The Effect of the Choice of the Primitive Variables on the Numerical Solution Efficiency of Highly Transient Flows

Haroun Mahgerefteh and Adeyemi O. Oke
Department of Chemical Engineering, University College London,
London WC1E 7JE

Abstract

The numerical solutions for different formulations of the conservation equations based on the dependent variables, pressure (P), enthalpy (h), density (ρ), entropy (s) and flow velocity (u) for highly transient flows are presented. Their application for simulating the fluid flow dynamics following the rupture of a real pressurised pipeline produces a ten fold reduction in the computational run time for Phu and Psu based conservation equations as compared to the conventional Pρu formulation.

* Author for correspondence (h.mahgerefteh@ucl.ac.uk)

Introduction

Pressurised pipelines are increasingly used for the transport of large quantities of highly flammable hydrocarbons and their rupture can give rise to catastrophic consequences. Indeed in recent years there have been many instances of pipeline rupture (Bond, 2002; Fletcher, 2001) which have caused enormous damage to the environment and numerous fatalities, the most recent example being the Belgium pipeline rupture (Georges and Louvain-la-Neuve, 2005) leading to 25 deaths and 50 injuries. In the United States alone there are over 420,000 km of high pressure gas pipelines, over 250,000 km of oil and products pipelines and many thousands of kilometres of lower pressure local distribution gas lines. Data published by the U.S. Department of Transport (1997) on reportable incidents reveals that action by third parties alone during 1982 – 1997 caused more than 104,000 incidents of pipeline damage.

The accurate prediction of outflow and its variation with time following pipeline rupture is therefore extremely important since this information dictates all the major consequences associated with such type of failure including fire, explosion and environmental pollution.

The development of a transient two-phase fluid outflow model for pipeline rupture entails three main steps. The first requires the formulation of the conservation equations governing the flow incorporating heat transfer and frictional effects. The conventional approach has invariably involved expressing these equations in terms of the dependent variables, pressure, density and flow velocity (see for example Picard and Bishnoi 1988,1989; Chen et al., 1992,1993; Mahgerefteh et al., 1999,2000). The resulting quasi-linear partial differential equations are hyperbolic and cannot be solved analytically as they contain terms that are unknown or complex functions of their dependent and independent variables (see Flatt, 1986; Mahgerefteh et al., 1999). The second step involves the transformation of these non-linear equations into a finite difference form. The final step requires their solution in conjunction with the relevant boundary conditions using a suitable numerical technique. As all of these techniques involve the numerical discritisation of the pipeline into a large number of elements, the solution for a typical pipeline often requires very long CPU time (e.g 5 days on a Pentium IV processor for a

300 km, 1 m dia pipeline transporting a condensable hydrocarbon mixture at 100 bar pressure). This is despite significant advances involving the use of nested grid systems (Chen et al., 1992, Mahgerefteh et al., 1999, Oke et al., 2003) and higher speed computer processing powers.

In this study a more fundamental approach is described which for the first time demonstrates the significant effect of the choice of the dependent variables in the formulation of the conservation equations on the computational run time and accuracy. The model's efficacy is demonstrated based on comparison with recorded data for the rupture of a real pipeline.

Theory

Conservation Equations

The conservation equations are in essence the fundamental building blocks for formulating the transient fluid flow process. The following describes their derivation for 1-D flow in pipes based on different combinations of the primitive parameters including density, entropy and enthalpy. The modelling takes account of heat transfer and friction but assumes homogeneous equilibrium flow with negligible fluid/structure interactions. Comparisons with real data have shown (Chen et al., 1995) that the homogeneous flow assumption in which the constituent phases are at thermal and mechanical equilibrium is valid in the case of rupture of long (>100 m) pipelines. As such only one set of mass, momentum and energy conservation equations suffice for both single and two-phase flows. The pressure waves generated within the contained fluid following rapid depressurisation of a pipeline exert forces that may cause a compliant (freely suspended) system to move or vibrate. This dynamic phenomenon is known as fluid-structure interaction. In this work, such forces are ignored as the pipeline is assumed to be rigidly clamped and inelastic.

