Modelling transient leaks from pressure vessels including effects of safety systems

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A new fast time-varying discharge model with safety system capabilities has been developed to replace the existing model in the consequence modelling package Phast. The new model explicitly models normal operation production inflow and outflows and their impact on the accidental leak. Furthermore safety system capabilities allow the user to model the effects of isolation and blowdown. Successful isolation results in the shut-off of these flows; its failure results in a merging of inventories with upstream isolatable sections. Blowdown allows vapour to be released from the top of the vessel through a pre-defined valve, thereby reducing pressure and mitigating the accidental release. An example case is given to illustrate how this can help provide an understanding of how the failure/success of the safety systems will impact in case of an accidental outflow.

The above new time-varying discharge model has been verified against the Bernoulli equation for liquid leaks and ideal isentropic flow for gas leaks. Validation against experimental results for carbon dioxide releases shows accurate results with run times sufficiently short to support the needs of consequence analysis and QRA.

Keywords: discharge; consequence modelling; Phast; blowdown; safety systems; pressure vessels; QRA

Introduction

Conventionally quantitative risk assessment (QRA) has used either steady-state or instantaneous source term models to characterise accidental outflow of hazardous materials from pressure vessels. However, in reality source terms will often be highly dynamic, with reducing release rates as pressure drops and inventories reduce following the initial loss of containment. Furthermore the consequences of such a release may be mitigated by the operation of safety systems, including blowdown and isolation, and to evaluate their effectiveness it is crucial to include time-varying effects. QRA studies often include variations in hole sizes, detection times and safety system behaviour, resulting in a large number of release cases where the use of computational fluid dynamics models or process simulators may be prohibitively expensive. To address these specific QRA needs, a new version has been developed of the time-varying discharge model TVDI in the Phast (consequence) and Safeti (risk) software packages. The new version is planned to be made available in a future version of Phast and Safeti.

This paper discusses the main features of the new TVDI model and its treatment of safety systems. The new model allows fluid in the vessel to be stored as pure vapour, pressurised liquid, stratified two-phase fluid (liquid at bottom and vapour at top) at saturated conditions, and pressurised vapour. The accidental outflow is through a circular orifice, and the fluid phase approaching the orifice may be either vapour or liquid; the phase is determined by the transient liquid height in relation to the outflow height. The outflow calculations are split into two distinct stages: first an expansion of the fluid from stagnation conditions within the vessel to the orifice conditions, and secondly a final expansion from the orifice conditions to atmospheric pressure. When relevant, flashing liquid is taken into account both within the vessel and during the expansion to atmospheric pressure, and condensation is also modelled in case of significant cooling of vapour. In case of a two-phase fluid then vapour and liquid are assumed to be in thermal equilibrium.

A new key feature is that normal operation production inflow and outflows can be explicitly modelled and their impact on the accidental leak is accounted for. The user can specify an isolation time and a blowdown time and whether each of these safety measures is successful or not. Successful isolation results in the shut-off of these flows; its failure results in a merging of inventories with upstream isolatable sections. Blowdown allows vapour to be released from the top of the vessel through a pre-defined valve, thereby reducing pressure and mitigating the accidental release.

Modelling assumptions and governing equations of the new model are presented in this paper together with verification and validation results. An example case also illustrates how the new TVDI safety system capabilities can help provide an understanding of how the failure/success of the safety systems will impact in case of an accidental outflow.

New time-varying discharge model with safety systems

This section discusses key features of the new TVDI model for the case of an accidental leak from a circular orifice of a pressure vessel. The model determines the variation in time of storage (containment) and exit conditions. The contained fluid may be single phase or two-phase, and homogeneous equilibrium is assumed within the containment throughout the release. The model 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. The fluid phase approaching the orifice may be either vapour or liquid; the phase is determined by the transient liquid height in relation to the outflow height. The accidental leak calculations are split into two distinct stages:

i. Firstly an expansion of the fluid from stagnation conditions within the vessel to the orifice. These calculations are carried out by the Phast steady-state discharge model DISC - see the DISC theory manual for details (Harper et al., 2011)

ii. Secondly a final expansion from the orifice to atmospheric pressure. These calculations are carried out by the Phast atmospheric expansion model ATEX - see the ATEX theory manual for details (Witlox et al., 2011)

A fluid leaves the vessel, the transient flow is calculated by the model. The control volume considered consists only of the fluid contained in the vessel and excludes vessel walls. Conservation equations for mass M and internal energy U are applied to this control volume, and with added equation of state, a complete description of the dynamic evolution of the vessel can be obtained.

Governing equations – mass and energy balance

A schematic overview of the inflows and outflows taken into account by the model is given in Figure 1. With regards to the mass balance, the adopted 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 and (in case of saturated conditions) a user-specified liquid fraction.
    - 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). The modelling of these is simplistic and is determined from the vessel pressure in relation to a user-specified downstream pressure (production outflows stop when vessel pressure drops to the downstream pressure).
- Accidental outflow: The accident is modelled as fluid leaving the system through one single orifice, either as vapour or liquid, depending on whether the hole is located above the liquid level or below it. The multiple simultaneous 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 from the vapour space through a blowdown valve with a user-specified diameter. This evacuation commences at a user-specified blowdown time.

The mass balance may thus be expressed as

$$\frac{dM(t)}{dt} = \dot{m}_{in} - \dot{m}_{acc} - \dot{m}_{BD} - \dot{m}_{out}^{vap} - \dot{m}_{out}^{liq} \tag{1}$$

where M(t) is the total mass (kg) of the fluid in the system at time t (s). The production inflow rate (kg/s) 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.

