the liquid space – a situation that can be better reflected using a genuine multi-component (MC) approach.

It is on this basis that an MC version of the TVDI model has been developed, and the associated theory will be described in this section.

The theory described in Sections 2 and 3 is generally still valid for the MC version of the model except when specifically mentioned here, in which case it supersedes the theory presented earlier.

4.2 Time and phase dependent compositions

A key to the multi-component version of the model is that unlike the PC version, the composition will be time-dependent and generally be different in the vapour and liquid space, i.e. for stratified two phase vessels and padded liquid vessels. Nevertheless, the idea is to still use one single stream only for the entire system when extending to MC. This is possible by taking advantage of the MC functionality present in the discharge sub-model DISC:

- the overall bulk stream will be sent into DISC for discharge calculations
- when the discharge is from the vapour/liquid space, send a corresponding “phase to release” flag into DISC. DISC will then do a phase split and carry out vapour/liquid discharge calculations accordingly.

It should be noted that both the PC and MC models make use of a separate liquid and vapour stream for padded liquid vessels.

4.3 Governing equations

The PC model applies one single set of governing equations for the entire system, where the system is defined as the fluid within the vessel excluding any potential pipe. For ease of extension to an MC version, one single set of governing equations will be applied to the same system, though the actual governing equations will in part have to be changed. Note that considering one single system for both vapour and liquid space entails an assumption of the vapour and liquid space always being in thermal equilibrium. This is consistent with the PC treatment.

4.3.1 Mass balance equations

The TVDI PC model made use of one single ODE to describe the overall change of mass in the system. This could be done as the composition of the liquid and vapour space were the same and remained constant throughout the release. In the MC model, however, the liquid and vapour space composition will generally not be the same and will furthermore change with time. As such it will be necessary to track the mass of each component of the mixture in the system, resulting in N ODEs for the mass balance if the multi-component mixture has N components. If we define

- X_i^{tot}: mass fraction of component *i* in the total system of fluid

- X_i^{liq} : mass fraction of component *i* in the liquid space
- X_i^{vap} : mass fraction of component *i* in the vapour space,

then the mass balance for the *i*-th component may be expressed as

$$\frac{dM_i(t)}{dt} = X_{t=0,i}^{tot}\,\dot{m}_{in} - X_i^{ph}\,\dot{m}_{acc} - X_i^{vap}\,\dot{m}_{BD} - X_i^{vap}\,\dot{m}_{out}^{vap} - X_i^{liq}\,\dot{m}_{out}^{liq}\,, \qquad (62)$$

where the superscript *ph* is liquid, vapour or two-phase depending on the leak location and vessel type.
The component masses M_i will all be primary variables; these masses are needed to determine the composition of fluid in the system, and the composition is needed before any flash calculations can be carried out. The total system mass M , which is a primary variable for the PC model, will become a secondary variable for the MC model: $M = \sum_{i=1}^{N} M_i$.

4.3.2 Energy balance

The energy balance from the PC model can be directly applied also to the MC model:

$$\begin{aligned}\frac{dU}{dt} = {} & \dot{m}_{in}\left[h\left(P(t=0), T(t=0); \eta_{in}^{liq}\right) + \frac{1}{2}u_{in}^2\right] \\ & - \dot{m}_{acc}\left[h\left(P_{acc}, T_{acc}; \eta_{acc}\right) + \frac{1}{2}u_{acc}^2\right] \\ & - \dot{m}_{BD}\left[h\left(P_{BD}, T_{BD}; \eta_{BD}\right) + \frac{1}{2}u_{BD}^2\right] \\ & - \dot{m}_{out}^{vap}\left[h\left(P, T; \eta_{out}^{vap}\right) + \frac{1}{2}\left(u_{out}^{vap}\right)^2\right] \\ & - \dot{m}_{out}^{liq}\left[h\left(P_{st}, T; \eta_{out}^{liq} = 1\right) + \frac{1}{2}\left(u_{out}^{liq}\right)^2\right].\end{aligned}$$

The liquid/vapour enthalpies in the equation above can be obtained by using a property system model to carry out flash calculations of the overall multi-component stream.

4.4 Specification of initial storage conditions

A new approach for the initial storage condition specification for the MC vessel has been adopted. The revised approach aims to as far as possible match the required model inputs with the data that the analysts are likely to have at their disposal. Three specification flags must be set in the following order:

1. Initial fluid storage state:
   a. Pure gas / super-critical conditions
   b. Stratified two-phase
   c. Homogeneously mixed two-phase
   d. Pressurized liquid
   e. Atmospheric liquid

2. Specified fluid conditions:
   a. Pressure P
   b. Temperature T
   c. Liquid flash fraction η_{flash}

3. Inventory
   a. Mass M
   b. Volume V

c. Liquid fill level (by volume fraction) η_{fill}

Table 1 shows the valid combinations of initial storage specification inputs.

Table 1: Overview of valid input combinations for setting up the initial vessel state

Initial fluid storage state	Specified fluid conditions	Inventory	Notes
Pure gas / super-critical	P & T	M	
		V	
Homogeneously mixed two-phase	Same as below for stratified two-phase		In reality homogeneous two-phase should not be liquid fill regulated[xxviii]
MC Stratified two-phase	P or T	M & V	η_{fill} implies η_{flash}
	P&T or P&η_{flash} or T&η_{flash}	M	
		V	
		M & V	η_{fill} indepdent of η_{flash}
		M & η_{fill}	
		V & η_{fill}	
PC Stratified two-phase	P or T	M & V	
		M & η_{fill}	
		V & η_{fill}	
Pressurized liquid	P & T	M_{Haz} & V	Flash fraction not an option for pressurized liquid
		M_{Haz} & η_{fill}	
		V & η_{fill}	
Atmospheric liquid	T	M	Atm liq always 100% liquid
		V	

4.4.1 Initial storage condition for TVDI MC - details

Table 1 is elaborated here:

- Total fluid composition always input
- User must specify fluid phase in containment:
  - Pure vapour (same for single comp. and mixtures):
    - P,T,M: Vessel shape assumed spherical with diameter to accommodate the specified inventory
    - P,T,V: Vessel shape and dimensions input, mass M is then a calculated value.
  - MC two-phase:
    - Two out of (P,T,η_{flash}) and
      - M: volume calculated, spherical storage assumed and $\eta_{fill} = \eta_{flash}$
      - V: Vessel shape and dimensions input, mass M is then a calculated value and $\eta_{fill} = \eta_{flash}$
      - M&V: both mass and volume given which determines the liquid fill fraction, so $\eta_{fill} \neq \eta_{flash}$
      - M&η_{fill}: volume calculated, spherical storage assumed and $\eta_{fill} \neq \eta_{flash}$
      - V&η_{fill}: Vessel shape and dimensions input, mass M is then a calculated value and $\eta_{fill} \neq \eta_{flash}$
    - P or T and M&V: Iterate on T or P to satisfy the given mass and volume. In this case $\eta_{fill} = \eta_{flash}$.
  - PC two-phase:

[xxviii] Liquid fill level would typically be an input in a separator situation where the liquid level is regulated based on certain criteria. For homogeneous two-phase conditions, like modelling release from hole in a pipe with two-phase fluid, such liquid fill level control is unlikely; rather the thermodynamic liquid flash fraction is likely to govern the amount of liquid present.

- P or T given (in PC mode, two-phase means being on the saturation curve so a given P automatically determines T and vice-versa):
  - M&V: liquid fill fraction η_{fill} calculated
  - M&η_{fill}: vessel volume V is calculated, spherical vessel assumed
  - V&η_{fill}: the mass M is calculated
- Pressurized liquid – PC and MC mode the same:
  - Both P&T and
    - M_{haz} & V : calculate η_{fill}
    - M_{haz} & η_{fill} : calculate volume V, assume spherical vessel
    - V_{haz} & η_{fill} : calculate mass M
  - MC mode : same as above PC mode
- Atmospheric liquid – pressure always atmospheric:
  - T&M: calculate volume V, assume spherical vessel
  - T&V: calculate mass M

4.4.2 Pure gas vessel

- No distinction between a single-component and multi-component mixture required
- Check that the input (P,T) does indeed correspond to pure gas or super-critical phase by carrying out a (P,T) flash on the stream and check the resulting phase.
  - Issue error if (P,T) does not correspond to pure gas.
  - In the GUI perhaps there can be interactive checks on (P,T) to ensure valid user inputs.
- If the inventory is specified in terms of mass M, then assume a spherically shaped containment with diameter given by $D = \left[\frac{6M}{\pi \rho_{vap}(P,T)}\right]^{\frac{1}{3}}$.
- If the inventory is given in terms of volume V, then:
  - a spherical containment with diameter $D = \left[\frac{6M}{\pi \rho_{vap}(P,T)}\right]^{\frac{1}{3}}$ is assumed with gas mass $M = V\rho_{vap}(P,T)$.
  - The inventory may also be given in terms of a specific vessel shape and dimensions, in which case the volume V is calculated as appropriate with mass inventory $M = V\rho_{vap}(P,T)$.

4.4.3 Stratified two-phase vessel

A distinction between a pure component or a single-component mixture on one hand and a multi-component mixture on the other hand is required as different specification options will apply. Pure/single-component mixture should effectively just correspond to PC mode.

<u>Pure component/single-component mixture</u>

- For a pure/single component the phase envelope collapses so if the pressure P is given then the temperature T is automatically known and vice-versa.
- P or T, and two out of V, M, η_{fill}:
  - P/T, V and M
    - See Equation (11) on how the liquid fraction η_{fill} can be obtained.
  - P/T, V and η_{fill}
    - The mass can be obtained from $M = \frac{\rho_V \rho_L V}{(1-\eta_{\text{fill}})\rho_L + \eta_{\text{fill}}\rho_V}$
    - Above derived from the three basic equations:
      - $V = V_L + V_V$
      - $M = \rho_L V_L + \rho_V V_V$

- $\eta = \frac{\rho_L V_L}{M}$

  - P/T, M and η_{fill}
    - Volume can be obtained from $V = \frac{\eta_{\text{fill}} M}{\rho_L} + \frac{(1-\eta_{\text{fill}})M}{\rho_V}$

Multi-component mixture

- P,T,M/V
  - Liquid fraction η_{flash} from (P,T) flash
  - Volume/Mass can be obtained from
    - $V = \frac{\eta_{\text{flash}} M}{\rho_L} + \frac{(1-\eta_{\text{flash}})M}{\rho_V}$
    - $M = \frac{\rho_V \rho_L V}{(1-\eta_{\text{flash}})\rho_L + \eta_{\text{flash}}\rho_V}$
- P, η_{flash}, M/V
  - Temperature T from (P, η_{flash}) flash
  - V or M from above equations
- T, η, M/V
  - Pressure P from (T, η_{flash}) flash
  - V or M from above equations
- Two of (P,T, η_{flash}) and two of (M, V, η_{fill})
  - In this case $\eta_{\text{flash}} \neq \eta_{\text{fill}}$
  - $M = V\{\eta_{\text{fill}}(\rho_L - \rho_V) + \rho_V\}$
  - $V = \frac{M}{\{\eta_{\text{fill}}(\rho_L - \rho_V) + \rho_V\}}$
  - $\eta_{\text{fill}} = \frac{M\left\{\rho_L - \frac{V}{M}\rho_V \rho_L\right\}}{\rho_L V\{\rho_L - \rho_V\}}$

Initial liquid level can then be calculated based on the geometry of the vessel.

4.4.4 Homogeneous two-phase vessel

Similar to the stratified two-phase vessel with exception of liquid level and phase to release.

4.4.5 Pressurized liquid vessel

A pressurized liquid vessel will always have both pressure and temperature specified as input and in additional two out vessel volume, vessel mass, and liquid fill fraction.

- P, T, V and M
  - See Equation (22) on how the liquid volume (and thus) the liquid fill fraction η_{fill} can be obtained.
- P, T, V and η_{fill}
  - The mass can be obtained from $M = V\left(\eta_{\text{fill}}\,\rho_L + x_V \rho_V (1 - \eta_{\text{fill}})\right)$
  - Here x_V is the mass fraction of hazardous material in the vapour space
- P, T, M and η_{fill}
  - The volume V can be obtained by a simple manipulation of above equation

5. MODELLING NEAR THE CRITICAL POINT

Difficulties around the critical point has been partly addressed by introducing “exclusion zones” – regions in pressure-temperature which are “not allowed” to enter during depressurisation. Further work has been carried out to understand these difficulties, and the purpose of this chapter is to describe how TVDI deals with challenging situations related to the critical pressure and critical temperature.

5.1 EXCLUSION ZONES AND ADJUSTMENTS

“Exclusion zones” here refer to certain ranges of pressures and temperatures that are avoided in the TVDI model so as to retain robustness of the model predictions. These zones are shown in **Figure 13** and defined in **Table 2**.

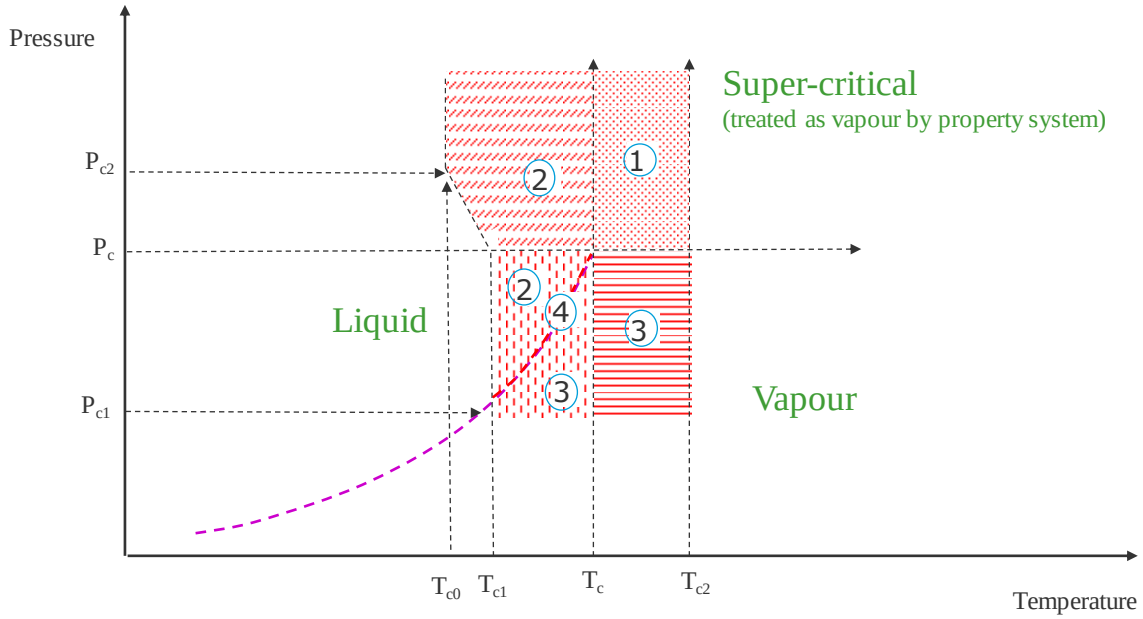


Figure 13: Exclusion zones near the critical point

Table 2: Definition of extended exclusion zones

Zone	P	T	Fluid state
1	Pc<P	Tc<T<Tc2	Super-critical
2	To be defined $P_{sat}(T)$<P	Tc0<T<Tc1 Tc1<T<Tc	Pressurized liquid
3	Pc1<P< $P_{sat}(T)$ Pc1<P<Pc	Tc1<T<Tc Tc<T<Tc2	Pure vapour
4	P=$P_{sat}(T)$	Tc1<T<Tc	Stratified two-phase

In **Table 2** the following definitions apply:

- $P_{c1}=P_{sat}(T_{c1})$
- $P_{c2}=P_c+10$ bar
- $T_{c0}=T_c-5.0$
- $T_{c1}=\min(T_{tricky}-0.2, T_c-1.0)$
- $T_{c2}=T_c+0.5$

Here T_{tricky} is a temperature defined as where the Soave-Redlich-Kwong (SRK) cubiq equation of state (EOS) has a zero discriminant along the saturation curve. The value is always below the critical temperature, varying from around 1 K to 5 K below critical temperature for a few typical materials. In case a non-default property template that does not use SRK EOS is chosen, then T_{tricky} is not defined and $T_{c1}=T_c-1.0$.