Mass conservation

For an element of fluid, the law of conservation of mass can generally be expressed as (Versteeg and Malalasekera, 1995):

$$\frac{d\rho}{dt} + \rho \frac{\partial u}{\partial x} = 0 \qquad (1)$$

where u and ρ are the fluid velocity and density with t and x, representing time and distance respectively.

Rearranging and using thermodynamics relations, the total derivative of density with respect to time in the mass conservation equation (1) may be expressed in terms of fluid pressure and enthalpy for 1D flow as given by:

$$\frac{d\rho}{dt} = \frac{1}{a^2}\left[\frac{dP}{dt}\left(1 + \frac{\varphi}{\rho T}\right) - \frac{\varphi}{T}\frac{dh}{dt}\right] \qquad (2)$$

Similarly the mass conservation equation expressed in terms of pressure and entropy for 1D flow may be shown to be given by:

$$\frac{dP}{dt} - \varphi\frac{ds}{dt} + \rho a^2 \frac{\partial u}{\partial x} = 0 \qquad (3)$$

The mass conservation equation expressed in terms of pressure and density for 1D flow:

$$[\rho T + \varphi]\frac{dP}{dt} - \rho\varphi\frac{dh}{dt} + \rho^2 a^2 T\frac{\partial u}{\partial x} = 0 \quad (4)$$

Where

$$\left(\frac{\partial P}{\partial s}\right)_\rho = \varphi \quad (5)$$

Momentum conservation

The derivation of the momentum conservation equation is based on the assumption that only the surface and gravitational body forces are of significance. Consequently, the momentum equation may be expressed in differential form as (Versteeg and Malalasekera, 1995):

$$\rho\frac{du}{dt} = -\frac{\partial P}{\partial x} - \rho g\sin\theta + \beta_{wx} \quad (6)$$

where g, θ and β_{wx} are the acceleration due to gravity, the angle of elevation and wall frictional force respectively.

Energy conservation

The energy conservation equation for 1-D flow expressed in terms of pressure and enthalpy is given by (Versteeg and Malalasekera, 1995):

$$\rho\frac{dh}{dt} - \frac{dP}{dt} = q_h - u\beta_{wx} \quad (7)$$

where q_h is the pipe wall/ambient heat transfer rate.

The energy conservation equation expressed in terms of fluid entropy:

$$\rho T\frac{ds}{dt} = q_h - u\beta_{wx} \quad (8)$$

Replacing the total derivatives with partial derivatives in space and time, the system of conservation equations (4), (6) and (7) expressed in terms of pressure, enthalpy and velocity (Phu) as dependent variables are respectively given by:

$$[\rho T + \varphi](P_t + uP_x) - \rho\varphi(h_t + uh_x) + \rho^2 a^2 T(u_x) = 0 \quad \text{\{mass\}} \quad (9)$$

$$\rho(u_t + uu_x) + (P_x) = \alpha \quad \text{\{momentum\}} \quad (10)$$

$$\rho(h_t + uh_x) - (P_t + uP_x) = \psi \quad \text{\{energy\}} \quad (11)$$

where:

$$\alpha = -\rho g\sin\theta + \beta_{wx} \quad (12)$$

$$\psi = q_h - u\beta_{wx} \tag{13}$$

Similarly applying the same treatment to equations (9), (11) and (13), the conservation equations expressed in terms of pressure, entropy and velocity (Psu) are given by:

$$\left(P_t + uP_x\right) - \varphi\left(s_t + us_x\right) + \rho a^2\left(u_x\right) = 0 \quad \text{\{mass\}} \tag{14}$$

$$\rho\left(u_t + uu_x\right) + \left(P_x\right) = \alpha \quad \text{\{momentum\}} \tag{15}$$

$$\rho T\left(s_t + us_x\right) = \psi \quad \text{\{energy\}} \tag{16}$$

The conservation equations represented by equations (9) - (11) and (14) - (16) are quasilinear. This is because all the derivative terms are linear. Furthermore they are hyperbolic as they can be shown (Prasad and Ravindran, 1985) to possess three real and distinct eigenvalues. These equations cannot be solved analytically as the coefficients of the partial derivatives such as density, ρ or flow velocity, *u* are themselves functions of some of the dependent functions, *P*, *s, h* and *u*.