With regards to the energy balance, the following assumptions are applied:

- Negligible potential energy
- No external work is added to the system by e.g. pumps
- No heat transfer between fluid and vessel wall
- Heat loss due to loss of fluid resulting from production vapour and liquid outflows, accidental outflow, and blowdown outflow
- Heat gain due to production inflow

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

$$\begin{aligned}\frac{dU}{dt} &= \dot{m}_{in}\, h\big(P(t=0), T(t=0); \eta_{in}\big) - \dot{m}_{acc}\, h\big(P, T; \eta_{acc}\big) - \dot{m}_{BD}\, h\big(P, T; \eta_{BD}\big) \\ &\quad - \dot{m}_{out}^{vap}\, h\big(P, T; \eta_{out}^{vap}\big) - \dot{m}_{out}^{liq} h\big(P_{out}^{liq}, T; \eta_{out}^{liq} = 1\big) \;.\end{aligned} \tag{2}$$

Here P is the vapour space pressure (Pa), T the uniform fluid temperature (K), h the specific enthalpy (J/kg) and η the liquid mass fraction; all quantities relate to fluid entering/leaving the vessel. The superscripts (*vap*) and (*liq*) refer to production vapour and production liquid outflow, respectively.

The internal energy of the system U is related to the system enthalpy H (J) through pressure-volume work, and assuming constant pressure P throughout the vessel, we get the relation

$$H(P,T) = U(P,T) + PV \,, \tag{3}$$

where V is the vessel volume (m^3) . Together with an appropriate equation of state, Equations (1), (2) and (3) are sufficient to solve for the four main unknowns: the total fluid mass M, the total fluid enthalpy H, the total fluid internal energy U and the system pressure P. From these all other quantities of interest (e.g. accidental flow rates, temperature, liquid volume, etc.) can be determined.

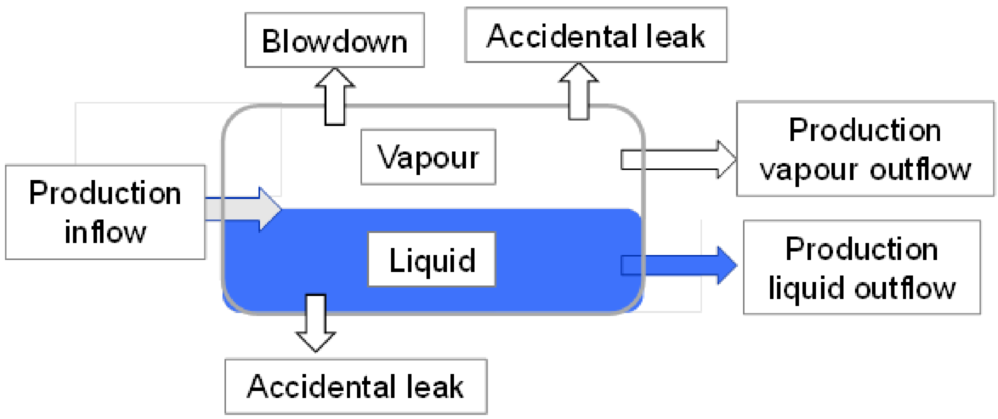


Figure 1. Schematic overview of inflows and outflows of the new TVDI model

Production flows and safety systems

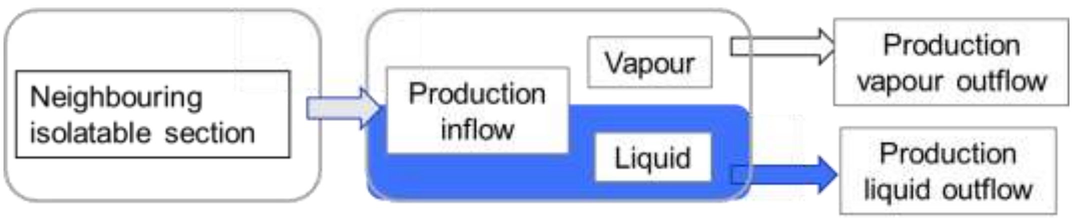
A key feature of the new TVDI model is that normal operation production inflow and outflows can be explicitly modelled and their impact on the accidental leak accounted for. Furthermore, the impact of safety systems following an accidental leak is taken into account: The user can specify an elapsed time t_{ESD} from the onset of the accidental leak until emergency shutdown (ESD) is intended to occur. Similarly the user can supply an elapsed time t_{BD} until blowdown (BD) occurs together with an associated blowdown valve diameter. Each of the two safety system measures may fail or succeed depending on the user input.

Consider a vessel with a stratified two-phase fluid with liquid at the bottom and vapour at the top – this 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 2a. In the following we will describe how the extended TVDI model handles production flows, emergency and safety system modelling for this system – this is best achieved by considering successive time periods defined by some key events:

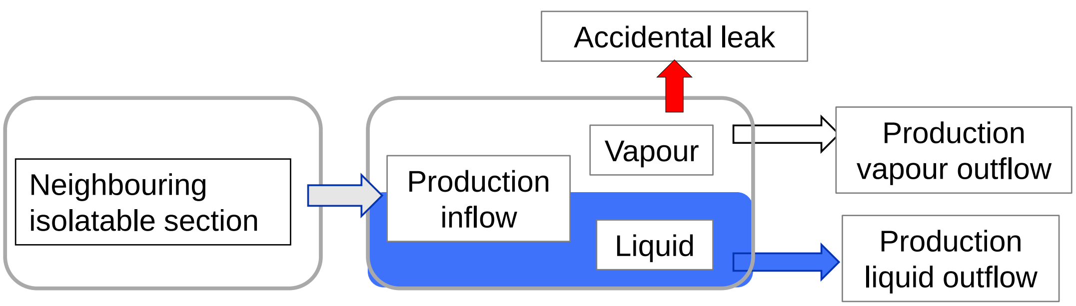
- Normal operation prior to accidental leak ($t<0$) as seen in Figure 2a:
  - The user specifies a constant production inflow rate from a neighbouring vessel and a constant liquid fraction of this inflow.
  - Fixed downstream pressures define the boundary conditions for the production vapour and liquid outflows.
  - Under normal operating conditions the production inflow rate is equal to the combined production outflow rates.
- After onset of accidental leak but before ESD ($0<t<t_{ESD}$) as seen in Figure 2b:
  - The accidental leak can be from either the vapour or liquid space and is calculated using the DISC sub-model
  - The production inflow remains constant while the production outflow rates decrease as the pressure in the vessel decreases due to the accidental outflow.
- After successful ESD before BD ($t_{ESD}<t<t_{BD}$) as seen in Figure 2c:
  - If the ESD is successful, then all production flows are assumed to be cut off instantaneously at time t_{ESD}. The only flow from the vessel is subsequently the accidental outflow.
- After unsuccessful ESD before BD ($t_{ESD}<t<t_{BD}$) as seen in Figure 2d:
  - If the ESD is unsuccessful, then the following occurs at time $t=t_{ESD}$:
    - The isolation valve between the vessel and the neighbouring (upstream) vessel is assumed to have failed. The main effect of this merging is that the mass of the neighbouring vessel is instantaneously added to vessel undergoing accidental leak.

- This merging of inventories essentially obviates the need for further production inflow into the merged vessel, which is thereafter assumed to be zero
- The production outflows are still assumed to be shut off correctly.

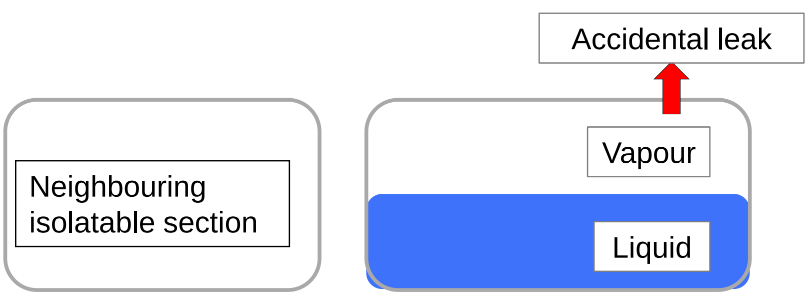
- After BD ($t>t_{BD}$) as seen in Figure 2e for the case of successful BD following successful ESD:
  - If blowdown is unsuccessful then nothing occurs at all at time t_{BD}.
  - If successful, the blowdown valve is assumed to open instantaneously at time t_{BD} and the pressure in the vessel is subsequently relieved by evacuation of vapour through the BD valve.
  - The blowdown valve is assumed to be a circular orifice with user-specified diameter d_{BD}.
  - The backpressure of the blowdown valve is assumed to be equal to the ambient pressure
  - The blowdown outflow is assumed to be located at the top (roof) of the vessel so that vapour is evacuated (i.e. not connected to the liquid)
  - The blowdown outflow rate is calculated using the same approach as for the accidental release rate – using the DISC sub-model.



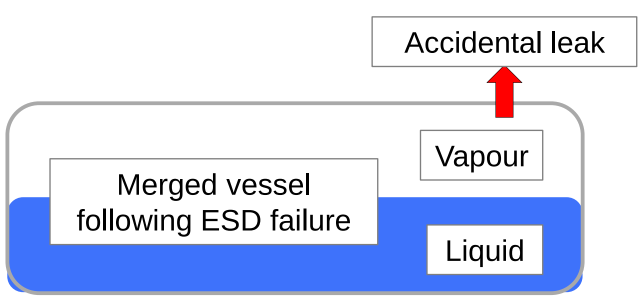
(a) normal operation prior to accidental leak ($t<0$)



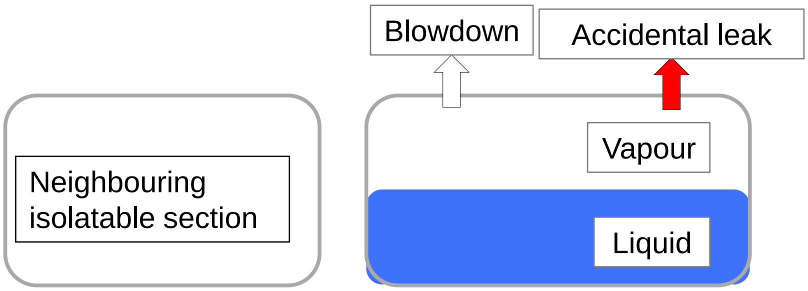
(b) after accidental leak has occurred but prior to ESD time ($0<t<t_{ESD}$)



(c) following successful isolation and before blowdown ($t_{ESD}<t<t_{BD}$)



(d) following unsuccessful isolation and before blowdown ($t_{ESD}<t<t_{BD}$)



(e) following successful isolation and after blowdown ($t>t_{BD}$)

Figure 2. Schematic overview of production flow and safety system modelling as a function of time

Verification and validation of the new model

Verification against Bernoulli for water leaks

For incompressible liquid leaks from an orifice in a vessel, we may verify the TVDI model predictions against results obtained using the well-established Bernoulli equation:

$$\dot{m}_{acc} = C_D \; A_o \; \rho \sqrt{2\left(\frac{P(t)-P_a}{\rho} + g\Delta H_L(t)\right)} \qquad (4)$$

Here $\dot{m}_{acc}$ is the flow rate, C_D is the discharge coefficient, A_o is the orifice area, ρ is the liquid density, P is the vapour space pressure in the vessel, P_a is the atmospheric pressure, g the gravitational acceleration, ΔH_L the liquid head and t the time since the start of the release. Equation (3) may be integrated over time to find the transient flow rate as predicted by the Bernoulli equation.