5.1.1 STARTING INSIDE AN EXCLUSION ZONE

This section considers the situation when the user has specified initial pressure and temperature that fall within one of the exclusion zones defined above. In such situations, the adjustments made by the TVDI model to the initial conditions are given in Table 3.

Table 3: Starting within an exclusion zone

Zone	Pnew	Tnew	Mnew	Vnew	LFnew	Hole height
1	P_{c1}	T_{c1}	M	V	Set as to preserve M&V	Bottom of tank except for disk rupture and relief valve at top to the tank. Assuming stratified two-phase.
2	P	T_{c1}	M	V	Adjust as needed	Leave unchanged
3	P_{c1}	T_{c1}	M	V	Set as to preserve M&V	Top of the tank. Assuming homogeneous two-phase release.
4	P_{c1}	T_{c1}	M	V	Set as to preserve M&V	Leave unchanged

Special cases

In certain special cases the general adjustments given in Table 3 are not possible and some further adjustments are required:

- If the vapour density increases after (P,T) adjustments such that the total mass is less than the vapour density times the tank volume, then we have an inconsistency. The model handles this by decreasing the tank volume while preserving the total fluid mass.

- It's possible that some mass may be lost after adjustments are made. This would happen in cases where the liquid density is so small after adjustment that even if 99% of the tank is liquid, then the fluid mass is still below the initial fluid mass. Such cases are rare, and a warning is issued if encountered (TVDI warning 1015).

5.1.2 STARTING OUTSIDE BUT LATER ENTERING AN EXCLUSION ZONE

When we *start outside* an exclusion zones but the thermodynamic trajectory during depressurization takes us into an exclusion zone, then adjustments are also made to the pressure and temperature to avoid modelling in the challenging exclusion zones. The adjustments are basically very similar to those made when starting within an exclusion zone – an overview of the behaviour is given in **Table 4**.

Table 4: Starting outside but later entering an exclusion zone

Into zone	Original conditions	Transition	Note
1	$P>P_c$, $T>T_{c2}$	Same as when starting within Zone 1	
2	Not possible		
3	$P>P_{c1}$, $T>T_{c2}$	Same as when starting within Zone 3	Can only enter Zone 3 from a pure vapour state, but could have been super-critical originally.
4	Not possible		

5.2 EXAMPLE OF EXCLUSION ZONES

Below in **Table 5** examples of exclusion zones are given for a range of typical materials.

Table 5: Exclusion zones for selected materials

Material	T_{c0}	T_{c1}	Tricky temperature, T_{tricky}	Critical Temperature, T_c	T_{c2}
Methane	185.55	189.47	189.67	190.55	191.05
Propane	364.83	366.78	366.98	369.83	370.33
Heptane	535.2	536.56	536.76	540.2	540.7
Ammonia	400.65	404.46	404.66	405.65	406.05
CO2	299.21	303.21	303.77	304.21	304.71
H2S	368.53	371.41	371.61	373.53	374.05
Chlorine	412.15	411.99	412.19	417.15	417.65

5.3 REMAINING ISSUES AND FUTURE WORK

- Some cases may still fail due to issues near the critical temperature. In particular it is thought that some pressurized liquid cases involving very high pressures just below Tc0=Tc-5.0 K may cause difficulties. In case of failures it is recommended to try reducing the initial temperature and see if that helps.
- Some short pipe cases near the critical region run very slowly and this should be looked into. More details attached to B-16083.
- Rather than having a pre-defined exclusion zone, one could apply more intelligent adjustments to the pressure and temperature only when the solver actually runs into difficulties. This restart logic would be a more refined approach and avoid adjusting P and T unnecessarily when it may not be needed.

6. FUTURE RECOMMENDATIONS / SUGGESTED IMPROVEMENTS (INCOMPLETE)

The following summarises the key improvement tasks to be conducted on TVDI. Note that this list needs to be reviewed and updated in line with comments and footnotes in preceding chapters.

Thermodynamics and heat transfer:

- Permitting thermal non-equilibrium between fluid phases
- Include heat transfer between tank walls and fluid
- Include heat transfer between surroundings and tank walls

Geometry Modelling:

- Implement additional tank geometry models (e.g. dome-ended tanks, octagonal membrane tanks etc)

Discharge Modelling:

- Improve the modelling of air ingestion to determine ingestion duration

APPENDICES

Appendix A. Guidance on input and output for the TVDI model

A.1 Input data

1. Material specification. This section sets the material and what property template to use.
   - 1.1. Pre-existing stream?
     - 1.1.1.0 – No: stream to be defined in spreadsheet.
     - 1.1.2.1 – Yes: stream defined in relevant matls file. If using a pre-existing stream, then that renders the remaining inputs in the Material specification section irrelevant.
   - 1.2. Mole or mass basis for spreadsheet composition specification?
     - 1.2.1.0 – mass basis
     - 1.2.2.1 – mole basis
   - 1.3. Number of components in stream defined in spreadsheet. Maximum 5 components allowed.
   - 1.4. Mass or mole fraction of each of the mixture components.
   - 1.5. Component of interest. Specify which of the mixture components for which to get additional outputs.
   - 1.6. Property template specification for spreadsheet-defined stream. Default template is PhastMC (=100).

2. Storage state.
   This section sets up the initial conditions within the vessel at the time the accident starts.
   - 2.1. Initial fluid storage state. To ensure consistency between what the user expects and the calculated fluid state at given input conditions, the user is required to input the initial fluid storage state.
     - 2.1.1.1 - Pure gas
     - 2.1.2.2 - Homogeneous two-phase (liquid uniformly dispersed in the tank)
     - 2.1.3.3 - Stratified two-phase (liquid settled at bottom with vapour above)
     - 2.1.4.4 - Padded liquid (pressurized liquid with padding nitrogen)
     - 2.1.5.5 - Atmospheric storage tank (subcooled liquid at ambient pressure)
   - 2.2. Specification choice. Which storage state inputs should be used to set the initial conditions in the vessel?
   - 2.3. Pressure (Pa). Initial storage pressure (absolute), excluding liquid head.
   - 2.4. Temperature (K). Initial storage temperature.
   - 2.5. Liquid fraction (kg/kg). Initial liquid fraction in the vessel.
   - 2.6. Fluid characteristic at storage (-); only applicable to two-phase conditions.
     - 2.6.1.0 – stratified liquid; liquid at the bottom with vapour on top
     - 2.6.2.1 – vapour and liquid homogeneously mixed

3. Vessel data.
   - 3.1. Inventory specification. Initial inventory based on: mass only (=1), volume only (=2), mass and volume (=3), mass and liquid fill fraction (=4), volume and liquid fill fraction (=5).
   - 3.2. Inventory (kg). The total fluid mass contained in the vessel; excluding padding nitrogen for pressurized liquid scenarios.
   - 3.3. Liquid fill fraction by volume (-). For stratified two-phase and padded liquid vessels, it is possible to input the liquid fill fraction by volume when the inventory specification flag is set to (4) or (5).
   - 3.4. Fraction of liquid volume trapped (-). For stratified two-phase and padded liquid vessels, it is possible to specify fraction of liquid volume trapped. When greater than 0 this means that a certain liquid volume is not available to be discharged.
   - 3.5. Pump head (m). Allows the specification of a potential additional pump head [mainly used for pipe releases]
   - 3.6. Vessel shape (-):
     - 3.6.1.1 – Vertical cylinder
     - 3.6.2.2 – Horizontal cylinder
     - 3.6.3.3 – Sphere

3.6.4.4 – Rectangular box (cuboid)

3.7. Vessel dimensions (m):

3.7.1. Diameter – specify for all vessel types except the rectangular box

3.7.2. Length – required for horizontal cylinder and rectangular box

3.7.3. Height – required for vertical cylinder and rectangular box

3.7.4. Width – required for rectangular box only

4. Accident scenario data

4.1. Scenario (1: Line rupture, 2: Disc rupture, 4: Leak, 6: Relief valve)

4.2. Orifice diameter (m). The hole in the vessel is assumed to be circular.

4.3. Orifice elevation (m). Height from vessel bottom to the orifice. For the purpose of elevation, the orifice is assumed to be a point source.

5. Pipe and valve data (not used for Leak scenario):

5.1. Pipe diameter (m)

5.2. Pipe length (m)

5.3. Pipe roughness (m)

5.4. Frequency of pipe fittings (m^{-1}); their presence increases the overall friction on the fluid in the pipe:

5.4.1. Couplings

5.4.2. Junctions

5.4.3. Bends

5.5. Valve velocity head losses (-). These head losses are added to the pressure drop calculations along the pipe:

5.5.1. Excess flow valves

5.5.2. Non-return valves

5.5.3. Shut-off valves

5.6. Number of valves (-):

5.6.1. Excess flow valves

5.6.2. Non-return valves

5.6.3. Shut-off valves

6. Safety system data

6.1. Does isolation work? (-)

6.1.1.0 – Isolation fails; (all production flows are shut off at isolation time while the neighbour vessel mass is added at the isolation time to account for the isolation failure)

6.1.2.1 – Isolation works; (production inflow and outflows all shut off at isolation time)

6.2. Time delay until isolation occurs (s)

6.3. Inventory of neighbouring vessel to be added in the event of isolation failure (kg)

6.4. Does blowdown work? (-)

6.4.1.0 – Blowdown fails

6.4.2.1 – Blowdown works

6.5. Time delay until blowdown occurs (s)

6.6. Diameter of blowdown valve (m)

7. Specification of production flows

7.1. Production flow modelling approach

- 0 – simple:
  - Accidental flow rate assumed constant until isolation time, i.e. production inflow and outflows are assumed to behave such that steady state is maintained until time of isolation.
  - None of production flow inputs are being used when simplistic approach is chosen.
- 1 – detailed:
  - Production inflow: constant user-specified flow rate is assumed until the time of isolation.

- Production outflows: variable flow rates proportional to the difference between the vessel pressure and downstream pressure.

7.2. Production inflow mass flow rate (kg/s): the amount of mass coming into the vessel per second during normal operation
7.3. Production inflow mass liquid fraction (-): mass liquid fraction of inflow. Only used for two-phase storage; pressurized liquid storage always has liquid inflow fraction equal to 1 while pure gas scenarios have an inflow liquid fraction of 0.
7.4. Production vapour outflow pressure difference (Pa): This is the initial difference between the storage pressure in the vessel and the downstream pressure for the production vapour outflow
7.5. Production liquid outflow pressure difference (Pa): This is the initial difference between the storage pressure at the bottom of the vessel and the downstream pressure for the production liquid outflow (liquid outflow always assumed to be at bottom of vessel)
7.6. The following table shows when the various production flow inputs are being used (U=Used, NU=Not Used):

Input argument:	**Detailed approach**				**Simple approach**
	Pure gas storage	Pressurized liquid	Two-phase storage, stratified	Two-phase storage, homogeneous	All scenarios
Production inflow mass flow rate (constant)	**U**	**U**	**U**	**U**	**NU**
Production inflow mass liquid fraction	**NU**	**NU**	**U**	**U**	**NU**
Production vapour outflow downstream pressure difference	**U**	**NU**	**U**	**U**	**NU**
Production liquid outflow downstream pressure difference	**NU**	**U**	**U**	**NU**	**NU**

8. Atmospheric expansion data – ambient data:
   8.1. Ambient pressure (Pa)
   8.2. Ambient temperature (K)
   8.3. Ambient humidity (-)
   8.4. Ambient wind speed (m/s)

3	Input	Description	Units	Limits		Orifice-A
4	Index			Lower	Upper	
10		**Material specification**				
11	A	Pre-existing stream? (0=no, 1=yes)	-			0
12	A	Mole (=1) or mass (=0) basis for composition specification?	-			0
13	A	Number of components in stream	-	1	5	1
14	6	Component name 1 or stream name	-			Ammonia
15	A	Mass or Mole fraction of component 1		0	1	1
16	7	Component name 2	-			Ammonia
17	A	Mass or Mole fraction of component 2		0	1	0
18	8	Component name 3	-			Ammonia
19	A	Mass or Mole fraction of component 3		0	1	0
20	9	Component name 4	-			Ammonia
21	A	Mass or Mole fraction of component 4		0	1	0
22	10	Component name 5	-			Ammonia
23	A	Mass or Mole fraction of component 5		0	1	0
24	11	Component of interest	-			=N14
25	A	Property template specification (PhastMC = 100, Phast6.4 = 101, Acid = 102, SRK = 103, PR = 104, Ideal&SRK = 105, PRIdealFugacity = 106, SRKIdealFugacity = 107	-	100	107	100
26		**Storage state**				
27	A	Initial fluid storage state: 1: Pure gas, 2: Homogeneous 2 phase, 3: Stratified 2 phase, 4: Padded liquid, 5: Atmospheric liquid	-	1	5	4
28	A	Specification choice: 31=P only, 32=T only, 33=P&T, 34=P&LiqFrac, 35=T&LiqFrac	-	0	35	33
29	A	Initial absolute pressure (excluding any liquid head)	Pa	0		=3000000
30	A	Initial temperature	K	0	5000	283
31	A	Initial liquid fraction	-	0	1	0
32	A	Fluid characteristics at storage (0=stratified, 1=homogeneous)	-	0	1	0
33		**Vessel data**				
34	A	Inventory specification: 1:Mass only, 2:Volume only, 3: Mass & Volume, 4: Mass and liquid fill fraction, 5: Volume and liquid fill fraction	-	1	5	3
35	A	Inventory	kg	0.1	10000000	5000
36	A	Liquid fill fraction by volume	-	0	1	0
37	A	Fraction of liquid volume trapped	-	0	1	0
38	A	Pump head	m	0		0
39	A	Vessel shape (1=vert.cyl , 2=hor. cyl , 3=sphere , 4=cuboid)	-	1	4	1
40	A	Vessel diameter	m		100	2
41	A	Vessel length	m			0
42	A	Vessel height	m		50	3
43	A	Vessel width	m			0
44		**Accident scenario data**				
45	A	Scenario (1: Line rupture, 2: Disc rupture, 4: Leak, 6: Relief valve	-			4
46	A	Orifice diameter	m	0.001	50	0.025
47	A	Orifice elevation from vessel bottom	m	0		0
48		**Pipe and valve data (not used for leak)**				
49	A	Pipe diameter	m	0.001	50	0.001
50	A	Pipe length	m	0.01	1000000	750
51	A	Pipe roughness	m	0	0.01	0.0000457
52	A	Frequency of couplings	m-1	0	10	0
53	A	Frequency of junctions	m-1	0	10	0
54	A	Frequency of bends	m-1	0	10	0
55	A	Excess Flow Valves velocity head losses	-	0	100	0
56	A	No Return Valves velocity head losses	-	0	100	0
57	A	Shut-off valve velocity head losses	-	0	100	0
58	A	Number of Excess Flow Valves	-	0	10	0
59	A	Number of Non-Return Valves	-	0	10	0
60	A	Number of Shut-off Valves	-	0	10	0

Figure 14. TVDI model input data – part 1.