Numerical Solution of the Conservation Equations

In the main, 3 different types of numerical techniques have found widespread use in resolving quasilinear hyperbolic partial differential equations. These include the finite difference methods (Chen et al., 1993, Chen et al., 1995, Bendiksen et al., 1991), finite element methods (Lang, 1991, Bisgaard et al., 1987) and the Method of Characteristics (MOC) (Zucrow and Hoffman, 1976, Mahgerefteh et al., 1997, 2000).

In this work, the MOC is employed as the numerical solution technique for the resolution of the governing conservation equations. This is because both the finite difference and finite element methods have difficulty in handling the choking condition at the rupture plane (Chen et al., 1992). The MOC handles choked flow intrinsically via the mach line characteristics. Moreover, MOC is considered to be more accurate than the finite difference method as it is based on the characteristics of wave propagation. Hence, numerical diffusion associated with a finite difference approximation of partial derivatives is avoided.

MOC involves replacing the conservation equations with the corresponding characteristics and compatibility equations and solving them numerically at selected space and time intervals along the pipeline subject to the Courant-Friedrich-Lewy stability criterion (Zucrow and Hoffman, 1976).

The following investigates the effects of the three different forms of the compatibility equations based on the Phu, Psu and Pρu system of conservation equations on the simulation run time and accuracy using the results of Isle of Grain pipeline rupture tests (Richardson and Saville, 1996 a,b) as a case example.

Results and Discussion

The Isle of Grain experiments conducted jointly by BP and Shell involved the rapid depressurisation of extensively instrumented carbon steel, 154 mm i.d, 100 m pipeline containing commercial propane or LPG (95 % propane, 5% n-butane). Pressure transducers and thermocouples were attached along each line. Inventory and hold-up were measured using load-cells and neutron back scattering.

A number of tests involving both full bore rupture as well as puncture at different starting line pressures were conducted. Of these, the full bore rupture test (P40) initiated by the rupture of a disc at the downstream end of the pipeline is chosen as an example as it starts with the highest line pressure of 21.6 bara representing the longest discharge process. The feed and the ambient temperatures are both 20 ^{o}C. The heat transfer calculations are based on the lumped capacitance method (Myers, 1971), for which respective wall density, specific heat capacity and thermal conductivity of 7854 kg/m^3, 434 J/kgK and 53.60 W/mK for carbon steel are assumed (Perry, 1997). The pipeline thickness and roughness factors are given as 0.0073 m and 0.00005 m respectively. The discretisation scheme used for the numerical simulations is based on the specified time intervals using a uniform grid spacing of 2.5 m. Smaller grid sizes were found to have negligible effect on the simulation results.

Figures 2-5 respectively show the measured pressure (open and intact end), temperature and inventory variations with time for test P40 in comparison with simulated results using the Pρu, Phu and Psu models.

Referring to figure 2, the transition of the liquid inventory to the 2-phase mixture upon full bore rupture results in an almost instantaneous drop in the rupture plane pressure from 21 bara to ca. 6.5 bar. This is followed by a slower, almost monotonous drop in pressure corresponding to vaporisation of the 2-phase mixture to the gaseous state at around 20s following depressurisation. Similar trends in behaviour may be observed for the variations of the intact end pressure (figure 3) and fluid temperature (figure 4) with time with exception of the effects being less marked. The inventory versus mass data indicates that almost the entire content of the pipeline is discharged in approximately 20s.

Returning to the simulation data, all three models produce good agreement with measured data (curves A) with the Phu model (curves C) producing the best fit followed by the Psu (curves D) and the P□u (curves B) based predictions. Also, at any given time, the three models predict lower pressures and temperatures when compared to measured data. The P□u model generally predicts the lowest pressures and temperatures at a given time, hence the fastest depressurisation rate, followed by the Psu and Phu models. The Pρu model's estimation of the depressurisation time is the most conservative of the three.