Scenario data

The key scenario data are selected as follows:

- Material: water with density 996.479 kg/m^3 (from Phast 6.54; at both ambient pressure and at 6 atm.)
- Initial temperature: 20° C
- Initial pressure: 101325 Pa (unpressurised; 1atm.) and 607950 Pa (pressurised; 6atm.)
- Ambient pressure: 101325 Pa (1 atm.)
- Orifice: circular hole (0.3 m diameter) located 2.0 m above bottom of the vessel
- Discharge coefficient 0.6
- Initial liquid head: 6.028268 m
- Vessel geometry: horizontal cylinder (10.0 m in diameter and 10.7 m long).

The TVDI model has two different calculation methods for the flow rate: the default approach uses the compressible flow equations while there also is a non-default option based on the above Bernoulli equation – details about these two calculation approaches can be found in the DISC theory document (Harper et al., 2011). Both approaches were applied here, giving a total set of 4 TVDI runs.

Results

The flow rates from the orifice of a horizontal cylinder for both unpressurised and pressurised water releases can be seen in Figure 3. The flow rate predicted by the TVDI model with the Bernoulli option closely coincides with the flow rate calculated by solving the Bernoulli equation manually. The initial flow rate predicted by TVDI default option is about 15% higher than the Bernoulli flow rate.

Very similar results were obtained for three other vessel geometries, i.e. a horizontal cylinder, a rectangular box or a sphere. The total released mass was also compared with very close agreement between TVDI default, TVDI Bernoulli and analytical Bernoulli for all four vessel geometries.

Verification against ideal gas for release of air

Sallet and Palmer (1980) present analytical formulas describing both the choked and unchoked flow of ideal gas through an orifice assuming isentropic expansion. These formulas were applied to the release of pressurised air, and the analytical flow rate was then compared to the flow rate predicted by the TVDI model as seen in Figure 4. The scenario input data are selected as follows:

- Material: air (molecular weight 28.95 kg/kmol, compressibility factor 1)
- Initial storage data: temperature 323.15 K; pressure 40 bar; mass 8620 kg (corresponding to a tank volume of 200 m^3)
- Accident data: orifice diameter 0.1 m; discharge coefficient 0.88
- Ambient pressure : 101325 Pa

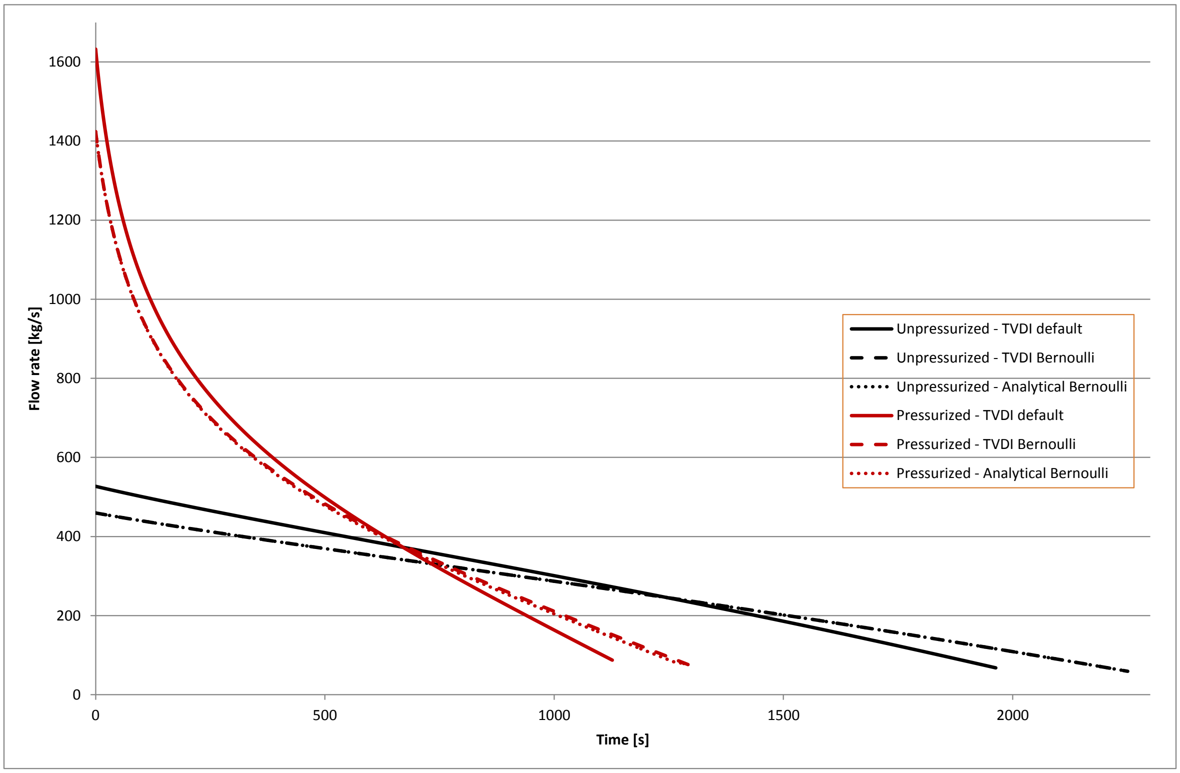


Figure 3. **TVDI predicted flow rates compared to analytical Bernoulli flow rates for unpressurised and pressurised release of sub-cooled water**