Parameters (to be changed only by expert users):

1. Include orifice kinetic energy in energy balance (-):
   1.1. 0 – Do not include kinetic energy of fluid leaving the orifice (consistent with old TVDI model)
   1.2. 1 – Do include kinetic energy of fluid leaving the orifice

2. Vacuum relief valve operating (-):
   2.1. 0 – Valve not operating
   2.2. 1 – Valve operating

3. Vacuum relief valve set point (Pa): If the vacuum relief valve is operating, it will open at a pressure equal to ambient pressure – relief valve set point. E.g: If the ambient pressure is 100000 Pa and the valve set point is 10000 Pa, then the valve will open at 90000 Pa.

4. Maximum number of discharge calculation steps (-): This number should not be changed from 1000 as it must match a hard-coded value in the model.

5. Multi-component modelling flag (-):
   5.1. 0 – pseudo-component modelling
   5.2. 1 – multi-component modelling

6. Convert MC final results to PC?
   6.1. 0 – No. Use MC results as produced.
   6.2. 1 – Yes. Results converted to PC for use by downstream PC models. Temperature/liquid fraction adjusted in such a way as to preserve fluid density.

7. Atmospheric molecular weight (kg/kmole):

8. Model termination and numerical control

   8.1. Maximum release duration (s): The model will at terminate if the release duration exceeds this maximum release duration
   8.2. Minimum flow rate (kg/s): The model will terminate if the accidental release rate drops below this value
   8.3. Max pressure reduction (-): The model will terminate when a certain pressure reduction has been achieved. This reduction is input as a fraction, where a value of 0 would mean immediate termination, a value of 0.5 would mean termination when the initial gauge pressure has been halved, and a value of 1 would mean termination when ambient pressure has been reached. A value greater than 1 disables any termination due to pressure reduction and would allow the vapour space pressure for certain scenarios to drop below ambient pressure.
   8.4. The initial time step size (s): The size of the first time step used to control the output times of results.
   8.5. Time step increase ratio (-): Each subsequent time step size is increased with this ratio. If for example the first time step size was 1 s and the increase ratio equal to 2, then the sequence of output time steps would be 0 s, 1 s, 3 s, 7 s, 15 s. If supplying a value < 1, then the solver will output all internally used time steps.
   8.6. IDA solver relative tolerance (-): used to control the accuracy of the solver of the governing differential-algebraic set of equations.

9. Safety systems:
   9.1. Is the blowdown discharge coefficient specified by the user? (-)
      9.1.1.0: Not specified, calculated by model.
      9.1.2.1: User-specified value used
   9.2. User-specified discharge coefficient for blowdown (-): only used if the previous input has a value of 1.

10. Parameters only applicable to Leak scenarios:

10.1. Use Bernoulli model for metastable liquid releases (-):
10.1.1. 0: Don't use Bernoulli but use standard compressible set of flow equations
10.1.2. 1: Use the Bernoulli equations
10.2. Is the discharge coefficient for accidental leak specified by the user? (-)
10.2.1. 0: Not specified, calculated by model.
10.2.2. 1: User-specified value used
10.3. User-specified discharge coefficient for accidental leak (-): only used if the previous input has a value of 1.
10.4. Forced phase flag: the discharge phase will be attempted forced as follows below.
10.4.1. 0 – unknown
10.4.2. 1 – vapour
10.4.3. 2 – two-phase
10.4.4. 3 – liquid
10.5. 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.

11. Parameters unique to pipe scenarios:
11.1. Capping method for flow rate short pipeline (-): For very short pipes the flow rate predicted by pipe model sometimes exceeds the flow rate computed by the corresponding orifice model, i.e. 0 pipe length. This appears unphysical and inconsistent, and this parameter allows the user to cap the pipe flow rate by the corresponding orifice flow rate. A warning is issued to inform the user whenever capping occurs. The options are as follows:
11.1.1. 0 – no capping
11.1.2. 1 – capped by the orifice flow rate with flashing
11.1.3. 2 – capped by the orifice flow rate without flashing
11.2. Non-equilibrium to equilibrium flow rate ratio for Relief valves (-): the constricted valve orifice area for the relief valve scenario is assumed to be 'over-drilled' by this ratio. Thus the orifice will be less constricted than suggested by the ratio of orifice and pipe diameters.

12. Atmospheric expansion – parameters relevant to the post-expansion model ATEX:
12.1. 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
12.2. Maximum velocity capping method (-). The post-expansion velocity is capped by one of the two possible methods:
12.2.1. 0 – fixed maximum velocity. The post-expansion velocity is capped by a fixed user-defined maximum value (see the next parameter)
12.2.2. 1 – sonic velocity capping. The post-expansion velocity is capped by the sonic velocity of the discharged material.
12.3. Maximum release velocity (m/s): The fixed, maximum velocity that caps the post-expansion velocity when 'fixed maximum velocity' option is chosen in the preceding parameter. Default value 1e8 m/s, i.e. uncapped.

13. Droplet-related parameters:
13.1. 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.
13.1.1. 0 – the original CCPS (Phast 6.4) method – default in Phast 6.6 and earlier versions.
13.1.2. 1 – the JIP method uses the correlation proposed by the Flashing Liquid Jets Phase II project.
13.1.3. 2 – the TNO Yellow Book correlation

13.1.4. 3 – the droplet size correlation developed by Tilton and Farley
13.1.5. 4 – the Melhem correlation.
13.1.6. 5 – the correlation proposed in the JIP Phase III
13.1.7. 6 – the Modified CCPS correlation – new default since Phast 6.7
13.1.8. 7 – the Modified CCPS correlation but not for two-phase pipes

13.2. Force mechanical of flashing break-up (-)?
13.2.1. 0 – no forcing
13.2.2. 1 – force mechanical break-up
13.2.3. 2 – force flashing break-up
Note that not all correlations may be forced:
- Phast 6.4. Can force either flashing or mechanical break-up.
- JIP (phase II or III). Can force mechanical break-up only
- TNO. Purely a mechanical break-up correlation, so this parameter has no effect.
- Melhem. Can force either flashing or mechanical break-up.

13.3. Critical Weber number (-). Used for the CCPS/Phast 6.4 mechanical droplet size correlation. See ATEX model documentation for further details.

13.4. Minimum droplet diameter (m): Lower cut-off value for the calculated droplet diameter

13.5. Maximum droplet diameter (m): Upper cut-off value for the calculated droplet diameter

3	Input	Description	Units	Limits		Orifice-A
4	Index			Lower	Upper	
61		**Safety system data**				
62	A	Does isolation work? (0=no, 1=yes)	-	0	1	1
63	A	Time delay until isolation occurs	s	0		0
64	A	Inventory neighbour vessel to be added upon isolation failure	kg	0		1000
65	A	Does blowdown work? (0=no, 1=yes)	-	0	1	0
66	A	Time delay until blowdown starts	s	0		0
67	A	Diameter of blowdown valve	m	0		0.01
68		**Specification of production flows**				
69	A	Production flow modelling approach (0=simple, 1=detailed)	-	0	1	1
70	A	Production inflow mass flow rate (constant)	kg/s	0		0
71	A	Production inflow mass liquid fraction	-	0		0
72	A	Production vapour outflow downstream pressure difference	Pa	0		10000
73	A	Production liquid outflow downstream pressure difference	Pa	0		10000
81		**Atmospheric expansion data**				
82	A	Ambient pressure	Pa			101325
83	A	Ambient temperature	K	200	350	283
84	A	Ambient humidity	-	0	1	0.7
85	A	Ambient wind speed	m/s	0		0
86		**PARAMETERS (below input to be changed by expert users o**				
87	A	Include orifice kinetic energy in energy balance?	-			0
88	A	Vacuum relief valve operating? (0=no, 1=yes)	-	0	1	1
89	A	Vacuum relief valve set point if operating	Pa	0	50000	0
90	A	Generate debug file (currently not active) (0=no, 1=yes)	-			0
91	13	Maximum number of discharge calculation steps (don't change)	-			1000
92	A	Multi-component modelling flag (1 = MC, 0 = PC)	-	0	2	1
93	A	Convert MC final results to PC? 0=No, 1 = Convert to PC	-	0	1	0
94	A	Atmospheric molecular weight	kg/kmole			28.966
95		**Model termination and numerical control**				
96	A	Maximum release duration	s			3600
97	A	Minimum flow rate (stop model when flow rate below this value)	kg/s	0		0
98	A	Max pressure reduction fraction (1=reduce to ambient pressure)	-	0		1.5
99	A	Initial time step size	s	0		0.1
100	A	Time step increase ratio	-	1		1.05
101	A	IDA solver relative tolerance	-	0		0.00001
102		**Safety systems**				
103	A	Is the blowdown discharge coefficient specified by user?	-	0		0
104	A	User-specified blowdown discharge coefficient	-	0.6	1	1
105		**Leak only**				
106	A	Use Bernoulli model for metastable liquid releases? (0=N,1=Y)	-			0
107	A	Is the Discharge Coefficient specified by user? (0=N,1=Y)	-			0
108	A	User-specified Discharge Coefficient	-	0.6	1	1
109	A	Forced phase flag (0=unknown, 1=vap, 2=2PH, 3=Liq)	-	0	3	0
110	A	Allow Flashing across the orifice (0=N,1=Y)	-			0
111		**Pipe only**				
112	A	Pipe flow rate cap (0=none, 1=orif allow flash, 2=orif no flash)	-	0	2	2
113	A	Non-equilibrium to equilibrium flow rate ratio for Relief valves	-			1.2
114		**ATEX parameters - expansion method**				
115	A	Expansion method flag (0=min thermal change, 1=isentropic, 2= conservation of momentum, 4=DNV GL recommended)	-	0	4	4
116	A	Maximum velocity capping method (0=fixed, 1=sonic)	-	0	1	0
117	A	Maximum release velocity (Not applicable to sonic velocity capping)	m/s	0		100000000
118		**ATEX Droplet data**				
119	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
120	A	Force breakup? (0=don't force, 1=mechanical, 2=flashing)		0	2	0
121	A	Critical Weber number	-	1	50	12.5
122	A	Minimum droplet diameter	m	0	0.01	0.00000001
123	A	Maximum droplet diameter	m	0	1	0.01

Figure 15: TVDI model input data – part 2.

A.2 Output data

1. Number of time steps used for outputting results (-)

2. Time (s). The output times at which the model has produced results.

3. Storage state and tank data:
   - 3.1. Stagnation vapour space pressure (Pa).
   - 3.2. Stagnation vapour space temperature (K).
   - 3.3. Volume of vapour in tank (m^3)
   - 3.4. Liquid head (m) : distance from centre of orifice to the liquid-vapour interface
   - 3.5. Total liquid height (m): distance from vessel bottom to liquid-vapour interface (excluding swelling)
   - 3.6. Swell height (m): Total liquid height including entrained vapour (current model assumes zero vapour entrained in liquid phase)
   - 3.7. Pressure at hole inlet (Pa): vapour space pressure plus pressure exerted by liquid head
   - 3.8. Mass of nitrogen (kg): Mass of padding nitrogen – only nonzero for pressurized liquid vessels.
   - 3.9. Total vapour mass (kg).
   - 3.10. Vapour mass of component of interest (kg).
   - 3.11. Total liquid mass (kg).
   - 3.12. Liquid mass of component of interest (kg).
   - 3.13. Total fluid mass (kg).
   - 3.14. Total fluid mass of component of intereset (kg).

4. Orifice state (or pipe exit for pipe scenarios):
   - 4.1. Orifice pressure (Pa)
   - 4.2. Orifice temperature (K)
   - 4.3. Orifice liquid fraction (-).
   - 4.4. Orifice liquid fraction of component of interest (-).
   - 4.5. Orifice velocity (m/s)
   - 4.6. Orifice discharge coefficient (-)

5. Final (post-expansion) state:
   - 5.1. Expanded diameter (m)
   - 5.2. Post-expansion temperature (K)
   - 5.3. Post-expansion liquid fraction (-)
   - 5.4. Post-expansion liquid fraction of component of interest (-)
   - 5.5. Post-expansion velocity (m/s)
   - 5.6. Post-expansion droplet diameter (SMD) (m)

6. Accident outflow results
   - 6.1. Expelled mass (kg). – total mass expelled by accidental release
   - 6.2. Expelled mass of component of interest (kg). – total mass expelled by accidental release of the component of interest
   - 6.3. Accident mass release rate (kg/s)
   - 6.4. Accident mass release rate of component of interest (kg/s)

7. Various mass flow rates
   - 7.1. Blowdown flow rate (kg/s) – rate at which mass is evacuated through the blowdown valve
   - 7.2. Production inflow rate (kg/s)
   - 7.3. Production vapour outflow rate (kg/s)
   - 7.4. Production liquid outflow rate (kg/s)

3	Input	Description	Units	Limits		Orifice-A
4	Index			Lower	Upper	
124	**Outputs**					
125	Output	Description	Units			
126	Index					
127		*ERROR STATUS*				WARN
128	1	Size of output arrays (number of time steps)	-			109
129	2	Time	s			
130		**Storage state and tank data**				
131	3	Stagnation vapour space pressure	Pa			
132	4	Stagnation vapour space temperature	K			
133	5	Volume of vapour in tank	m^3			
134	6	Liquid head	m			
135	7	Total liquid height	m			
136	8	Swell height	m			
137	9	Tank liquid fraction	-			
138	10	Pressure at hole inlet	Pa			
139	11	Mass of nitrogen (padding gas)	kg			
140	12	Current total vapour mass	kg			
141	13	Current vapour mass of component of interest	kg			
142	14	Current total liquid mass	kg			
143	15	Current liquid mass of component of interest	kg			
144	16	Current total fluid mass	kg			
145	17	Current total fluid mass of component of interest	kg			
146		**Orifice state (pipe exit for pipe scenarios)**				
147	18	Orifice pressure	Pa			
148	19	Orifice temperature	K			
149	20	Orifice liquid fraction	-			
150	21	Orifice liquid fraction of component of interest	-			
151	22	Orifice velocity	m/s			
152	23	Orifice discharge coefficient	-			
153		**Final (post-expansion) state**				
154	24	Expanded diameter	m			
155	25	Post-expansion temperature	K			
156	26	Post-expansion liquid fraction	-			
157	27	Post-expansion liquid fraction of component of interest	-			
158	28	Post-expansion velocity	m/s			
159	29	Post-expansion droplet diameter (SMD)	m			
160		**Accident outflow results**				
161	30	Expelled mass	kg			
162	31	Expelled mass of component of interest	kg			
163	32	Total accident mass release rate	kg/s			
164	33	Accident mass release rate of component of interest	kg/s			
165		**Various mass flow rates**				
166	34	Blowdown flow rate	kg/s			
167	35	Production inflow flow rate	kg/s			
168	36	Production vapour outflow rate	kg/s			
169	37	Production liquid outflow rate	kg/s			

Figure 16: TVDI model output data.

