

Computational Fluid Dynamic Modelling of Atomisation Processes in Turbulent Flows

N. Beheshti^a, A.A. Burluka^{a*} and M. Fairweather^b

^aSchool of Mechanical Engineering,

^bSchool of Process, Environmental and Materials Engineering,
University of Leeds, Leeds LS2 9JT, UK

Abstract

Atomisation of liquids is frequently encountered in the liquid-gas flows used in many practical chemical and process engineering applications, and an ability to reliably predict such flows is of benefit to the optimisation and performance improvement of existing equipment and processes, as well as the evaluation of retrofit options and the design of new equipment, systems and plant. This paper considers the ability of an Eulerian, two-equation continuum model of the atomisation process, embodied within a computational fluid dynamic framework, to reproduce the experimentally established behaviour of air-assisted atomisation. The influence of injector exit velocity profile, surface tension, gas velocity, and liquid and gas densities on predictions of the model is examined, and results found to be in good agreement with available experimental data.

Keywords: two-phase flow, spray, atomisation, continuum model, validation.

1. Introduction

In a recent survey (Fairweather, 2001) of users of computational fluid dynamic (CFD) codes within industries across Europe, carried out as part of the definition phase of the CAPE Alliance, the most frequent shortcoming of existing codes was identified as their inability to accurately predict multi-phase flows. Given the broad range of chemical and process engineering problems that involve such flows, and their often complex nature, multi-phase flow modelling for such applications is in its infancy, with available models generally considered (Fairweather, 2001) to be inaccurate and unreliable. This review also identified another shortcoming, high on the list of work required, namely the lack of validation of CFD models of such flows against reliable experimental data, with user confidence in multi-phase flow models being low as a consequence.

Atomisation and vaporisation of liquids is encountered in the liquid-gas flows used as the basis of many practical chemical and process engineering applications, and a predictive numerical model of such flows must contain embedded sub-models for these phenomena. Atomisation, that is the reduction of the characteristic size of liquid-containing structures, is involved in the working processes of numerous operations. Atomisation results in an increase in the liquid surface area which defines the rate of

* Author to whom correspondence should be addressed: a.a.burluka@leeds.ac.uk

vaporisation, and in many flows, such as those involving combustion, atomisation may be the rate determining process. Despite its importance, however, the description of atomisation remains largely at the level of semi-empirical formulae that need to be adjusted on a case-by-case basis during application.

An attempt to fill this gap was undertaken in a recent paper by Vallet et al. (2001). The latter paper proposed a relatively simple, Eulerian, two-equation model for predicting atomisation that solves transport equations for the average liquid mass fraction and the mean area of the liquid-gas interface per unit mass of media. The present paper describes an assessment of the model of Vallet et al. (2001) with regard to its ability to reproduce the experimentally established behaviour of air-assisted (or air-blast) atomisation.

2. Fluid Dynamic and Atomisation Models

The atomisation model used in this work consists of two transport equations, one for the mass fraction of liquid phase $\tilde{Y}_{liq}$ and the other for the mean surface area of the gas-liquid interface per unit mass of two-phase media $\tilde{\sigma}$ (Vallet et al., 2001). Expressed as conservation equations for incorporation in a CFD methodology, these equations are:

$$\frac{\partial \bar{\rho} \tilde{Y}_{liq}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{Y}_{liq}}{\partial x_j} = \frac{\partial}{\partial x_j} \bar{\rho} \frac{D_T}{Sc_{liq}} \frac{\partial \tilde{Y}_{liq}}{\partial x_j} - \dot{m}_{vap} \bar{\rho} \tilde{\sigma} \quad (1)$$

$$\frac{\partial \bar{\rho} \tilde{\sigma}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{\sigma}}{\partial x_j} = \frac{\partial}{\partial x_j} \bar{\rho} \frac{D_T}{Sc_\sigma} \frac{\partial \tilde{\sigma}}{\partial x_j} + \frac{\bar{\rho} \tilde{\sigma}}{\tau_c} (1 - \frac{\tilde{\sigma}}{\tilde{\sigma}_{eq}}) \quad (2)$$

where tilde denotes density-weighted averaging, an over-bar conventional time-averaging, $\dot{m}_{vap}$ is the mean vaporisation rate per unit surface, D_T is the turbulent diffusivity, and τ_c is the rate of surface production. The latter term is here taken to be proportional to the turbulence time scale:

$$\tau_c = C_1 \frac{\tilde{k}}{\tilde{\varepsilon}} \quad (3)$$

In Eq. (2), $\tilde{\sigma}_{eq}$ is the liquid surface area defined in terms of the droplet radius characterising a mono-dispersed spray at equilibrium with the local turbulence (Vallet et al., 2001; Beheshti et al., 2003), taken as:

$$\tilde{\sigma}_{eq} = \frac{3 \tilde{Y}_{liq}}{\rho_{liq} r_{eq}} \quad r_{eq} = C_r \left(\frac{\bar{\rho} \tilde{Y}_{liq}}{\rho_{liq}} \right)^{2/15} \left(\frac{\eta}{\varepsilon^{2/3} \rho_{liq}} \right)^{3/5} \quad (4)$$

The atomisation model, Eqs. (1) and (2), requires a turbulent diffusivity and an integral scale τ_c , and the standard k - ε turbulence model was used to calculate these variables as well as providing closure of the fluid dynamic transport equations. Compared to homogeneous gaseous flows, modelling of two-phase mixtures also requires a different equation of state for the mean density, given by:

$$\frac{1}{\bar{\rho}} = \frac{\tilde{Y}_{liq}}{\rho_l} + \frac{(1 - \tilde{Y}_{liq})}{\rho_g} \quad (5)$$

Account must also be taken of the incompressibility of the liquid phase through:

$$\bar{p} = \frac{\bar{\rho}(1 - \tilde{Y}_{liq})R_g T_g}{1 - \bar{\rho}\tilde{Y}_{liq} / \rho_l} \quad (6)$$

It should be emphasised that in this approach the two-phase mixture is considered as a single continuum. The conservation equations solved, for mass and momentum as well as for turbulence and atomisation, are therefore expressed in their usual density-weighted (Favre) averaged form. This continuum approach therefore simplifies the prediction of atomisation phenomena, without the need for tracking individual droplets. Another advantage of using the continuum approach is its obvious compatibility with the majority of existing CFD codes which employ, in some form or another, algorithms for the calculation of the pressure field from a single continuity equation, such as the SIMPLE algorithm (Patankar and Spalding, 1972). Use of two separate continuity equations, one for the gas and the other for the liquid phase, would compromise such algorithms and the use of computer codes based upon them.

As noted above, the overall CFD model was based on solutions of averaged forms of the density-weighted transport equations, with closure achieved using a standard $k-\varepsilon$ turbulence model. Solution of the transport equations was achieved using a finite-volume technique based on the pressure correction algorithm. The large density variations encountered in the flows of interest entailed the use of small under-relaxation factors in order to promote numerical convergence. Further details of the numerical solution method employed may be found elsewhere (Fairweather et al., 1992; Beheshti et al., 2003).

3. Test Case

Air-assisted jet atomisation, as considered experimentally by Hopfinger and Lasheras (1994) and Lasheras et al. (1998), is chosen here as the test case because it is characterised by a relatively simple axisymmetric flow field, has high Reynolds and Weber numbers typical of those found in the injectors used in industry, and has been comprehensively studied in a number of experiments. A comprehensive review by Lefebvre (1980) also summarises the extensive measurements made regarding the dependency of the Sauter mean diameters (SMD) encountered in sprays on liquid properties such as surface tension η and viscosity μ , with different injection regimes also considered in terms of the inlet gas $u_{0,g}$ and liquid u_{liq} velocities. A tentative correlation for the SMD was proposed in this work as:

$$SMD = \left[1 + \frac{\dot{m}_l}{\dot{m}_g} \right] \left[0.073 D_l^{2/5} \left(\frac{\eta}{\rho_g u_{0,g}^2} \right)^{3/5} \left(\frac{\rho_l}{\rho_g} \right)^{1/10} + 0.015 \left(\frac{\mu_l^2 D_l}{\eta \rho_l} \right)^{1/2} \right] \quad (7)$$

where the second term is relevant only for atomisation of very viscous liquids, such as a heavy mazout oil. It can be easily seen that Eq. (7) characterises the spray SMD dependency on any particular variable x in terms of a corresponding exponent α , so that $SMD \propto x^\alpha$. An obvious first assessment of the atomisation model proposed is therefore to establish its ability to reproduce the measured exponents, such as those given in Eq. (7).