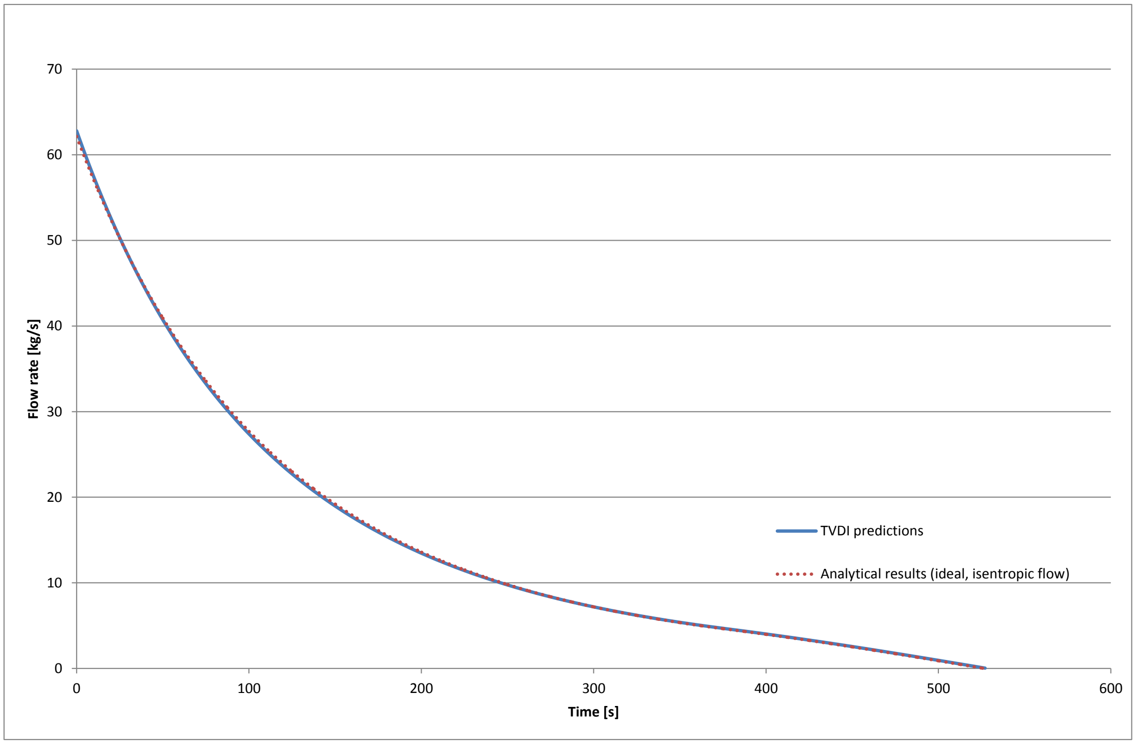


Figure 4. TVDI predicted flow rates compared to analytical flow rates for release of air

Figure 4 demonstrates a virtually perfect match between the TVDI and analytical results.

Validation against CO_2 experiments

Experiments involving pressurised CO_2 releases were carried out at Spadeadam by GL Noble Denton (previously Advantica) for BP in 2006 and for Shell in 2010. In these experiments the CO_2 was stored under high pressure in a horizontal cylindrical vessel. The modelled experiments include time-varying cold releases (liquid storage; Shell tests 1,2,4) and hot supercritical releases (dense vapour storage; BP tests 8, 8R, 9 and Shell tests 14,16).

A summary of the key input data required for the TVDI model is given in Table 1 for the cold releases only, and Figure 5 presents TVDI validation results for these tests. The TVDI predictions were obtained by using the Peng-Robinson equation of state and allowing potential flashing in the expansion to the orifice. Figure 5 shows generally good agreement for the flow rate predicted by the model and observed in experiments. When deviations do occur, the model predictions tend to be conservative. Note that the flow rate observed in the experiment dropping to 0 kg/s marks the end of the experiment.

A complete, detailed description of these experiments and associated validation of Phast models is described by Witlox et al. (2013, 2014).

Discharge input	**SHELL TRANSIENT TESTS**		
	Test1	**Test2**	**Test4**
initial storage phase	liquid	liquid	liquid
storage pressure (barg)	148.3	147.1	148.2
nozzle pressure (barg)	143	118	148.2
storage temperature (^oC)	26.7	24.6	20.1
nozzle temperature (^oC)	23	18	20.1
vessel volume (m^3)	6.3	6.3	6.3
orifice diameter (mm)	12.7	25.4	6.3
orifice length (mm)	47.78	46.84	47.79
release duration (s)	90	145	>700