A.3 Model warnings and errors.

Below are descriptions of the possible TVDI model error and warning messages that the user may encounter.

Errors:

`TVD2 1 "Flash type %1%integer% not supported"`
An invalid flash type has been requested during the initialization of the model – try changing the Specified Conditions.

`TVD2 2 "Failed to initialise the IDA solver"`
Error setting up the solver for the governing equations – this could be for a number of reasons including failure to allocate sufficient memory.

`TVD2 3 "Failed to set IDA solver tolerances"`
The solver returns an error when trying to set the absolute and relative tolerances.

`TVD2 4 "Failed to set the user data for IDA solver"`
Failure to set the user-defined data required by the solver.

`TVD2 5 "Failed to set IDA choice of linear solver"`
Error when setting the linear solver for required to solve the governing equations.

`TVD2 6 "Exception %1%integer% caught during call to IDASolve"`
A controlled but unrecoverable error has been encountered when trying to solve the system of governing equations. This can happen due to a number of reasons, including ill-behaved physical properties for certain pressure-temperature regions. Workarounds that may help:

- Try initial conditions that would avoid proximity to the critical point during depressurization
- If using a mixture: try simplifying the mixture by reducing the number of components.

`TVD2 7 "IDA failed to calculate consistent initial conditions"`
The solver encountered issues when setting initial conditions. Try adjusting the initial process conditions.

`TVD2 8 "Illegal value %1%integer% of vessel shape flag"`
Valid vessel shapes are vertical cylinders (1), horizontal cylinders (2), sphere (3) and cuboid (4).

`TVD2 9 "Specified input mass %1%Mass% too small for vessel volume"`
Error given if the user-specified inventory is too small for the given vessel dimensions. Example: the specified mass for a two-phase vessel is smaller than the mass of vapour with volume equal to vessel volume. Adjust inventory and/or vessel dimensions to obtain a consistent set of inputs.

`TVD2 10 "Specified input mass %1%Mass% too large for vessel volume"`
Error given if the user-specified inventory is too large for the given vessel dimensions. Example: the specified mass for a two-phase vessel is larger than the mass of liquid with volume equal to vessel volume. Adjust inventory and/or vessel dimensions to obtain a consistent set of inputs.

`TVD2 11 "Failed to bracket root"`
Numerical error – failing to bracket a root. Try adjusting initial processing conditions.

`TVD2 12 "Outflow height %1%Length% out of range"`
The height of the accidental leak/line rupture is invalid – e.g. the accidental leak height is larger than the height of the vessel. Reduce the hole height or increase the vessel height.

`TVD2 13 "Outflow diameter %1%Length% out of range"`
Invalid value of leak/line rupture diameter – e.g. the value is larger than the height of the vessel. Adjust hole diameter and/or vessel dimensions.

`TVD2 14 "Partial volume %1%Volume% out of range"`
Volume of liquid in vessel inconsistent with vessel dimensions. Try adjusting initial inventory and/or vessel dimensions.

`TVD2 15 "Partial height %1%Length% out of range"`

Height of liquid in vessel inconsistent with vessel dimensions. Try adjusting initial inventory and/or vessel dimensions.

TVD2 16 "Outflow height %1%Length% above liquid level for padded liquid vessel"
The height of accidental outflow is above the liquid level for a pressurized liquid scenario – the model then terminates immediately as this scenario only supports accidental outflow from the liquid side. Reduce the outflow height or increase the inventory to avoid this error message.

TVD2 17 "Specified time step index out of range"
A request for a non-existent time step has been made internally in the model.

TVD2 18 "Invalid value of scenario flag %1%integer% (not supported by TVD2)"
Invalid specification of accident scenario. The model supports OrificeScenario (4), LineRuptureSceneario (1), DiscRuptureScenario (2) and ReliefValveScenario (6).

TVD2 19 "Invalid value of vessel type flag %1%integer% (not supported by TVD2)"
Invalid specification of vessel type when setting up the model. The model supports these vessel types initially at time t=0s: PureGasVesselType (1), HomogeneousVesselType (2), Stratified2PhVesselType (3), PadLiqVesselType (4) and AtmLiqVesselType (5).

TVD2 20 "New shape volume %1%Volume% is not positive"
Something has gone wrong when re-sizing the vessel following adding mass from neighbouring vessel upon isolation failure. Try adjusting the mass to add in the event of isolation failure.

TVD2 21 "User-specified input mass %1%Mass% too small; must be larger than 0.1 kg"
Increase the inventory to avoid this error.

TVD2 22 "Time to isolation %1%Time% exceeds time to blowdown"
The time to isolation is not allowed to exceed time to blowdown. Decrease/increase the isolation/blowdown time to avoid this error.

TVD2 24 "Temperature above bubble point temperature %1%Temperature% for padded liquid vessel"
Increase pressure or reduce temperature to avoid this error.

TVD2 25 "Equation of state fails to find two distinct phases - try changing processing conditions or material specification"
This error is given if for a two-phase vessel the liquid density equals the vapour density, indicating that only one fluid phase is present.

TVD2 27 "Property identifier not supported - cannot perform requested property evaluation"
The model has internally requested an unsupported property evaluation.

TVD2 28 "Multi-component padded liquid vessels not yet supported"
Try switching to pseudo-component (PC) modelling if encountering this error.

TVD2 29 "Invalid number of components in mixture"
This error is issued if running the model through the MDE test spreadsheet interface and specifying a number of components outside of the valid range 1 to 5.

TVD2 30 "Invalid mixture composition specified"
This error is issued if running the model through the MDE test spreadsheet interface and all components are given 0 composition.

TVD2 31 "User-specified input material is not a pre-existing stream"

This error is issued if running the model through the MDE test spreadsheet interface and the requested material cannot be found in the associated materials file.

```
TVD2  32 "Input temperature %1%Temperature% too low for chosen
specification; increase temperature or try padded liquid vessel"
```

```
TVD2  33 "Invalid value %1%integer% for the inventory specification
flag"
```
Valid values for inventory specification are “mass only” (1), “volume only” (2) and “both mass and volume” (3).

```
TVD2  34 "Invalid value %1%integer% for the multi-component modelling
flag"
```
Valid values are “PC modelling” (0), “MC modelling with single aerosol” (1) and “MC modelling with multiple aerosol” (2).

```
TVD2  36 "The specified conditions (P,T) do not correspond to a two-
phase fluid (Liquid fraction=%1%real%)"
```
Inconsistent inputs: try modifying the specified processing conditions if expecting two-phase conditions inside the vessel.

```
TVD2  37 "A pure gas vessel does not support this value of the
specification flag: %1%integer%"
```
If you expect pure gas storage conditions, this must be done by a “Pressure and temperature” specification.

```
TVD2  38 "A padded liquid vessel must have all of pressure, temperature,
mass and vessel volume specified"
```
If you expect pressurized liquid storage conditions, this must be done by supplying all of pressure, temperature, fluid mass and vessel volume as input.

```
TVD2  39 "Failure to adapt MC discharge results for use by downstream PC
models"
```

```
TVD2  40 "Calculated phase at given pressure and temperature does not
correspond to pure vapour"
```
Try adjusting input pressure and temperature if expecting pure vapour fluid state.

```
TVD2  41 "Invalid combination of pressure, temperature, liquid fraction,
mass and volume for two-phase storage"
```
See table in Section 4.4 for valid combinations of inputs for two-phase storage.

```
TVD2  42 "Temperature above boiling point temperature %1%Temperature%
for atmospheric liquid vessel"
```
Reduce the input temperature to below the given boiling point temperature to avoid this error.

```
TVD2  43 "Vacuum relief valve closed; tank not open to atmosphere so
cannot run atmospheric liquid vessel"
```
Open the vacuum relief valve to enable running the atmospheric storage tank scenarios.

```
TVD2  45 "Generic error message: The TVDI model failed to run but the
cause is unknown."
```

```
TVD2  47 "Invalid mixture definition: component number %1%integer% has
zero contribution"
```

```
TVD2  48 "Liquid phase cannot exist as fluid is super-critical with
temperature above critical temperature %1%Temperature%"
```
Reduce the input temperature if expecting pressurized liquid as initial fluid state.

TVD2 49 "Unsuccessful adjustment attempted by model near critical point (tank volume reduction too large). Try different initial pressure/temperature."

TVD2 50 "Error thrown in short pipe discharge calculations"
An unspecified error has occurred while calculating the flow in the pipe. Consider using the time-varying leak scenario instead; alternatively try the steady-state short pipe scenario.

TVD2 51 "An unrecoverable model error has been encountered at time %1%Time%."
Consider using the steady-state leak model as an alternative.

TVD2 53 "Unable to change property template."
The model encountered difficulties and tried switching property template internally, but this was unsuccessful. Consider using the steady-state leak model as an alternative.

TVD2 54 "Too large increment %1%real% in tank volume after adjustment made around the critical point"
The model tried a simplified approach to deal with difficulties near the critical point but failed. Try adjusting the initial pressure and temperature, or alternatively consider using the steady-state leak model.

TVD2 56 "The liquid fill fraction specified (%1%real%") must be greater than 0 for a vessel with liquid present"
There has to be liquid present when the calculated fluid state is indicates presence of liquid. Supply a positive liquid fill fraction or change the fluid storage conditions.

TVD2 57 "The liquid fill fraction must be smaller than %1%real% to allow some vapour to exist in the vessel"
If the user chooses to set up the vessel inventory by specifying liquid fill fraction, then this fraction cannot exceed an upper threshold level (less than 1). This is to ensure that there is some vapour present in the stratified two-phase vessel. Reduce the liquid fill fraction below the maximum value to run the case.

TVD2 58 "Failed to create matrix for the IDA solver."
TVD2 59 "IDA solver error: Failed to attach matrix and linear solver modules."
Both of these errors indicate that something has gone wrong with the initialisation of the numerical solver deployed by the TVDI model. It is difficult to provide any general advice in this case – it is recommended to contact DNV technical support.

TVD2 60 "Liquid fraction to be trapped is input as %1%real% which is above maximum value allowed of 0.999."
Pressurized liquid vessels only allow releases from the liquid side. It is therefore not possible to trap all the liquid in case of pressurized liquid vessels as there would then not be any release at all. Therefore, the upper limit of the fraction of liquid volume trapped is set to 0.999 for pressurised liquid vessels. Reduce the amount of liquid trapped to a value below the maximum value of 0.999 to run the case.

TVD2 61 "Liquid fill fraction specification is not allowed for a homogeneous two-phase vessel."
The user has specified a vessel with homogeneously mixed two-phase fluid. In this case the liquid is assumed to be uniformly distributed throughout the vessel and it does not make sense to have a certain liquid fill level, hence this error message. Liquid fill fraction input is only supported for stratified two-phase vessels and pressurized liquid vessels.

Warnings:
TVD2 1001 "Model terminated prematurely due to IDA solver failure"
The solver failed unrecoverably leading to premature model termination.

TVD2 1002 "Model terminated due to exceeding maximum number of time steps (1000)"
The model stops when having output 1000 time steps. If you encounter this warning, try increasing the time step size.

TVD2 1003 "Model terminated with positive liquid head %1%Length%"
For some reason the model terminated while the liquid head is still positive.

TVD2 1004 "Model terminated with pressurized vapour space (%1%Pressure%)"
For some reason the model terminated while the vapour space is still pressurized. This is fairly common for pressurized liquid vessels as these terminate when the liquid level drops below the hole height.

TVD2 1005 "Model terminated immediately as initial flow rate %1%MassFlow% less than minimum flow rate"
Decrease the minimum flow rate threshold to avoid this warning.

TVD2 1006 "Model terminated immediately due to minimum pressure too close to initial pressure"
Increase the maximum pressure reduction factor to avoid this warning.

TVD2 1007 "Model terminated immediately since initial stagnation pressure %1%Pressure% < ambient pressure"
Increase the initial vapour space pressure in the tank to avoid this warning.

TVD2 1008 "Initial user-specified pressure difference %1%Pressure% for production outflow too small - production outflow set to zero."
Increase the pressure difference for production outflows to avoid this warning.

TVD2 1009 "Initial user-specified pressure difference %1%Pressure% for production outflow too large; set equal to gauge storage pressure."
Warning issued as the difference between vapour space pressure in vessel and downstream production outflow pressure cannot be larger than the vapour space gauge pressure as this would imply sub-atmospheric pressure in the downstream production outflow. The downstream pressure is therefore set equal to the ambient pressure.

TVD2 1010 "Significant amount of mass (vapour) removed in transition to atmospheric liquid vessel"
A padded liquid vessel can undergo a transition to an atmospheric liquid vessel if the vapour space pressure drops to atmospheric. When such a transition occurs, the subsequent modelling ignores the part of the hazardous material that was present in the vapour space of the vessel. In some rare cases the disregarded vapour mass may be significant (more than 5%) compared to the liquid mass, in which case this warning is issued.

TVD2 1011 "Simplified transition from super-critical fluid to saturated liquid after time %1%Time%."
This warning is issued when the pressure-temperature trajectory during depressurization goes from the super-critical region to the pressurized liquid region. When this occurs the model drops the pressure and restarts as saturated liquid.