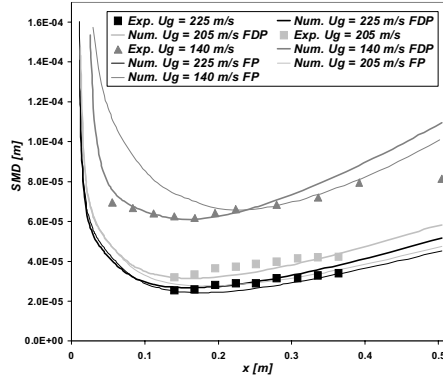


Figure 1. Axial distribution of droplet SMD for different inlet U_{air} values.

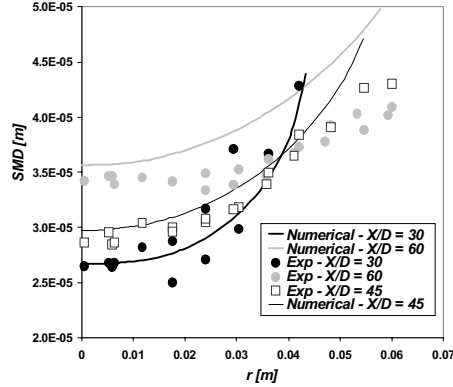


Figure 2. Radial distribution of droplet SMD for $U_{air}=225 \text{ m s}^{-1}$.

The simulated atomiser (Hopfinger and Lasheras, 1994) considered in this work consisted of a round water jet issuing from a nozzle of $D_l = 3.5 \text{ mm}$ diameter, with a coaxial high speed air flow passing through an annulus of outer diameter of $D_{air} = 5.6 \text{ mm}$.

4. Results and Discussion

The values of the constants in Eqs. (3) and (4) providing the best agreement with measurements were found for one particular set of conditions as $C_r = 0.73$ and $C_l = 4.38$. These values were then kept unchanged for all subsequent simulations. Figure 1 presents a comparison of calculated and measured (Hopfinger and Lasheras, 1994; Lasheras et al., 1998) droplet SMD values on the flow centre-line for different inlet air velocities. The conditions at the nozzle exit were not measured, therefore two sets of calculations were undertaken to verify the sensitivity of predictions to these inlet conditions. Calculations performed assuming uniform velocity profiles at the injector exit are shown as thin lines, denoted FP in the figure legend, with thick lines showing the results obtained with the exit profiles corresponding to fully-developed round pipe turbulence (FDP in the legend). For the strongest atomisation, $U_{o,g} = 225 \text{ m s}^{-1}$, the nozzle exit velocity profile has a very limited effect on the results. However, its importance increases with decreasing air velocity. For small gas velocities, the use of a uniform inlet velocity profile results in primary atomisation rate significantly slower than was observed by Lasheras et al. (1998). This is hardly surprising as the nozzles used in obtaining measurements were made using pipes that were sufficiently long to give rise to flows that most likely corresponded to fully developed pipe flow on exit. It is also appropriate to note that in the model used in this work the primary atomisation rate is governed solely by turbulent straining of the liquid surface. Turbulence generation is sensitive to the inlet velocity profile employed, and this explains the unrealistically slow primary atomisation predicted when using an unrealistic injector exit condition. Unfortunately, no measurements of turbulence quantities are available for the test cases considered, and this precludes a direct verification of the $k-\epsilon$ model predictions. However, indirect support is provided by the fact that the spreading rate of the jet is predicted with reasonable accuracy. This can be seen in Figure 2 which compares measurements (Hopfinger and Lasheras, 1994) and predicted radial profiles of SMD, calculated with a fully-developed inlet profile, for an air jet velocity of 225 m s^{-1} .

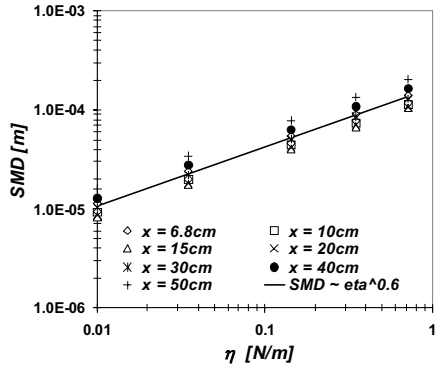


Figure 3. Power-law dependence of droplet SMD on surface tension η .