Table 1. Experimental conditions for and Shell CO_2 cold tests

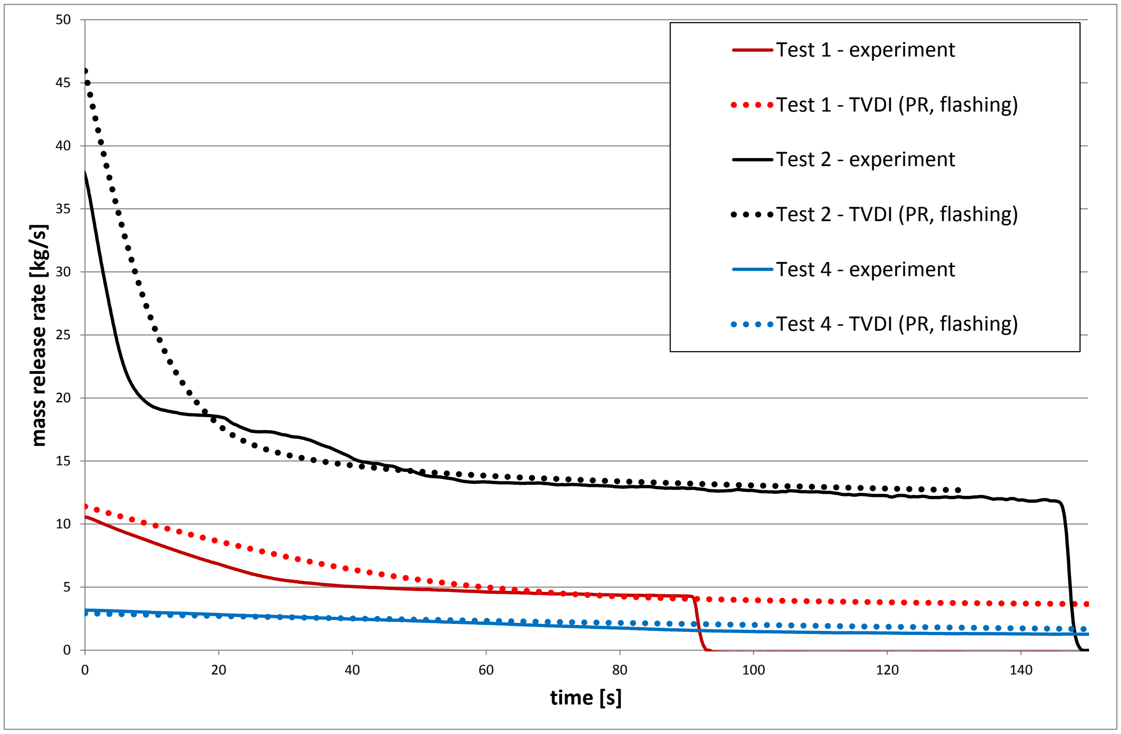


Figure 5. **TVDI validation of flow rate for time-varying cold releases (Shell tests 1, 2, 4)**

Illustrative example of production flows and safety systems

This section includes an example case illustrating the impact on results of various safety system options and parameters. A cylindrical tank is filled with saturated propane with liquid up to a level of 1.3 m. An accidental vapour release occurs from a height of 1.6 m. There are a production inflows and outflows of 5 kg/s. Safety systems include a blowdown valve of 100 mm that operates after 120 s and ESD valves that operate after 30 s to isolate the vessel from upstream. The inventory of the upstream isolatable section is 3000 kg.

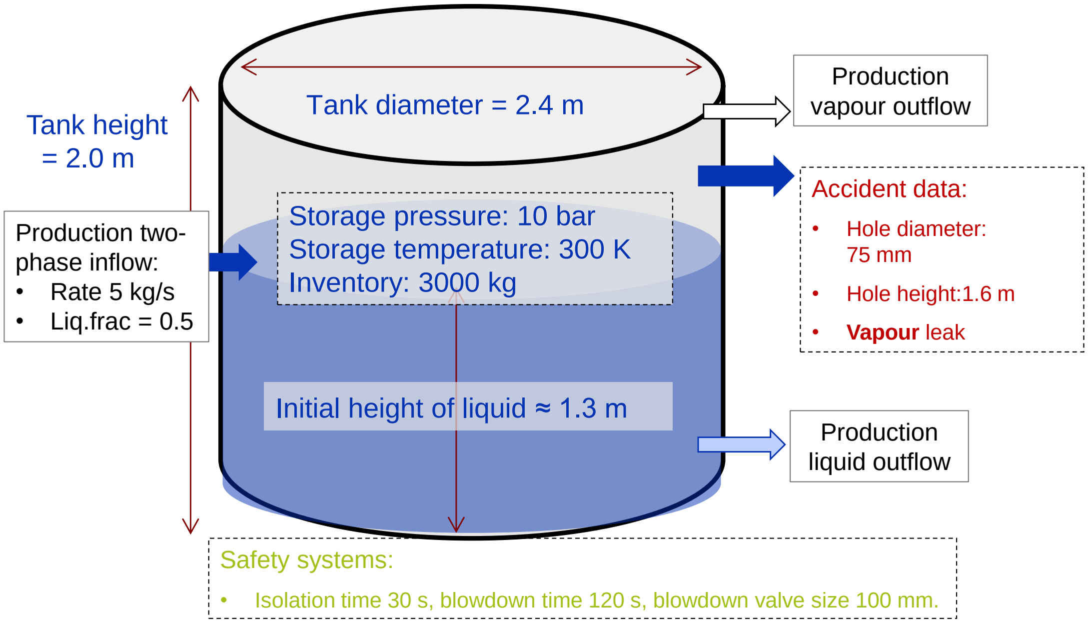


Figure 6. **Scenario description of the example case with a propane leak**

Figure 7 shows how the success and failure of isolation and blowdown impacts on the accidental flow rate and the total released mass. We see how failure of isolation sustains flows for longer than otherwise might be expected, due to the increased inventory.

Figure 8 gives the mass flow rate of the various fluid flows into and out of the vessel in the case when both isolation and blowdown is successful. The red dashed line shows how the production inflow is constant at 5 kg/s until isolation takes place at 30 s, after which it is instantaneously cut off. The production outflows both decrease as the pressure inside the vessel drops, with the production liquid outflow seen in black already dropping to 0 kg/s before isolation takes place. The production vapour outflow shown in green is cut off at isolation time 30 s. Also note the blowdown flow rate in blue which is zero until blowdown commences at 120 s, when it jumps to about 6 kg/s before gradually reducing as the vessel depressurises.