TVD2 1012 "Requested component of interest not found - first component of mixture set as component of interest"

TVD2 1015 "Lost %1%Mass% of inventory due to critical transition: pressure dropped to saturated pressure"

TVD2 1016 "Multi-component padded liquid vessels not yet supported, switching to PC mode"

TVD2 1017 "Tank has become completely filled with liquid at %1%Time%, assume steady-state thereafter"
In rare cases it is possible that production inflow can cause the tank to fill up completely with liquid. If this happens then a steady-state outflow is assumed thereafter.

TVD2 1018 "Inventory increased by %1%Mass% on isolation failure despite production inflow set to 0 kg/s"
This warning is issued to inform the user that despite specifying a production inflow of 0 kg/s, at time of isolation failure the inventory has been increased by the non-zero mass specified in upstream vessel.

TVD2 1019 "Initial temperature reduced to %1%Temperature% for robustness reasons as too close to critical temperature"
Due to limitations in the property evaluations very near the critical point, the initial temperature has been reduced to a value slightly further away from the critical temperature.

TVD2 1020 "Initial pressure close to saturation pressure (%1%Pressure%); consider starting at saturated conditions"
This warning is issued for pressurized liquid vessels when conditions in the vessel are very close to saturated conditions.

TVD2 1021 "Could not find a suitable temperature where SRK CEOS has a 0 discriminant"
The model has encountered difficulties characterizing the solution set of the Soave-Redlich-Kwong (SRK) cubic equation of state (CEOS).

TVD2 1022 "Simplified transition from gas near critical point to homogeneous two-phase after time %1%Time%."
The model makes an adjustment to the pressure and temperature to avoid difficulties very close to the critical point.

TVD2 1023 "Temperature reduced after time %1%Time% for robustness reasons to avoid near critical temperature modelling."
The model reduces the temperature to avoid difficulties very close to the critical temperature.

TVD2 1024 "Tank volume reduced to ensure continuity in mass inventory after adjustment made near critical point."

TVD2 1025 "Switch to SRK-IdealFugacity property template at %1%Time%. Liquid density may subsequently be underpredicted."
The model encountered an error and switched to the SRK-IdealFugacity template to try to overcome the error. The only difference between the default PhastMC template and the SRK-IdealFugacity template is the liquid density evaluation: the former uses the DIPPR saturated liquid density, while the latter uses the liquid density based on the Soave-Redlich-Kwong cubic equation of state.

TVD2 1026 "Tank volume increased by %1%real% after adjustment made near critical point to ensure continuity in mass inventory."

Modelling near the critical point is challenging and various adjustments may be applied as described in detail in Chapter 5. If such adjustments causes an increase in the tank volume, then this warning is issued.

TVD2 1027 "The new time-varying discharge model will be run and results may therefore change."
The old TVDI model is no longer supported; the new model will be run instead.

TVD2 1028 "The time-varying discharge model has encountered difficulties at time %1%Time%. Subsequently discharge the material assuming a steady-state release."

Time-varying calculations cannot continue after the given time. Therefore steady-state results are applied after this time. For details see Section 2.3.8.

TVD2 1029 "Blowdown ignored at time %1%Time%" due to calculation difficulties. Results may be conservative."

When steady-state results are applied due to calculation difficulties (see Section 2.3.8), this warning is issued if blowdown was supposed to have commenced during the steady-state period of the release.

TVD2 1030 " Switch from metastable liquid assumption to allow flashing to the orifice at time %1%Time%."

The model switched the fluid expansion assumption from stagnation to the orifice at the given time to be able to continue the discharge calculations.

Messages:

TVD2 2001 "Maximum release duration is reached with the vapour space still pressurised (%1%Pressure%)"

The time-varying release model stops calculations when the maximum release duration has been reached (default 3600 s). If the vapour space is still pressurized at this time, then this message is issued.

TVD2 2002 "Maximum release duration is reached with positive liquid head %1%Length%"

The time-varying release model stops calculations when the maximum release duration has been reached (default 3600 s). If there is still liquid above the hole at this time, then this message is issued.

TVD2 2003 "The time-varying release terminated with vapour space still pressurised (%1%Pressure%) as only liquid contents is discharged"
The model only releases liquid for pressurized liquid vessels, so there is no subsequent vapour release after the liquid has been discharged. This message informs the user accordingly if the vapour space is still pressurised after the release calculations have stopped.

Appendix B. A Memo on Liquid Swell Modelling

MEMO TO:	MEMO NO. : M-DNVS-TVDI-Liq-Swell-Mod-003 : M-DNV-TI-002
Henk Witlox, Stene Jan	**FROM** : Ade Oke **DATE** : 22nd June 2009
SUBJECT: **Review of liquid swell modelling in TVDI (Phast 7.21 and earlier) – rev 3**	

CONTENTS

B.1 Introduction

This memo presents a review of the liquid swell modelling in the PHAST time varying discharge model (old TVDI present in Phast versions 7.21 and earlier) against the DIERS[xxix] (1992) and more recently, the Cumber (2002)[xxx] models.

The memo is structured as follows:

- Section B.2 presents an overview on various liquid swell modelling approaches
- Section B.3 describes the key equations and algorithms adopted within the DIERS (1992) bubbly and churn–turbulent liquid swell (vessel flow) models.
- Section B.4 presents an overview of recommended modifications to the DIERS (1992) bubbly and churn–turbulent liquid swell models as prescribed in Cumber (2002).
- Section B.5 sets out the (bubbly and churn–turbulent) liquid swell modelling in the Phast time varying discharge model (old TVDI present in Phast 7.21 and earlier).

B.2 Overview

Liquid swell occurs during the depressurisation of a flashing liquid due to two major reasons: increase in volume due to entrainment of vapour bubbles created from the flashing process and slight increase in liquid specific volume due to the expansion process. The level of swell observed at any given time is dependent on the generation and disengagement rate of vapour bubbles (i.e. ratio of superficial vapour velocity and bubble rise velocity) from the surface of the liquid.

A number of models exist in literature that attempt to estimate the degree of vapour-liquid disengagement (i.e. liquid swell) during vessel depressurisation as a function of vapour throughput. These models are also known as “vessel flow models” and include[xxix]:

[xxix] Fisher, H. G., Forrest, H. S., Grossel, S. S., Huff, J. E., Muller, A. R., Noronha, J. A., Shaw, D. A., and Tilley, B. J., Emergency Relief System Design Using DIERS Technology, The Design Institute for Emergency Relief Systems, American Institute of Chemical Engineers, New York, 1992

[xxx] Cumber, P., “Modelling Top Venting Vessels Undergoing Level Swell,” Journal of Hazardous Materials, A89 (2002), 109 – 125.

- The homogenous (no-slip) vessel model: this model assumes the vapour and liquid phases are in thermodynamic and mechanical equilibrium (i.e. zero vapour-liquid disengagement, maximum liquid swell)
- The bubbly vessel model: this model assumes vapour generation throughout the liquid is uniform with limited vapour – liquid disengagement (i.e., significant liquid swell) in the vessel
- The churn – turbulent model: this model assumes vapour generation throughout the liquid is uniform but with considerable vapour – liquid disengagement (limited liquid swell) in the vessel.
- The non-boiling height vessel model: this model is essentially a churn – turbulent model but assumes vapour generation, and hence liquid swell, is only limited to the top portion of the fluid.
- The no-drag vessel model: this model assumes uniform vapour generation but with near instantaneous (i.e. maximum) vapour – liquid disengagement (negligible liquid swell).

There are two vessel flow models currently supported in TVDI: the bubbly and the churn – turbulent models. It is not clear why the no-drag, homogenous and non-boiling height vessel flow models are not supported in TVDI.[xxxi]

The bubbly and the churn – turbulent models have been formulated from the drift flux theory[xxxii] with empirical adjustments to match available experimental data[xxix] and are primarily expressed as a function of three variables: the average void fraction in the swelled liquid (α_{vap}), the superficial vapour velocity at the liquid surface (u_{sv}) and the characteristic bubble rise velocity (u_{bub}).

The aim of this report is to review the implementation of the bubbly and churn – turbulent models in TVDI against similar models described in the DIERS (1992)[xxix] and Cumber (2002)[xxx] reports.

Note that the no-drag, homogenous and non-boiling height vessel models have valid applications. In particular, the no-drag vessel model is best suited for the modelling of venting involving non-boiling (sub-cooled / padded / evaporating) non-foamy liquids, while the homogenous vessel model is most suitable for modelling venting resulting from runaway reactions (i.e. reactive mixtures) or involving foamy fluids. The non-boiling height vessel model, as compared to and the bubbly and churn-turbulent models, was observed to perform best against the DIERS (1992) large-scale experimental data involving non-foamy fluids. The non-boiling height model is particularly suited for the modelling of venting involving partially boiling non-foamy liquids (i.e. liquids with enough hydrostatic pressure exerted at the non-boiling height to maintain the total pressure at this height below or equal to the fluid's saturation pressure).[xxxiii]

B.3 DIERS (1992) Bubbly and Churn-Turbulent Vessel Flow Model and Algorithm

The following presents the key liquid swell modelling equations and algorithm based on the bubbly and churn – turbulent vessel flow models described in the DIERS (1992)[xxix] report.

Note that DIERS (1992) recommends the following simple criteria as means of identifying the governing vessel flow model[xxxiv]:

[xxxi] The only postulation that may be proffered is that: the homogenous and no-drag vessel models represent the extremes of liquid swell modelling, while the non-boiling height model is rather expensive to implement (i.e. mathematically and computationally). Furthermore, the thermodynamics modelling supported in TVDI are currently unsuitable for modelling vapour generation resulting from chemical reactions (i.e. as per modelling liquid swell due to runaway reactions using the homogenous vessel model).

[xxxii] Zuber, N., and Findlay, J. A., "Average volumetric concentration in two-phase flow systems" Trans. Am. Soc. Mech. Engrs. Journal of Heat Transfer, 87, 453 (1965);

Ishii, M., "One –dimensional drift-flux model and constitutive equations for relative motion between phases in various flow regimes, Argonne National Laboratory Report ANL-77-47 (1977)

Ishii, M., and Zuber, N., "Drag coefficient and relative velocity in bubbly, droplet or particulate flows, AIChE Journal, 25, 843 (1979)

[xxxiii] DIERS (1992) mention that for non-foamy fluids, the bubbly and churn-turbulent models were generally observed to be "unable to exactly reproduce the pressure and vessel void fraction histories measured in the DIERS large-scale experiments without including a "non-boiling region" in the lower section of the vessels". For these experiments, the non-boiling height vessel model was observed to predict measured data best (i.e. as compared to and the bubbly and churn-turbulent models).

[xxxiv] Cumber (2002) reports the following criteria as being recommended by DIERS for identifying the governing vessel flow model:

$f(\alpha_{vap,tank}) \leq 0.2$ bubbly flow regime,

$0.2 < f(\alpha_{vap,tank}) \leq 20$ churn-turbulent flow regime,

$20 < f(\alpha_{vap,tank})$ homogenous flow regime

In the above selection criterion f appears to be defined by Cumber (2002) by the churn-turbulent definition given by Eq. (66) [although this is not explicitly mentioned]. The origin of the above transition criteria remains to be substantiated / confirmed. Figure I-B1 in DIERS(1992) includes graphs of f (dimensionless superficial vapour velocity) versus versus averaged void fraction for both bubbly vessel and churn-turbulent vessel flow

- The bubbly and churn-turbulent vessel flow models are only applicable to fluids with no foaming tendency (i.e. non-reactive mixtures), while the homogenous vessel flow model may only be applied to reactive mixtures.[xxxv]
- The churn-turbulent vessel flow model may only be applied to non-reactive fluids with liquid viscosity less than 100 cp (i.e. μ_{liq} (T_{liq}) < 100 cp); for μ_{liq}(T_{liq}) ≥ 100 cp, the bubbly vessel flow model applies.

B.3.1 DIERS BUBBLY AND CHURN-TURBULENT VESSEL FLOW MODEL

The degree of vapour-liquid entrainment (or disengagement, α_{vap}) in a boiling fluid is defined as the volume (or mole or void) fraction of vapour in the vapour-liquid mixture.

α_{vap} and the total vessel void fraction ($\alpha_{vap,tank}$) can be expressed in terms of the total vessel volume (V_{tank}), swelled liquid volume (V_{swell}), liquid volume (i.e., excluding entrained vapour, V_{liq}) as:

$$\alpha_{vap} = \frac{V_{swell} - V_{liq}}{V_{swell}} \quad (63)$$

$$\alpha_{vap,\text{tank}} = \frac{V_{\text{tank}} - V_{liq}}{V_{\text{tank}}} \quad (64)$$

Based on the DIERS (1992)[xxix] model, α_{vap} may be estimated as follows:

For the bubbly vessel flow model:

$$f(\alpha_{vap}) = \frac{\alpha_{vap}(1-\alpha_{vap})^2}{(1-\alpha_{vap}c_k)(1-\alpha_{vap}^3)} \quad (65)$$

For the churn-turbulent vessel flow model:

$$f(\alpha_{vap}) = \frac{2\alpha_{vap}}{(1-\alpha_{vap}c_k)} \quad (66)$$

Note that c_k is a data correlating parameter with normal values ranging from 1.0 to 1.5. As a best estimate, for churn / turbulent flow c_k = 1.5, while for bubbly flow c_k = 1.2.

Also:

$$f(\alpha_{vap}) = \frac{u_{sv}}{u_{bub}} \quad (67)$$

For bubbly flow, the characteristic bubble rise velocity (u_{bub}) is given by:

$$u_{bub} = 1.18\left\{\sqrt[4]{\frac{\sigma_{liq} g(\rho_{liq} - \rho_{vap})}{\rho_{liq}^2}}\right\} \quad (68)$$

While for churn-turbulent flow:

[xxxv] For homogenous two-phase flow conditions to prevail within a vessel, the rate of vapour generation must far outstrip the rate of vapour disengagement (i.e. due to buoyancy effects etc.). This sort of behaviour (i.e. extremely rapid / "uncontrolled" vapour generation) may only be observed in vessel venting involving reactive mixtures / runaway reactions. As such, the homogenous vessel model is generally untenable for modelling vapour-liquid disengagement dynamics commonly prevalent during the venting of non-reactive containment.

$$u_{bub} = 1.53\left\{\sqrt[4]{\frac{\sigma_{liq} g\left(\rho_{liq} - \rho_{vap}\right)}{\rho_{liq}^2}}\right\} \quad (69)$$

The superficial vapour velocity at the liquid surface (u_{sv}) is given by:

$$u_{sv} = \frac{\dot{m}_{vap}}{\rho_{vap} S_{area}} \quad (70)$$

Where: σ_{liq}, ρ_{liq}, ρ_{vap}, g, S_{area} and $\dot{m}_{vap}$ are the liquid surface tension, liquid density, vapour density, gravitational acceleration, vessel cross-sectional area and "vapour only" release rate[xxxvi] respectively.