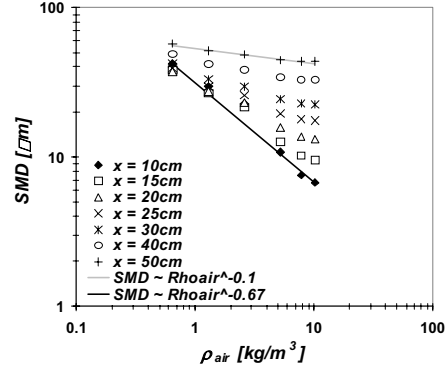


Figure 4. Power-law dependence of droplet SMD on air density ρ_{air} .

Figure 3 presents calculated SMD values obtained by varying the surface tension η by a factor of 80. Practically, the surface tension is reduced at conditions approaching the liquid critical state, e.g. with temperature and pressure rise. The distribution of temperature is usually very non-uniform inside a typical industrial combustion chamber; therefore a predictive atomisation model should be able to account for wide variations in η . The modelling results in $SMD \propto \eta^{0.6}$, in excellent agreement with Eq. (7), while other experimentally observed exponents generally range between 0.5 and 0.7 (Lefebvre, 1980).

Turbulence is generated by the shear between the high velocity co-flow gas and the low velocity liquid jet. The gas velocity affects the atomisation strongly, and the corresponding exponent measured by Lasheras et al. (1998) is close to -1.7, while Eq. (7) predicts a value of -2.2. The modelling results of the present work predict $SMD \propto u_{0,g}^{-5/3}$, in close agreement with the more recent measurements. It should be noted that the present results also show that variations in gas velocity do have a considerable effect upon the flow pattern and turbulence properties, and change a number of other factors such as momentum and mass flux ratios in an interdependent way.

Figure 4 presents the droplet SMD calculated using different values of the air/gas density. It can be clearly seen that the exponent α_g in $SMD \propto \rho_g^{\alpha_g}$ is not constant over the entire flow domain, indeed, near the injector $SMD \propto \rho_g^{-2/3}$ while further downstream $SMD \propto \rho_g^{-1/10}$. Decreases in air density result in poorer atomisation (Lefebvre, 1980), and this effect is clearly captured both qualitatively and quantitatively by the present model.

Similar results were obtained when varying the liquid density. The Eq. (7) results in $SMD \propto \rho_{liq}^{11/10}$ if the liquid density is changed, provided all other variables are kept the same. It also gives $SMD \propto \rho_{liq}^{1/10}$ if the density is changed and the liquid/gas mass flux ratio is kept constant. The calculation yields SMD values approximately independent of liquid density near the injector, in line with the latter expression, while further downstream SMD scales approximately as $SMD \propto \rho_{liq}^{3/5}$.

The observed lack of a single value of an exponent in $SMD \propto \rho_g^{\alpha_g} \cdot \rho_{liq}^{\alpha_{liq}}$ suitable for the entire flow field also deserves comment. Indeed, a vast number of formulae similar to Eq. (7) have been proposed, both for droplet size and liquid core length, e.g. Reitz and Bracco (1982). The present model assumes that the only mechanism for the primary atomisation is the flow turbulence, and the liquid or gas density affects the atomisation quality only in as far as it affects the turbulence. The influence of the flow field and turbulence inside the nozzle itself on the atomisation process, taken into account through the inlet conditions in the calculations, is the most likely explanation for the effect of nozzle geometry observed in practice (Reitz and Bracco, 1982; Lefebvre, 1980).

5. Conclusions

The predictive capability of an Eulerian atomisation model, originally proposed by Vallet et al. (2001), has been demonstrated for air-assisted atomisers. The influence of injector exit velocity profile, surface tension, gas velocity, and liquid and gas densities on predictions of the model has been examined, and results found to be in good agreement with experimental data. There is a need for more detailed data on atomising flows, particularly in regard to gas-phase turbulence properties, to permit a more rigorous validation of the present model.

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