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Modelling and validation of atmospheric expansion and near-field dispersion for pressurised vapour or two-phase releases

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A B S T R A C T

The consequence modelling package Phast includes discharge models for vessel orifice releases. These models first calculate the depressurisation between the stagnation and orifice conditions and subsequently impose the 'ATmospheric EXpansion model' ATEX for modelling the expansion from orifice conditions to the final conditions at atmospheric pressure. The latter post-expansion conditions are used as the source term for the Phast 'Unified Dispersion Model' UDM.

The current paper summarises the results of a literature review on atmospheric expansion modelling and provides recommendations on selection of ATEX model equations to ensure a most accurate prediction for the near-field UDM jet dispersion against available experimental data.

First, the correctness of the numerical solution to the ATEX equations has been verified analytically and the importance of non-ideal gas effects is investigated.

Secondly, both ATEX expansion options have been applied to known available experimental data for orifice releases. For these experimental data it was confirmed that the ATEX conservation-of-momentum option without a velocity cap provides overall more accurate concentration predictions than the isentropic assumption. However the existing default 'minimum thermodynamic change' option was found to mostly impose conservation of entropy (velocity cap not applicable) for two-phase releases and conservation of momentum (velocity cap applicable) for sonic gas jets. Rainout calculations for flashing two-phase releases are currently always based on the isentropic assumption, which is inconsistent with the recommended conservation of momentum; a further investigation is recommended.

1. Introduction

The consequence modelling software package Phast and the QRA software package Safeti include steady-state (DISC) and time-varying (TVDI) discharge models for vessel orifice releases of toxic or flammable materials. These models first calculate the depressurisation between the stagnation and downstream orifice (vena contracta) conditions by conserving energy and entropy. Subsequently the 'Atmospheric Expansion model' ATEX is imposed for modelling the expansion from downstream orifice conditions to the final conditions at atmospheric pressure. The latter post-expansion conditions are used as the source term for the Phast dispersion model UDM.

Fig. 1a illustrates the subsequent flow regimes for the case of the discharge from an orifice:

- (st) stagnation point (zero velocity, pressure P_{st}, temperature T_{st})
- (o) upstream orifice (nozzle entrance; area A_o, velocity u_o, pressure P_o, temperature T_o)
- (vc) downstream orifice (nozzle throat; vena contracta area A_{vc}, velocity u_{vc}, pressure P_{vc}, temperature T_{vc})
- (f) end of atmospheric expansion zone (area A_f, velocity u_f, pressure P_f = ambient pressure P_a, temperature T_f)

The vena contracta area equals $A_{vc} = C_d A_o$, where C_d equals the discharge coefficient. At the vena contracta, DISC and TVDI applies the metastable liquid assumption (100% liquid, pressure = ambient pressure) in case of liquid storage, and thermodynamic equilibrium in case of vapour storage. At the final conditions (f) the flow is presumed to be thermodynamically stable. ATEX presumes the final surface to be a plane surface (Fig. 1b), while Paris et al. (2005) presume the final surface to be part of a sphere (Fig. 1a).

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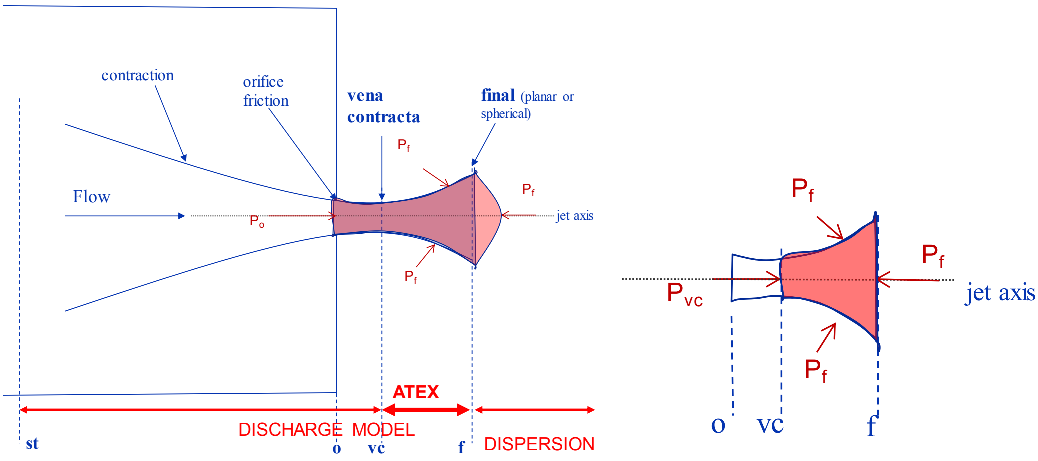

(a) Flow regimes for discharge from orifice (b) ATEX control volume

Fig. 1. Control volume for expansion to ambient conditions.