For the bubbly flow model, the void fraction at the liquid surface ($\alpha_{vap,surf}$) is assumed equal to the average void fraction in the swelled liquid (α_{vap}), while for the churn-turbulent flow model:

$$\alpha_{vap,surf} = \frac{2\alpha_{vap}}{\left(1 + \alpha_{vap} c_k\right)} \quad (71)$$

Furthermore, $\alpha_{vap,surf}$ is related to the stagnation or thermodynamic vapour quality at the liquid surface ($x_{vap,surf}$)[xxxvii] by:

$$\alpha_{vap,surf} = \frac{\rho_{liq} x_{vap,surf}}{\rho_{liq} x_{vap,surf} + \left(1 - x_{vap,surf}\right)\rho_{vap}} \quad (72)$$

B.3.2 ALGORITHM FOR THE DETERMINATION OF SWELL INDUCED TWO-PHASE FLOW

The primary objective of liquid swell modelling is the determination / prediction of conditions leading to two-phase flow at the orifice and the pertinent orifice upstream conditions (i.e. vapour quality, Pressure, Temperature etc) should two-phase flow occur.

The following presents the recommended algorithm in the DIERS (1992) report for determining conditions leading to two-phase flow and the pertinent orifice upstream conditions for top vented vessels (i.e. vessels with aperture at the top of the vessel).

1. Determine the all vapour mass flow rate ($\dot{m}_{vap}$) through the aperture from upstream stagnation conditions
2. Calculate the superficial vapour velocity at the liquid surface (u_{sv}) from Equation (70)
3. Calculate the characteristic bubble rise velocity (u_{bub}) for the appropriate vessel model (i.e. from Equation (68) or Equation (69).
4. Set f(α_{vap}) from Equation (67) and determine the average void fraction (α_{vap}) from the appropriate vessel model (i.e. from Equation (65) or Equation (66)).
5. Calculate the vessel average void fraction ($\alpha_{vap,tank}$) from Equation (64)[xxxviii]
6. If $\alpha_{vap} \leq \alpha_{vap,tank}$, then all vapour discharge (i.e. liquid swelling is not sufficient enough to lead to two-phase flow at the orifice); else, a two-phase mixture (of swelled fluid) is assumed to be discharged.

[xxxvi] $\dot{m}_{vap}$ may be initially estimated assuming pure vapour upstream conditions (i.e. zero liquid entrainment)

[xxxvii] $x_{vap,surf}$ = liquid mass fraction at the liquid surface

[xxxviii] Note that for apertures located other than at the top of the vessel, Equation (72) will need to be modified accordingly, i.e., V_{tank} will correspond to the total volume of the vapour and liquid spaces below the aperture.

7. If all vapour discharge, EXIT; else, if two-phase flow is predicted, recalculate u_{sv} from equations (65) or (66) by assuming $\alpha_{vap} = \alpha_{vap,tank}$.[xxxix]
8. Calculate $\alpha_{vap,surf}$ for the appropriate vessel model (e.g. from Equation (71))
9. Determine the stagnation quality at the liquid surface (i.e. $x_{vap,surf}$) from Equation (72) as:

$$x_{vap,surf} = \frac{\rho_{vap}\alpha_{vap,surf}}{\rho_{vap}\alpha_{vap,surf} + \left(1-\alpha_{vap,surf}\right)\rho_{liq}} \quad (73)$$

10. Determine the vapour quality (x_o) at the entrance of the orifice and the two-phase mass flow rate exiting the orifice by solving appropriate conservation equations.

B.4 Cumber (2002) Churn-Turbulent Vessel Flow Model

Cumber (2002) describes a mathematical model for predicting release rates and vapour-liquid disengagement from top venting high-pressure vessels undergoing churn-turbulent liquid swell. As with the DIERS liquid swell models, the Cumber (2002) churn-turbulent model is derived from the drift flux theory. However, unlike the DIERS models, the Cumber (2002) model does not require any adjustments to pertinent modelling parameters (e.g. c_k) and is based on more accurate empirical correlations. Note that simulated liquid-swell results based on the empirical correlations adopted in the Cumber (2002) model have been extensively validated and observed to compare very well against experimental data.

The following presents the key liquid swell modelling equations adopted in the Cumber (2002) model. Note that the Cumber (2002) model adopts a similar algorithm as the DIERS model (see Section B.3.2).

Cumber (2002) recommends the following equations for the characteristic bubble rise velocity (u_{bub}) and average void fraction in the swelled liquid (α_{vap})[xl].

For the characteristic bubble rise velocity (u_{bub}):

$$u_{bub} = \begin{cases} 0.03\left\{\sqrt[4]{\frac{\sigma_{liq} g\left(\rho_{liq}-\rho_{vap}\right)}{\rho_{liq}^2}}\right\}\left[\frac{\rho_{vap}}{\rho_{liq}}\right]^{-0.157} N_v^{-0.562}, & N_v \le 0.00225 \\ 0.92\left\{\sqrt[4]{\frac{\sigma_{liq} g\left(\rho_{liq}-\rho_{vap}\right)}{\rho_{liq}^2}}\right\}\left[\frac{\rho_{vap}}{\rho_{liq}}\right]^{-0.157}, & 0.00225 < N_v \le 0.1 \end{cases} \quad (74)$$

$$N_v = \frac{\nu_{liq}\rho_{liq}}{\sqrt{\rho_{liq}\sigma_{liq}\sqrt{\sigma_{liq}/\left(g\left(\rho_{liq}-\rho_{vap}\right)\right)}}}$$

While, the degree of vapour-liquid entrainment (or disengagement, α_{vap}) may be estimated as:

$$\alpha_{vap} = 1 + \frac{f\left(\alpha_{vap}\right)\left(1-c_k\right)^2}{\ln\left[1+\left(c_k-1\right)f\left(\alpha_{vap}\right)\right] - c_k\left(c_k-1\right)f\left(\alpha_{vap}\right)} \quad (75)$$

Where, $f(\alpha_{vap})$ is given by Equation (67) and ν_{liq} is the liquid phase kinematic viscosity (i.e. μ_{liq}/ρ_{liq}).

c_k is calculated as:

[xxxix] Note that this step is only really required for top vented vessels. Where the aperture is located elsewhere, α_{vap} may actually be less than the actual $\alpha_{vap,tank}$ (i.e., the total tank void fraction based on the total tank volume).

[xl] The equations for the superficial vapour velocity at the liquid surface (u_{sv}) are unchanged in the Cumber (2002) and DIERS models.

$$c_k = \left[\frac{\rho_{vap}}{\rho_{liq}}\right]^{-0.05} \max\left\{1, 2.6 - 8.4\alpha_{vap}\right\} \quad (76)$$

Note that from Equation (76), Equation (75) can only be solved numerically for α_{vap} as it is implicit in terms of α_{vap}.

B.5 Bubbly and Churn-turbulent Liquid Swell Modelling in old TVDI

The following presents and reviews the key equations and algorithm employed in the PHAST time-varying discharge model (old TVDI in Phast 7.11 and earlier) for simulating bubbly and churn–turbulent liquid swell effects[xli] against the DIERS (1992) models.

The TVDI vessel flow models (i.e. bubbly and churn-turbulent) are essentially derived from the DIERS (1992) models. The equations for $f(\alpha_{vap})$, the bubbly and churn-turbulent characteristic bubble rise velocities (u_{bub}) are as defined in equations (67), (68) and (69) respectively. However, the adopted expressions for the superficial vapour velocity at the liquid surface (u_{sv}) and the degree of vapour-liquid entrainment (α_{vap}, i.e., for bubbly / churn-turbulent flow) differ from the DIERS equations.

In TVDI, the superficial vapour velocity at the liquid surface (u_{sv}) is calculated as:

$$u_{sv} = \frac{\dot{m}_{evap}}{\rho_{vap} S_{area}} \quad (77)$$

Where, $\dot{m}_{evap}$ is the simulated evaporation rate over a given time interval. Note that in the DIERS model, u_{sv} is derived from the pure vapour discharge rate (i.e., $\dot{m}_{vap}$, see Equation (70))[xlii].

Furthermore, the degree of vapour-liquid entrainment (or disengagement, α_{vap}) in a boiling fluid, is estimated in TVDI as follows:

For the bubbly vessel flow model:

$$f(\alpha_{vap}) = \frac{\alpha_{vap}(1-\alpha_{vap})^2}{(1-\alpha_{vap}c_k)^2(1-\alpha_{vap}^3)} \quad (78)$$

For the churn-turbulent vessel flow model:

$$f(\alpha_{vap}) = \left(\frac{\alpha_{vap}}{(1-\alpha_{vap}c_k)}\right)\left(\frac{1}{1-\left(\frac{\alpha_{vap}c_k}{1-\alpha_{vap}c_k}\right)\left(\frac{1-x_{vap,surf}}{x_{vap,surf}}\right)\left(\frac{\rho_{vap}}{\rho_{liq}}\right)}\right) \quad (79)$$

c_k is as recommended in the DIERS (1992) report, i.e., for churn / turbulent flow c_k = 1.5, while for bubbly flow c_k = 1.2.

[xli] NOTE: Only the churn-turbulent flow solution is enabled (i.e. hard-coded) in TVDI.

[xlii] Note that for discharge in the liquid space (i.e. no vapour discharge), it will be credible to use $\dot{m}_{evap}$ in place of $\dot{m}_{vap}$

Equations (78) and (79) differ from the pertinent DIERS equations (see equations (65) and (66) respectively)[xliii]. Furthermore, equations (78) and (79) are solved numerically in TVDI for α_{vap}, while in the DIERS formulation, only Equation (65) requires a numerical solution.

TVDI Liquid Swell Modelling Algorithm

The first six steps in the TVDI and DIERS liquid swell modelling algorithm are essentially the same (see Section B.3.2), albeit the equations solved in each step may differ. Where the predicted value of α_{vap} is greater than $\alpha_{vap,tank}$, α_{vap} is set to $\alpha_{vap,tank}$, i.e.:

$$\alpha_{vap} = \min\left[\alpha_{vap,\tan k}, \alpha_{vap}\right] \qquad (80)$$

Unlike the DIERS model, all effects of liquid swell within a given time interval (or depressurisation step) are assumed not to influence the release process within that time interval but in subsequent time intervals[xliv]. As such, steps 7 to 10 in the DIERS algorithm are applied (with simplifications) in the next calculation step / time interval without the need for a rigorous solution.

Summary of Discrepancies between the TVDI and DIERS Liquid Swell Models

The following summarises the key differences / discrepancies in the TVDI as compared to the DIERS bubbly and churn-turbulent liquid swell models. These modelling discrepancies need further justification / resolution:

- The churn-turbulent vessel flow model is currently adopted (via hard-coding) as default in TVDI, clear justification for this assumption is required. It is recommended to implement in TVDI the DIERS (or Cumber, 2002) recommended transition criterion in selecting the appropriate "non-foamy" vessel flow model.
- Difference in adopted equations for bubbly vessel model: TVDI Eq. (78) versus DIERS Eq. (65)
- Difference in adopted equations for churn-turbulent vessel model: TVDI Eq. (79) versus DIERS Eq. (66).
- Difference in adopted equation for superficial vapour velocity: TVDI Eq. (77) versus DIERS Eq. (70)

Furthermore, considering the pertinent applications of the no-drag, non-boiling height and homogenous vessel flow models, there is need to implement (or provide a clear justification for not implementing) these models in TVDI.

[xliii] It is not clear why these modified set of equations have been employed in place of the original DIERS correlations. To overcome numerical problems, perhaps?

[xliv] This approach was apparently adopted to avoid the need for an expensive iterative solution of the pertinent conservation equations derived as part of step 10.

Appendix C. A literature overview of blowdown modelling

C.1 Introduction

The purpose of this document is to give an overview of main contributions in the literature relevant to the improvement and extension of the time-varying discharge model TVDI.

C.1.1 BACKGROUND AND ORGANIZATION

C.2 Discharge modelling

The actual discharge calculations in TVDI are carried out by using the initial rate DISC model as a sub-model at each time step. The improvements and extensions that are currently planned are not focussed on the actual discharge calculations, but rather on the over-all transient vessel response and behaviour, taking various heat and mass transfer processes into account. Nevertheless, the actual discharge modelling in DISC will need to be reviewed and further validated at some stage, and some key papers and models are therefore included here.

C.2.1 HANNAH CONSULTANTS 2009: TOXIC INDUSTRIAL CHEMICAL SOURCE EMISSIONS MODEL IMPROVEMENTS – CHAPTER 3

This report[4] was produced by Hannah Consultants for the US Defense Threat Reduction Agency (DTRA) as a review of their Hazard Prediction Assessment Capability (HPAC) model. Recommendations are made based on state-of-the-art knowledge in terms of various discharge scenarios as well as dispersion. Chapter 3 of the report is of relevance to this section as it presents a suite of six model equations allowing for gas, two-phase or liquid storage and release. In particular, the ω-method by Leung (Section C.2.3) is used extensively.

Chapter 8 of the report is an evaluation of the modelling and may contain useful pointers and data for validation purposes – more details required.

It should be noted that the focus in the DTRA report is on Toxic Industrial Chemicals and discussions may therefore not necessarily be applicable to hydrocarbon mixtures.

C.2.2 WOODWARD 2009: VALIDATION OF TWO MODELS FOR DISCHARGE RATE

This validation exercise was carried out to evaluate two models implemented in the BakerRisk program SafeSite. These models are labelled the Energy Balance (EB) model and the Non-Equilibrium Model (NEM) and are described by Woodward[5] and references therein.

The article serves as a very useful overview of experimental data in the literature that can be used for validation purposes. Importantly, all validation results are here based on initial data; none are transient to show the evolution of mechanics in the vessel during blowdown. As such the experimental data used would be suitable for validation of the initial-rate DISC model rather than for the transient processes modelled by TVDI.

C.2.3 THE Ω-METHOD BY LEUNG

This section is to be further completed.

C.3 Transient vessel response

Measurements characterizing the blowdown and two-phase venting of multi-component hydrocarbon mixtures are presented in Haque et. al[6]. and Hewitt et. al.[7], respectively.