The open end pressure-time profile data based on the P□u model (figure 2, curve B) using density as the primitive variable fluctuate between ca 5 - 7.5 bara for the first 1.5 s of depressurisation. This is believed to be due to the rapid change in fluid density during the transition from the liquid to the 2-phase region, which is in turn manifested in instability in the data. No such marked fluctuations in the results based on the Psu and Phu models are observed (curves C and D). This is a consequence of the fact that the rates of change in fluid entropy and enthalpy with pressure as the phase transition is crossed are much less pronounced as compared to the variation in the fluid density. This leads to the greater observed stability of the Phu and Psu based simulation data.

Apart from agreement with field data, the most significant aspect of the simulated data is the associated computation run times. The computation run time for the conventional P□u based

model is 86 minutes. The corresponding values for the Phu and Psu models are only 7 and 9 minutes respectively, representing a remarkable 10 fold reduction in the computation run time.

Conclusion

The numerical solutions of three different formulations of the conservation equations based on the dependent variables, Phu, Psu and the conventional P□u for simulating the fluid dynamics following pipeline rupture were presented.

The above involved replacing the conservation equations with the corresponding characteristics and compatibility equations using MOC and solving them numerically at selected space and time intervals along the pipeline. The resulting positive and negative compatibility equations turned out to be identical for all of the three different formulations of the conservation equations. Only the path line compatibility was found to be different in each case thus being solely responsible for the observed 10 fold reduction in the computational run time for the Phu and Psu as compared to the commonly employed P□u based formulations. In the case of the former, the fluid properties at the solution point may simply be obtained directly from P/h and P/s flash calculations. However, the determination of the fluid properties from the P□u compatibility equation requires its iterative solution. The above becomes an extremely computationally expensive procedure especially for two-phase flows as numerous isothermal flash calculations are required in order to obtain an accurate solution.

Based on comparison with the Isle of Grain field data, the simulation results obtained using the Phu and Psu formulations were found to be more stable than those obtained using the P□u formulation. The above was attributed to the less marked changes in the fluid entropy and enthalpy as compared to the fluid density when crossing the two-phase boundary.

In conclusion, using a fundamental approach, the present study addresses a major practical drawback associated with the long computational run times expended in simulating the fluid dynamics for highly transient flows such as those following the rupture of pressurised pipelines. The 10 fold reduction in the computational run time will be of considerable benefit to safety assessment engineers particularly in view of the rapid increase in the use of pressurised pipelines for the transport of hydrocarbons. Data on the fluid flow dynamics following pipeline rupture forms the basis for all the major hazard consequence predictions associated with such type of failure including fire, explosion and environmental pollution.

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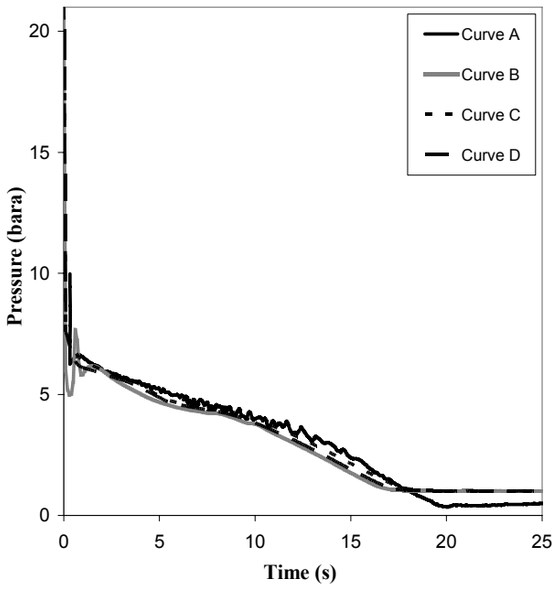

Figure 1: Experimental and simulated variations of the open end pressure with time following full bore rupture of the LPG pipeline.