Figure 9 shows how larger blowdown valves reduce flow rate and thereby shorten the accidental release significantly.

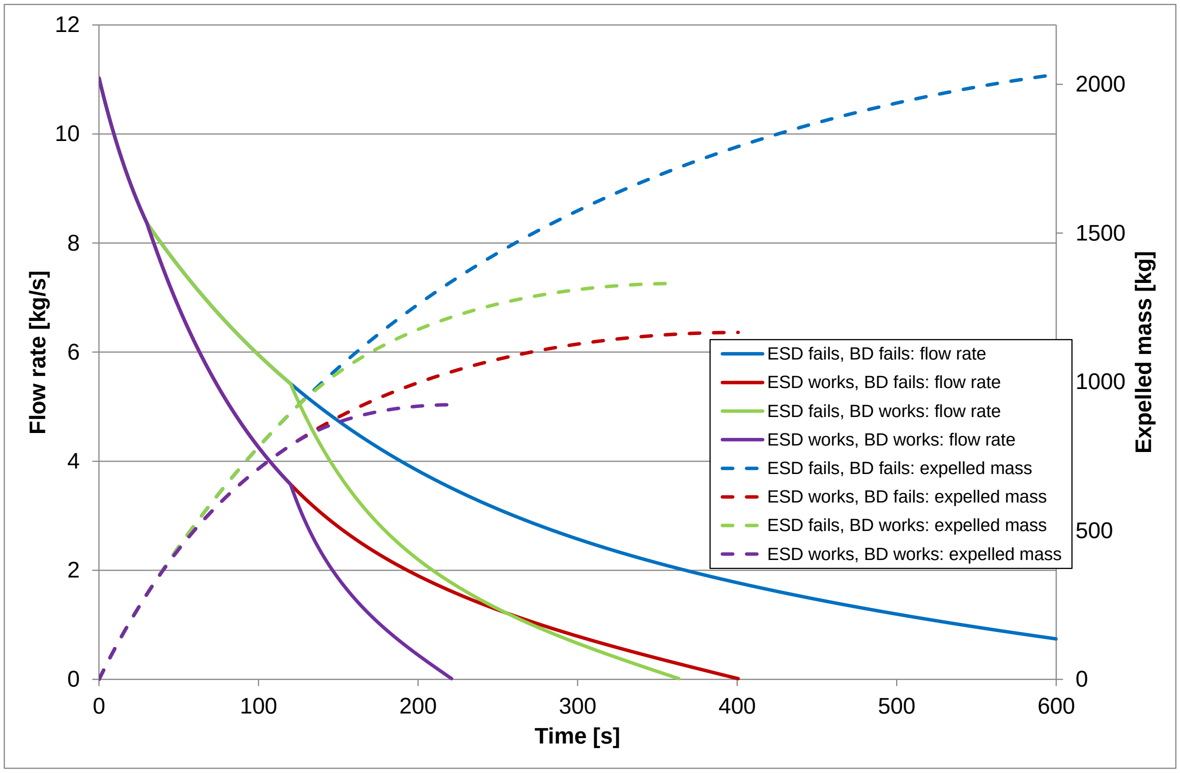


Figure 7. Mass flow rate (solid lines) and total expelled mass (dashed lines) for different safety system behaviour