C.3.1 HAQUE 1992: BLOWDOWN OF PRESSURE VESSELS

In the first paper[20] a computer model called BLOWDOWN is presented, and in the second paper[6] this model is validated against experimental data. The model is fairly sophisticated and includes the following features and assumptions:

- Can predict flow rate, pressure, fluid and vessel temperatures and multiphase composition (gas and liquid)
- Allows for additional pipework upstream or downstream of the choke
- Free liquid water can be added in the vessel
- Three fluid zones:
    - Gaseous hydrocarbon
    - Liquid hydrocarbon (including dissolved water)
    - Water (including dissolved hydrocarbon)
- Each zone assumed well-mixed and spatially uniform temperature
- The wall temperature in contact with each zone varies only across the wall thickness
- The heat and mass transfer effects taken into account are given in Figure 17.
- Thermo-physical properties calculated by the PREPROP computer package based on *corresponding states*.
    - Claim that this gives more accurate thermodynamic trajectories as compared to
- Depressurisation process based on discrete pressure decrements (not time)

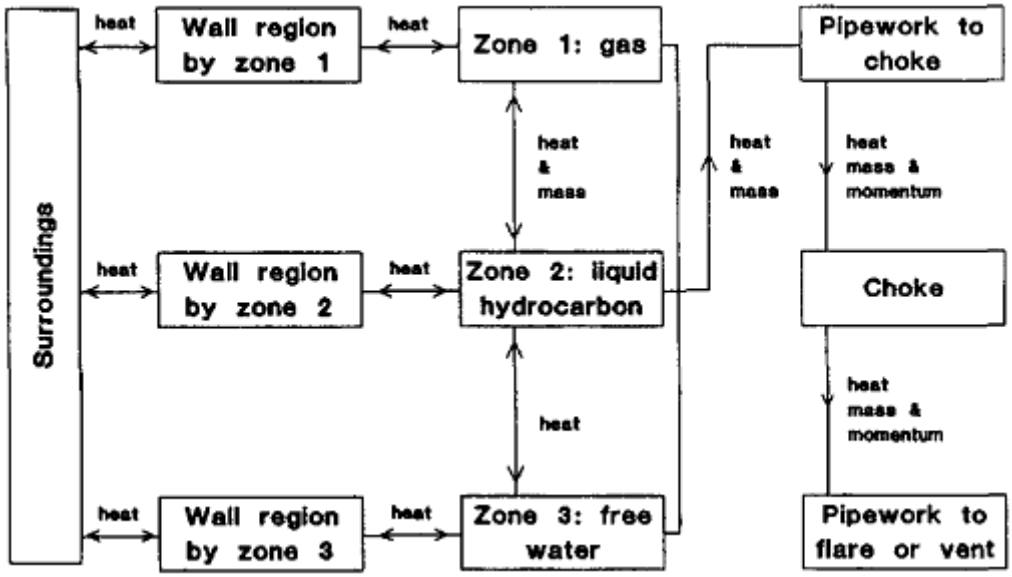


Figure 17: Heat and mass transfer effects in BLOWDOWN[Error! Bookmark not defined.].

C.3.2 OVERA 1994: SPLIT FLUID MODEL

In this paper[8] a model called the SPLIT FLUID MODEL is presented. This reference has not yet been obtained, but a description of the work is given by Wong, though I cannot obtain the reference…

Features and assumptions:

- Constant heat transfer coefficient assumed for the liquid phase
- Limited to single phase discharge

C.3.3 MONTGOMERY 1995: EFFECT OF HEAT TRANSFER FOR PURE GAS VESSEL BLOWDOWN

In the paper *"How to predict temperatures during gas depressuring"* [17] from 1995 by Montgomery, the effect of including heat transfer for pure gas vessel blowdown is considered. Model features and assumptions include:

- Pure gas vessel (non-condensable)
- Multiple inflows and outflows allowed
- Heat transfer from vessel walls to fluid taken into account, though vessel isolated from the surroundings
- Constant heat transfer coefficient assumed

The paper shows some interesting temperature plots showing the effect of the heat transfer from the vessel walls.

C.3.4 WONG 1998: MODELLING BLOWDOWN OF HYDROCARBON VESSELS

In the PhD thesis *"Development of a mathematical model for blowdown of vessels containing multi-component hydrocarbon mixtures"*[9] a fairly complex model named BLOWSIM is presented.

C.3.5 MAHGEREFTEH AND WONG 1999: MODELLING LIQUID SPACE BLOWDOWN

In this paper[10] a model named BLOWSIM is presented. Main features and assumptions:

- Blowdown of multi-component hydrocarbon mixture - from vapour space only
- Makes use of cubic equations of state rather than the principle of corresponding states used by Haque et.al.[20]. This is less complex and computationally more efficient, but may be problematic at or near the critical region.
- Non-equilibrium and heat transfer between phases
- Mass transfer between phases: evaporation and condensation
- Blows down using specified pressure decrements
- Heat transfer details:
    - Ignore heat transfer to/from the vessel surroundings, but include heat transfer between wall and fluid
    - Vessel wall split into two regions: dry and wet. Each region of the wall assumed to have a spatially uniform temperature, even across its thickness.
    - Introduces a film layer between zones and vessel wall with temperature equal to the average of the zone and wall temperature.

C.3.6 PETER CUMBER: BLOWDOWN OF HIGH PRESSURE VESSELS

Peter Cumber has authored a series of articles relevant to the blowdown of vessels in the process industry.

C.3.6.1 2001: Predicting Outflow from High Pressure Vessels

This paper[11] presents a very simple blowdown model and validates it against transient experimental results by Hervieu[12], Gebbeken and Eggers[13] and experiment S12 reported by Haque et. al.[6].

Key model assumptions and features:

- Homogenous equilibrium model
- Adiabatic vessel, i.e. not heat transfer to/from vessel walls
- No level swell modelling
- Vessel is treated as a single control volume, i.e. internal stratification is neglected
- Release phases: Liquid, gas or two-phase

C.3.6.2 2002: Modelling top venting vessels undergoing liquid swell

This paper[14] presents an extension of Cumber's previous model[11] by including liquid swell modelling. A further study of this paper will be done later when and if liquid swell modelling will be incorporated in the new TVDI model.

C.3.6.3 2002: Vessel outflow sensitivity to composition

This paper[15] studies the sensitivity of vessel outflow to the composition of the fluid in the vessel. The underlying model used is the one previously presented by Cumber[11,14]. It is shown how using methane to approximate an LNG mixture dominated by methane can lead to significant differences in the outflow.

C.3.7 OKE 2002: MODELLING LIQUID SPACE BLOWDOWN

This model[19] is a continuation of the work by Mahgerefteh and Wong[10].

Key features:

Further developed, focus on bottom space blowdown:
In Oke's MSc thesis, these are some of the assumptions for heat transfer through the vessel walls – very similar as those used by Mahgerefteh[10]:

- Heat transfer from vessel walls to the exterior is ignored (vessel perfectly insulated from the exterior, results completely independent of ambient temperature)
- Heat transfer from fluid to inside of the vessel walls is taken into account
- Involves entropy considerations in the heat transfer equations

C.3.8 SPERANZA 2005: BLOWDOWN OF HYDROCARBONS PRESSURE VESSEL WITH PARTIAL PHASE SEPARATION

This article[22] presents a mathematical model for a pure vapour blowdown of a multi-component hydrocarbon pressure vessel. The model is inspired by the one presented by Haque et. al.[20] and shares many features and assumptions with the current and new TVDI model and the article is as such interesting. Some of the key model features and assumptions include:

- For simplicity, only pure gas is considered to be discharged
  - *This limitation is not acceptable for TVDI – a generalization would be necessary*
- The stored material may be a multi-component mixture.
- The gas and liquid phase may be in thermodynamic non-equilibrium, i.e. the liquid and gas generally have different temperatures
- Thermodynamics assumed spatially uniform, i.e. each phase assumes perfectly mixed
- The inside vessel wall temperature is equal to the temperature of the fluid in contact with the wall. Thus there is a discontinuity in the wall temperature, and heat transfer across this discontinuity is ignored.
- Mass balance for each component in the mixture; energy balance for each of the two phases
- Heat transfer effects taken into account:
  - across the fluid interface
  - evaporation and condensation
  - discharged mass
  - heat exchange with the exterior through vessel wall
  - Solving 1D heat equation between exterior and interior vessel wall to obtain temperature of the latter (exterior temperature constant)
    - Complex as needs to be solved simultaneously with other equations
- Mass transfer between gas and liquid, introduces partial phase equilibrium:
  - Assumes that mass that evaporates/condenses is instantly transferred to the gas/liquid phase with properties evaluated at its original temperature, i.e. the liquid/gas temperature.
- The evaporation and condensation rates are found through use of chemical potentials.
  - *Can our current approach (Raoult, Dalton) still be used in a meaningful way for polydisperse phases/multi-component mixtures?*
- Equations are formulated in terms of moles rather than mass
- Can the property system calculate mixture properties? (E.g. internal energies, enthalpies etc)
- Can the current approach in TVDI with iterating on the evaporation rate be extended or is a new method needed?

C.3.9 HANNAH CONSULTANTS 2009: TOXIC INDUSTRIAL CHEMICAL SOURCE EMISSIONS MODEL IMPROVEMENTS – CHAPTER 4

Chapter 4 of this report (see Section C.2.1) deals with the transient vessel response during a blowdown process. The discussion is fairly top-level, focussing on the various phases that may be discharged depending on orifice location and liquid height: pure liquid, liquid/gas two-phase mixture and pure gas. Some details are provided for modelling of level swell[xlv], and here are some of the assumptions for the model that is introduced:

- Take into account a vertical void distribution
  - *Will we do this in TVDI or will we assume a uniform void distribution in the entire liquid? Initially no liquid swell modelling in the revised TVDI model*
- Thermodynamic equilibrium between vapour and liquid phases
  - *This assumption will also be present in the revised TVDI model (at least initially)*

Churn-turbulent flow regime with C_0=1.0m drift-flux model.

[xlv] Note that the TVDI theory document has an appendix with a review of liquid swell modelling

Appendix D. Energy balance and heat transfer modelling

D.1 Introduction

This Appendix contains a potential extension of the simple energy balance and heat transfer modelling in the new TVDI model. In particular, the first version of the new model completely ignores heat transfer between the fluid and vessel and between the vessel and the exterior surroundings. The following model includes heat transfer between fluid and vessel walls, but not between vessel walls and the surroundings.

D.2 Top-level theory

Top-level energy balance assumptions:

- Negligible potential and kinetic energy
- No shaft work done by the system
- Heat transfer between the vessel walls and the contained fluid is taken into account[xlvi].
- Heat loss due to discharged material
- The vessel is assumed to be adiabatic, i.e. no heat transfer between the vessel walls and the surroundings[xlvii].
- Vessel wall temperature is spatially uniform
- What about the situation with a short pipe attached? Same assumptions as for the vessel itself? What kind of heat transfer for the pipe?

The energy balance of the system may then be expressed in terms of the internal energy U, namely

$$\frac{dU}{dt} = -\dot{m}_{DISC} h_F + \lambda_L S_{LW} (T_W - T) + \lambda_G S_{GW} (T_W - T), \qquad (81)$$

where h_F is the specific enthalpy of the fluid being discharged, λ_L (λ_G) is the heat transfer coefficient between the liquid (gas) and the vessel wall, S_{LW} (S_{GW}) is the surface area of vessel wall in contact with liquid (gas), T is the fluid temperature and T_W is the temperature of the vessel wall.

Additionally, Newton's law of cooling governs the temperature evolution of the vessel wall:

$$\lambda_L S_{LW} (T_W - T) + \lambda_G S_{GW} (T_W - T) = M_V c_{p,V} \frac{dT_W}{dt}. \qquad (82)$$

Here M_V is the mass of the vessel wall and $c_{p,V}$ its specific heat capacity. The work carried out by the expanding gas is taken into account[xlviii] through the use of the total system enthalpy H,

$$H = U + PV_T, \qquad (83)$$

where P is the vapour space pressure and V_T is the constant system volume (vessel volume+possible pipe volume). This volume relates to the system mass M:

$$M(t) v_T(t) = V_T, \qquad (84)$$

[xlvi] In the Phast 7.21 multi-phase model, the liquid and vessel walls were lumped together and always assumed to be in thermal equilibrium – experiments show this is not the case.

[xlvii] The Phast 7.21 multi-phase model takes into account heat transfer between surroundings and the liquid-vessel system, though all coefficients are hard-coded.

[xlviii] The Phast 7.21 multi-phase model ignores this expansion energy. This differs from the Phast 7.21 pure gas model which assumes isentropic expansion

where v_T is the average specific volume of the fluid.

D.3 Detailed theory

D.3.1 ENERGY BALANCES AND HEAT TRANSFER EFFECTS

One of the decisions to make is which heat transfer effects to include in the model. The simplest approach is to assume no heat transfer at all between the fluid and the vessel walls – an approach that was investigated by Cumber[16]. The next step could be to include heat transfer between the vessel walls and the fluid but to ignore heat transfer between the vessel and its surroundings, and this was indeed done by e.g. Montgomery[17], Wong[18], and Oke[19]. Finally an option would be to consider heat transfer both from vessel walls to fluid and from exterior to vessel walls, e.g. Haque[20] , Overa[21] and Speranza[22]. Here the intermediate approach is chosen, i.e. assuming an adiabatic vessel. In practice this means that we assume that the heat transfer between the vessel and the immediate surroundings are negligible compared to other modes of heat transfer within the vessel, which may be reasonable in non-fire conditions. Furthermore the approach has the advantage of not needing to solve the heat equation across the thickness of the wall which would complicate the system (see e.g. Speranza[22]).

D.3.2 HEAT TRANSFER COEFFICIENTS

The modelling of heat transfer between the vessel walls and the fluid requires the estimation of certain heat transfer coefficients λ and this estimation will be discussed here.

Constant heat transfer coefficients

One simple approach is to model heat transfer using a constant heat transfer coefficient λ, see Montgomery[17]. The coefficient will be different for the part of the vessel wall in contact with liquid and gas, say λ_L and λ_G. A study of the impact of using constant vs variable heat transfer coefficients was done by Oke[19].

Variable heat transfer coefficients

We here relax the assumption of constant heat transfer coefficient from the previous section. The equations in Section 2.1 still apply, but the heat transfer coefficients λ_L and λ_G are no longer constants. Variable heat transfer coefficients have been used by Wong[18], Oke[19], Haque[20] and Speranza[22]. First we introduce some relevant notation and dimensionless numbers, namely the Prandtl number Pr, the Nusselt number Nu, the Grashof number Gr and the Rayleigh number Ra:

$$Pr = \frac{c_P \mu}{k}, \tag{85}$$

$$Nu = \frac{\lambda L}{k}, \tag{86}$$

$$Gr = \frac{\rho^2 g \beta \left(T_W - T\right) L^3}{\mu^2}, \tag{87}$$

and

$$Ra = Gr \cdot Pr. \tag{88}$$

Here k is the thermal conductivity of vapour, μ is the viscosity the vapour, L is the characteristic length of the geometric region containing vapour, ρ is vapour density, g is the gravitational acceleration, and β is the vapour thermal expansion coefficient.