Curve A: Measurement (Richardson and Saville, 1996a,b)
Curve B: Simulated data, Pρu model
Curve C: Simulated data, Phu model
Curve D: Simulated data, Psu model

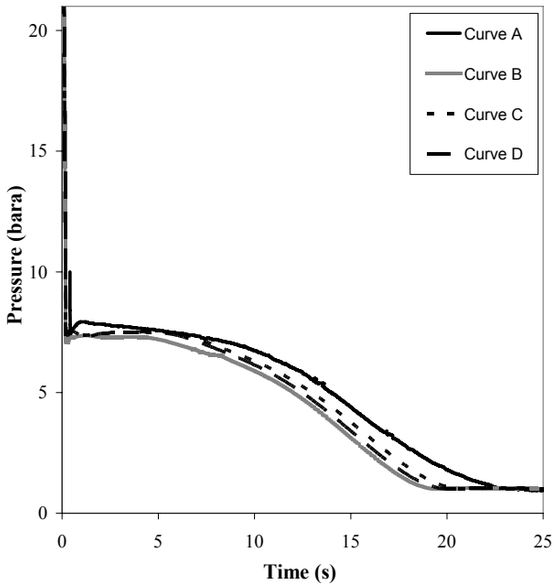

Figure 2: Experimental and simulated variations of the intact end pressure with time following full bore rupture of the LPG pipeline.

Curve A: Measurement (Richardson and Saville, 1996a,b)
Curve B: Simulated data, Pρu model
Curve C: Simulated data, Phu model
Curve D: Simulated data, Psu model

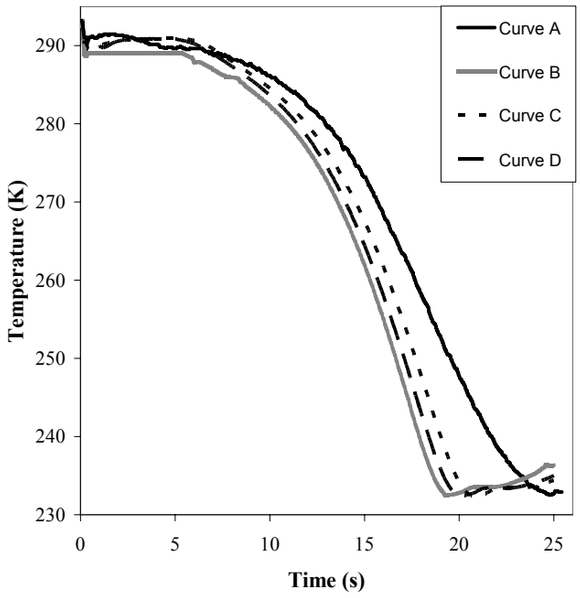

Figure 3: Experimental and simulated variations of the closed end temperature with time following full bore rupture of the LPG pipeline.

Curve A: Measurement (Richardson and Saville, 1996a,b)
Curve B: Simulated data, Pρu model
Curve C: Simulated data, Phu model
Curve D: Simulated data, Psu model

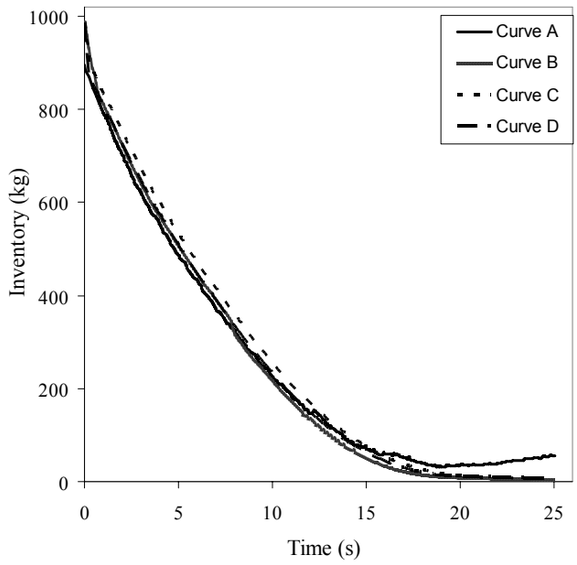

Figure 4: Experimental and simulated variations of the pipeline fluid inventory with time following full bore rupture of the LPG pipeline.

Curve A: Measurement (Richardson and Saville, 1996a,b)
Curve B: Simulated data, Pρu model
Curve C: Simulated data, Phu model
Curve D: Simulated data, Psu model