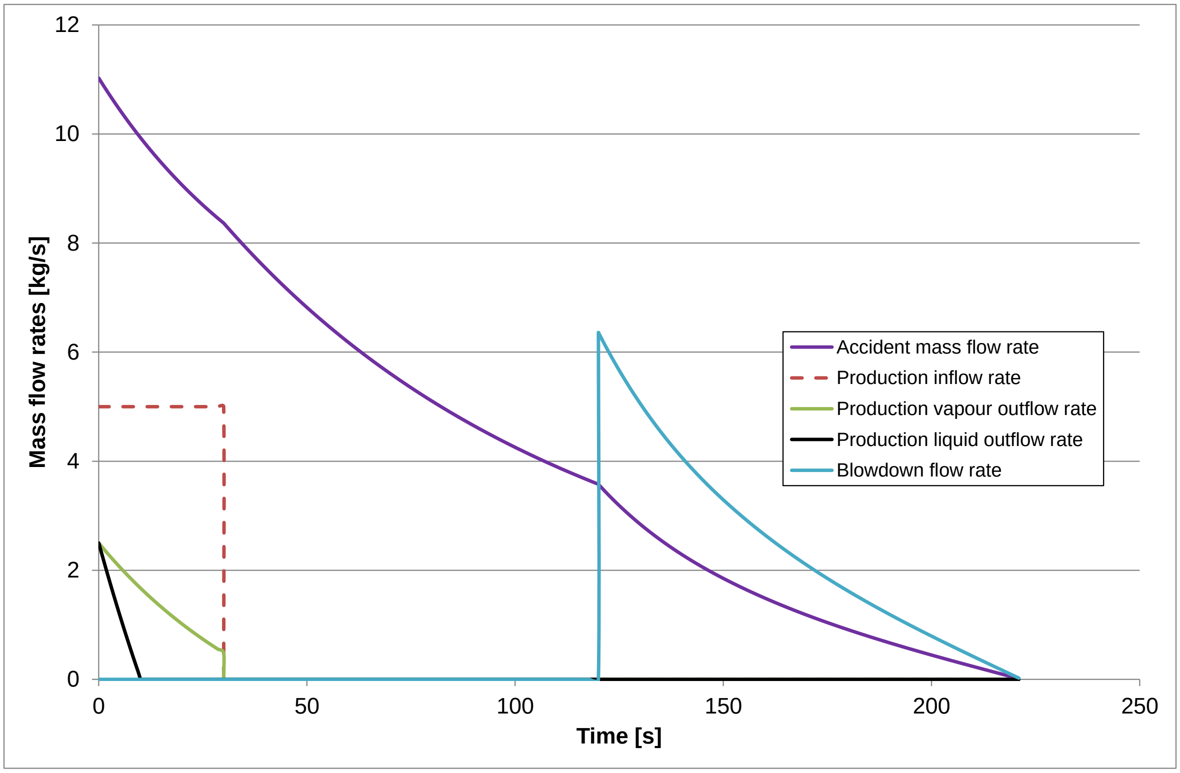


Figure 8. **The various flows in and out of the vessel for the case of successful isolation and blowdown**

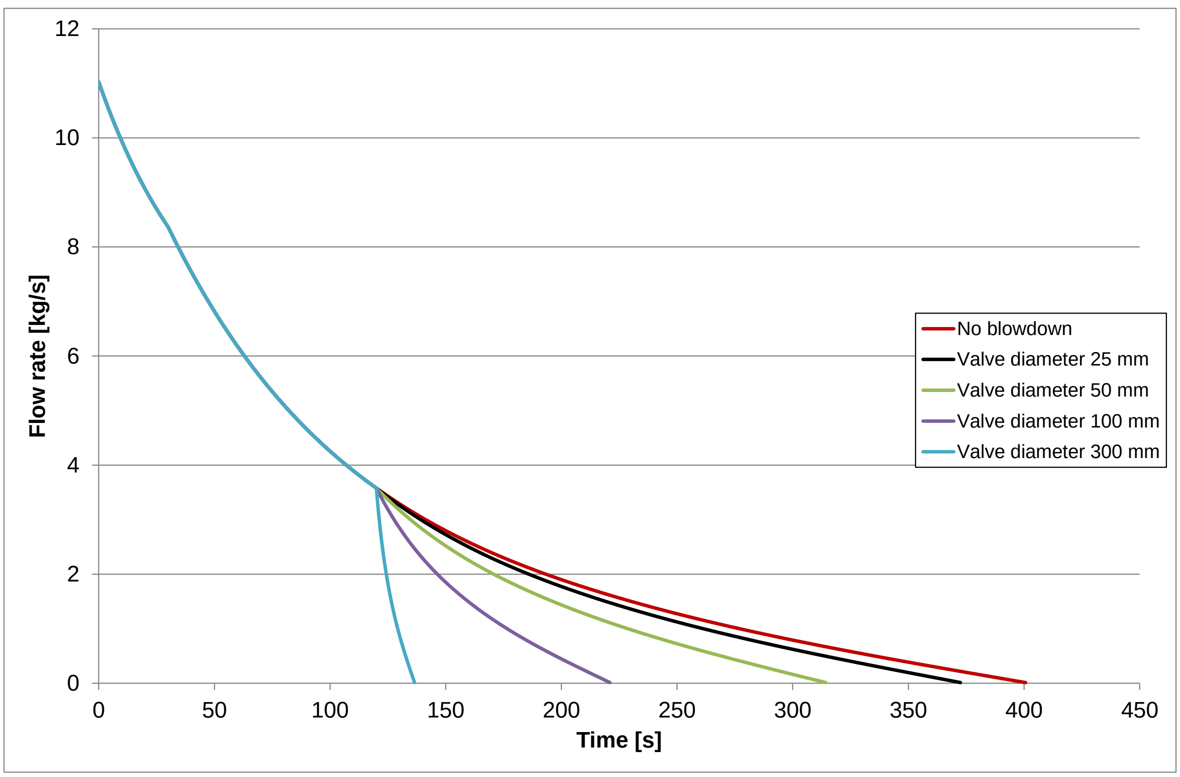


Figure 9. **Impact of different blowdown valve diameters on the accidental flow rates following successful isolation**

Conclusions and future work

The following main conclusions can be drawn:

- A new time-varying discharge model TVDI for vessel leaks has been developed for inclusion in future versions of the consequence modelling package Phast and QRA tool Safeti.
- The user may define normal operation production flows to and from the vessel so that their impact on the accidental leak can be accounted for.
- Safety measures in form of emergency shutdown (isolation) and vapour-space blowdown are explicitly modelled, allowing the user to study their effectiveness in reducing consequences of an accidental leak.
- Flow rates for liquid water leaks predicted by the model were successfully verified against the Bernoulli equation, while flow rates for vapour air leaks were verified analytically against isentropic flow for ideal gas.
- Flow rates were validated against experimental data in form of high-pressure CO_2 releases and excellent agreement was observed.

Ongoing and planned further work includes:

- The model currently uses a pseudo-component approach when dealing with vapour-liquid equilibrium for mixtures: the mixture is assumed to have a 'saturated' vapour pressure curve approximately matching the mixture's bubble point. Work is underway to overcome this limitation in form of a rigorous multi-component version of the model where the material properties of each individual component will be taken into account.
- The model currently ignores heat transfer between fluid and vessel walls, which can lead to too low fluid temperatures being predicted. As such heat transfer between the fluid and walls is intended to be included in a future version of the model. Further extension could be to also allow heat transfer from the surroundings to the vessel (e.g. heat flux term due to impinging external fires).
- Added model validation subject to availability of experimental data

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Acknowledgement

Input from Ade Oke in theoretical discussions and from David Worthington in model specification is gratefully acknowledged.