1.1. *ATEX atmospheric expansion model*

The ATEX model solves five equations to determine five unknown variables at the final surface, i.e. area A_f, velocity u_f, temperature T_f or liquid fraction f_{Lf}, density ρ_f and enthalpy h_f:

$$\rho_f A_f u_f = \rho_{vc} A_{vc} u_{vc}, \quad \textit{mass conservation} \tag{1}$$

$$\rho_f A_f u_f^2 = \rho_{vc} A_{vc} u_{vc}^2 + \left(P_{vc} - P_f\right) A_{vc}, \quad \textit{momentum conservation} \tag{2}$$

$$\rho_f A_f u_f \left[h_f + \frac{1}{2} u_f^2\right] = \rho_{vc} A_{vc} u_{vc} \left[h(P_{vc}, T_{vc}; f_{Lvc}) + \frac{1}{2} u_{vc}^2\right], \quad \textit{energy conservation} \tag{3}$$

$$\rho_f = \rho_f\left(P_a, T_f; f_{Lf}\right), \quad \textit{density equation of state} \tag{4}$$

$$\begin{aligned} h_f &= h\left(P_a, T_f; f_{Lf}\right) \\ &= f_{Lf} h_L\left(P_a, T_f\right) \\ &\quad + \left(1 - f_{Lf}\right) h_V\left(P_a, T_f\right), \quad \textit{enthalpy equation of state} \end{aligned} \tag{5}$$

Phast currently caps by default the final velocity u_f with 500 m/s. This capped velocity is then used in conjunction with the conservation-of-energy Equation (3) to determine the final temperature T_f and liquid fraction f_{Lf}.

Instead of imposing the conservation-of-momentum Equation (2), ATEX also allows imposing conservation of entropy (final entropy = vena-contracta entropy). By default Phast selects the method predicting the smallest thermodynamic change. Thus Phast will carry out both options of expansion modelling and use the results of the model which gives the highest final temperature. If both models give the same final temperature, then ATEX will use the results of the model which gives a final liquid fraction that is closest to the vena-contracta liquid fraction.

1.2. *Literature review*

Phases I-IV of the droplet-modelling JIP managed by DNV Software (Witlox and Harper, 2013) very much focussed on the correct evaluation of the flow rate (kg/s) and initial post-expansion droplet size distribution (micrometre), but did not focus on correct evaluation of the post-expansion velocity, post-expansion liquid fraction (case of 2-phase releases) and temperature (case of vapour releases). A very brief review of external expansion calculations available in the literature was carried out by Witlox and Bowen (2002) as part of the first phase of the droplet modelling JIP.

The arbitrary ATEX default cap of 500 m/s for post-expansion velocity is a known issue alongside the appropriate default choice of the ATEX expansion method (isentropic, conservation of momentum, or minimum thermodynamic change). The most common approach in the literature may be the absence of a cap combined with the conservation of momentum method (recommendation by EU project FLADIS and USA DTRA project; see e.g. Britter et al., 2011). ATEX currently also allows for an alternative cap (sonic velocity). However in case of choked flow (sonic velocity at orifice), supersonic turbulent flow (shock waves) is known to occur downstream of the orifice and the sonic cap may not be appropriate. Moreover the thermodynamic path may need to include non-equilibrium effects and/or slip. So far we are not aware of a published and validated formulation, which takes these effects into account.

Also important to note is that when modelling choked flows the final velocity u_f does not necessarily correspond to a physically real velocity, and is therefore sometimes referred to in literature as a ‘pseudo-velocity’. The key important aspect is that this pseudo-velocity produces the correct amount of (jet) entrainment in the UDM dispersion model to ensure accurate predictions of the concentrations in the near-field. It is therefore NOT important that the predicted post-expansion velocity is close to the actual post-expansion velocity. A larger selected value for the velocity will correspond to a larger temperature drop and this may affect e.g. the plume rise for buoyant plumes; to avoid a large temperature drop, sometimes also an isenthalpic expansion or an isothermal expansion is applied in the literature instead of the conservation-of-energy assumption (e.g. Birch et al., 1987). Thus the emphasis of the current work is on conventional pseudo-source models (as could be used in Phast). CFD modelling is not considered. For example, Leeds University (Wareing et al., 2013) developed a CFD method solving rigorously the Navier Stokes equations to define the shape, velocity and temperature distribution downstream of the Mach shock region, where the flow expands to atmospheric

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