Heat transfer coefficient for vapour and vessel wall
The approach used here is very similar to the one used by Wong[18] and Oke[19]. Key points:

- Assume natural convection only (so ignore forced convection)
- The material properties are to be evaluated at the film temperature $T_F = 0.5(T_W + T)$
- The overall heat transfer coefficient λ_G depends on the vessel geometry.
    - Vertical or horizontal cylinder:

$$\lambda_G = \lambda_{top}\frac{S_{top}}{S_{GW}} + \lambda_{bot}\frac{S_{bot}}{S_{GW}} + \lambda_{cyl}\frac{S_{cyl}}{S_{GW}}. \quad (89)$$

    - Rectangular box:

$$\lambda_G = \lambda_{top}\frac{S_{top}}{S_{GW}} + \lambda_{bot}\frac{S_{bot}}{S_{GW}} + \lambda_{side}\frac{S_{side}}{S_{GW}}. \quad (90)$$

    - Sphere[xlix]:

$$\lambda_G = \lambda_{top}\frac{S_{top}}{S_{GW}} + \lambda_{bot}\frac{S_{bot}}{S_{GW}}. \quad (91)$$

The actual heat transfer coefficients for each part of the vessel walls will depend on the geometry, curvature and orientation of the surface in question – several correlations have been developed to handle a variety of surface types.

For the vertical walls in a rectangular box and in a vertical cylinder and with the Prandtl number satisfying $1 < \mathrm{Pr} < 40$, Perry and Green[23] refers to Kato et al.[24] who recommend the relation

$$Nu = \begin{cases} 0.138\,Gr^{0.36}\left(Pr^{0.175} - 0.55\right) & \text{if } Gr > 10^9, \\ 0.683\left(\dfrac{GrPr^2}{0.861 + Pr}\right)^{0.25} & \text{otherwise.} \end{cases} \quad (92)$$

However, as the above relation is limited to Prandtl numbers $1 < \mathrm{Pr} < 40$, an alternative relation is used when either $\mathrm{Pr} \le 1$ or $\mathrm{Pr} \ge 40$. This relation is recommended by Incropera et al.[25] and was originally derived by Churchill and Chu[26] without any restrictions on the Prandtl or Rayleigh numbers:

$$Nu = \left[0.825 + \frac{0.387\,Ra^{1/6}}{\left[1 + \left(0.492/Pr\right)^{9/16}\right]^{8/27}}\right]^2 \quad (93)$$

It should be noted that the correlation (93) is applicable to vertical walls, but according to Incropera et al.[25] it may also be used for vertical cylinders with relatively large diameters, that is when

[xlix] JUSTIFY: This relation should be cross-checked against the literature

$$\frac{D}{L} \geq \frac{35}{Gr^{1/4}}. \qquad (94)$$

In the absence of known alternatives, the correlation (93) is used even if the inequality (94) does not hold.

For the horizontal walls in a rectangular box and in a vertical cylinder (top and bottom), correlations originating from McAdams[27] and later modified by Goldstein et al.[28] and Lloyd et al.[29] is recommended by Incropera et al.[25]:

Bottom wall with $T < T_W$ or top wall with $T > T_W$:

$$Nu = \begin{cases} 0.54Ra^{1/4} & \text{if } 10^4 < Ra < 10^7 \\ 0.15Ra^{1/3} & \text{if } 10^7 < Ra < 10^{11} \end{cases} \qquad (95)$$

Bottom wall with $T > T_W$ or top wall with $T < T_W$:

$$Nu = 0.27Ra^{1/4} \quad \text{if } 10^5 < Ra < 10^{10} \qquad (96)$$

Note that the following characteristic length must be used in conjunction with the correlations (95) and (96), namely

$$L = \frac{S_{top}}{P_{top}}, \qquad (97)$$

where S_{top} and P_{top} is the surface area and perimeter of the vessel wall in contact with the gas. In lack of further data, the correlations (95) and (96) may also be used outside of the indicated range for the Raleigh number .

Horizontal cylinders and spheres – what are the relevant correlations for these curved surfaces? A look to the literature is needed to establish this – postpone for now.

Heat transfer coefficient for liquid and vessel wall
Key assumptions:

- Two modes of heat transfer between vessel wall and liquid:
  - Natural convection:
    - When the liquid is sub-cooled or slightly superheated w.r.t. the vessel wall.
    - Can use the appropriate correlations as previously introduced for heat transfer between vapour and wall.
  - Nucleate boiling:
    - When the liquid is intermediately superheated w.r.t. the vessel wall.
    - Correlations to be presented below.
- Other modes of heat transfer not considered, e.g. transition and film boiling (see Oke[19] for justification).

Natural convection heat transfer is assumed when $T_W - T < 5K$, otherwise nucleate boiling is assumed. A common correlation for nucleate boiling is the Rohsenow correlation as mentioned by Incropera et al. [25]:

$$\dot{q}_{LW} = \mu_L h_{fg} \left[\frac{g(\rho_L - \rho_G)}{\sigma} \right]^{1/2} \left[\frac{c_{p,L}(T_W - T)}{C_{s,f} h_{fg} \, \mathrm{Pr}_L^n} \right]^3, \qquad (98)$$

where $\dot{q}_{LW}$ is the heat flux from wall to liquid, h_{fg} is the latent heat of vaporization for the liquid, σ is the surface tension and ρ is the fluid density, while $C_{s,f}$ and n depend on the solid-liquid combination. We here make the same choice as Wong[18] and Oke[19], namely $C_{s,f} = 0.006$ and $n = 1.0$. This corresponds to ground and polished stainless steel in contact with water – references to further combinations are given by Incropera et al.[25]. The Rohsenow correlation (98) is valid for nucleate boiling, i.e. for $5K < T_W - T < 30K$, but if in rare cases $T_W - T$ actually exceeds 30 K then we shall still apply the Rohsenow correlation[I,Ii].

[I] There are correlations for transition and film boiling in the literature, but this is not really relevant unless we want to consider a vessel subject to an external fire.

[Ii] It may be prudent to issue a warning in cases when $T_W - T$ exceeds 30K.

NOMENCLATURE

Roman Letters

a_k	Flow regime dependent constant used in void fraction calculations
A	Area (m^2)
c_p	Specific heat capacity (J/(kg K))
c_k	Flow regime dependent constant used in void fraction calculations
D	Diameter (m)
e	Pipe surface roughness length parameter
f	Frequency (m^{-1})
f	Fanning friction factor (-),
f_w	Fractional wetted area at the end of a horizontal cylinder
f	Fraction (-)
g	Gravitational constant (m/s^2)
h	Heat transfer coefficient ($W/(m^2K)$)
H	Height (m)
H_{cap}	Heat capacity of total system (J/K)
ΔH_{vap}	Heat of vaporisation (J/kg)
K	Number of velocity head losses (-)
L	Length (m)
$\dot{m}$	Mass flow rate out of system (kg/s)
M	Mass (kg)
ΔM_i	Change in mass during time step i (kg)
Nu	Nusselt number
N	Number of steps (-)
N_{comp}	Total number of components in the vapour phase (-)
P	Pressure (Pa)
P_{pp}	Partial vapour pressure (Pa)
P_{vap}^{sat}	Saturated vapour pressure
Pr	Prandtl number
Q	Heat (J)
ΔP_i	Pressure drop during time step i (Pa)
r	Radius (m)
Re	Reynolds number (-)

s	Specific entropy (J K^{-1} kg^{-1})
S	Surface area (m^2)
t	Time (s)
Δt_i	Duration of time step i (s)
T	Temperature (K)
u	Velocity (m/s)
U	Heat transfer coefficient (W/(m^2K))
V	Volume (m^3)
W	Width (m)
x	Mass fraction / Vapour quality (-)
y	Mole fraction (-)

Greek Letters

α	Void fraction (-)
χ	Thickness (m)
κ	Thermal conductivity (W/(Km))
μ	Viscosity (dynamic) (kg/(ms))
υ	Specific volume (m^3/kg)
ρ	Density (kg m^{-3})
σ	Surface tension (N/m)

Subscripts

X_{pipe}	Pipe attached to main vessel
X_{EF}	Excess flow rate valve
X_{NR}	Non-return valve
X_{SO}	Shut-off valve
X_{coup}	Pipe couplings
X_{junc}	Pipe junctions
X_{bend}	Pipe bends
X_{tank}	Tank
X_{liq}	Liquid
$X_{t\text{-}liq}$	Top liquid
$X_{b\text{-}liq}$	Bottom liquid
X_{vap}	Vapour phase

X_{evap} Evaporated mass

X_{ingest} Air ingested due to ‘gulping’

X_i Value of variable at time step number i

$X_{k,i}$ Component k at time step number i

X_{DISC} Calculated by the DISC model

X_{tot} Total system (i.e. vessel plus a potential pipe attached)

X_{avg} Averaged quantity

X_{st} Stagnation conditions (orifice inlet conditions)

X_a Ambient

X_o Vessel or pipe orifice/exit (pre atmospheric expansion)

X_{in} Indicating transfer into the system / inside the system

X_{out} Indicating transfer out of the system / outside the system

X_{Ins} Insulated component

X_{Unins} Uninsulated component

$X_{wet\text{-}wall}$ Wall covered by the liquid phase, i.e. wetted wall

X_{frac} Fraction of said quantity

X_{hole} Hole inlet conditions before the orifice

X_{hyd} Hydrostatic head

X_{Svalve} Safety valve

X_{inert} Inert padding gas

X_{bub} Bubbles rising in the liquid

X_{sv} Superficial vapour

X_{froth} Includes entrained vapour – ‘froth’

X_{mix} Takes entrained vapour into account – ‘froth’

X_{ref} Reference value

X_{char} Char

Superscripts

Xsat Saturated state

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REFERENCES

[1] Stene, J., Harper, M., and Witlox, H.W.M., *"Modelling transient leaks from pressure vessels including effect of safety systems"*, Hazards 24, Symposium Series No 159, 2014.
[2] Stene, J., Harper, M., and Witlox, H.W.M., *"Modelling Transient Leaks of Multi-Component Fluids Including Time-Varying Phase Composition"*, Chemical Engineering Transactions, Vol. 48, 2016.
[3] Cumber, P., *"Predicting Outflow from High Pressure Vessels"*, Trans IChemE Part B, 79, pp. 13-22, 2001.
[4] Britter, R., Leung, J., Weil, J., Sykes, I., and Hanna, S., *"Toxic Industrial Chemical (TIC) Source Emissions Model Improvements"*, Prepared for Defense Threat Reduction Agency, Report Number P098-4 (2009),
[5] Woodward, J.L., *"Validation of two models for discharge rate"*, J. Hazard. Mater. 170, pp. 219-229 (2009)
[6] Haque, M.A., Richardson, S.M., Saville, G., Chamberlain, G., and Shirvill, L., *"Blowdown of Pressure Vessels. II. Experimental Validation of Computer Model and Case Studies",* Trans IChemE Part B: Process Safety Environmental Protection, 70 (BI), pp. 10-17, 1992.
[7] Hewitt, G.F., Richardson, S.M., Saville, G., and Weil, C., *"Two-phase pressure relief sizing: An assessment study"*, Imperial College report MPS/73, HSE report H95475 / O96713, 1995.
[8] Overa, S.J., Stange, E., and Salater, P., *"Determination of temperatures and flare rates during depressurization and fire"*, Proceedings of 72nd GPA Annual Convention, pp. 235-247, 1994.
[9] Wong, S.M.A., *"Development of a mathematical model for blowdown of vessels containing multi-component hydrocarbon mixtures"*, PhD Thesis, Dept. Chem. Engin., University College London, 1998.
[10] Mahgerefteh, H. and Wong, S.M.A., *"A numerical blowdown simulation incorporating cubic equations of state"*, Comput. Chem. Eng., Vol. 23, pp. 1309-1317, 1999.
[11] Cumber, P., *"Predicting Outflow from High Pressure Vessels"*, Trans IChemE Part B, 79, pp. 13-22, 2001.
[12] Hervieu, E., *"Behaviour of a flashing liquid within a vessel following loss of containment. Application to propane."*, Final report CEC program: Major Technological Hazards, Contract no. AA-EV4T 00 19-F/GR-764279.
[13] Gebbeken, B., and Eggers, R., "Blowdown of carbon dioxide from initially supercritical conditions", J. Loss Prev. Process Ind., Vol 9, pp. 285-293, 1996.
[14] Cumber, P., "Modelling top venting vessels undergoing level swell", J. Hazard. Mater., Vol 89, pp. 109-125, 2002.
[15] Cumber, P., "Vessel outflow sensitivity to composition", J. Loss Prev. Process Ind., Vol 15, pp. 205-212, 2002.
[16] Cumber, P., *"Predicting Outflow from High Pressure Vessels"*, Trans IChemE Part B, 79, pp. 13-22, 2001.
[17] Montgomery, G., *"How to predict temperatures during gas depressuring"*, Hydrocarbon Processing, pp. 85-88, April 1995.
[18] Wong, S.M.A., *"Development of a mathematical model for blowdown of vessels containing multi-component hydrocarbon mixtures"*, PhD Thesis, Dept. Chem. Engin., University College London, 1998.
[19] Oke, A., "Modelling Liquid Space Blowdown", M.Sc. Thesis, UCL, 2000.
[20] Haque, M.A., Richardson, S.M., and Saville, G., "Blowdown of Pressure Vessels. I. Computer Model", Trans IChemE Part B: Process Safety Environmental Protection, 70 (BI), pp. 3-9, 1992.
[21] Overa, S.J., Stange, E., and Salater, P., *"Determination of temperatures and flare rates during depressurization and fire"*, Proceedings of 72nd GPA Annual Convention, pp. 235-247, 1994.
[22] Speranza, A., and Terenzi, A., "Blowdown of hydrocarbons pressure vessel with partial phase separation", Series on Advances in Mathematics for Applied Sciences, Vol. 69, pp. 508, 2005.
[23] Perry, R.H., Green, D.W., *Perry's Chemical Engineers' Handbook, Heat and Mass Transfer*, McGraw Hill, New York, 7th edition, Section 5, pp 5-12 to 5-23 (1999)
[24] Kato, H., Nishiwaki, N., and Hirata, M., *"On the turbulent heat transfer by free convection from a vertical plate"*, Int. J. Heat Mass Transfer, Vol. 11, pp. 1117-1125, 1968.
[25] Incropera, F.P., DeWitt, D.P., Bergman, T.L. and Lavine, A.S., "Fundamentals of heat and mass transfer", John Wiley & Sons, 6th ed., 2006.
[26] Churchill, S.W., and Chu, H.H.S., *"Correlating equations for laminar and turbulent free convection flow from a vertical plate"*, Int. J. Heat Mass Transfer, Vol. 18, pp. 1323-1329, 1975.
[27] McAdams, W.H., *"Heat Transmission"*, Chap. 7, McGraw-Hill, New York, 1954.
[28] Goldstein, R.J., Sparrow, E.M., and Jones, D.C., *"Natural convection mass transfer adjacent to horizontal plates"*, Int. J. Heat Mass Transfer, Vol. 16, pp. 1025-1035, 1973.
[29] Lloyd, J.R., and Moran, W.R., *"Natural Convection Adjacent to Horizontal Surfaces of various Planforms"*, ASME Paper 74-WA/HT-66, 1974.