Model for the Prediction of Internal Flow Conditions in Pressurised Metered Dose Inhalers (pMDIs)

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Summary

The mechanics of flow of propellant through the twin orifice of pMDIs (pressurized metered-dose inhalers) is complex and poorly understood. The quantitative prediction of flow variables inside pMDIs, from a fundamental point of view remains elusive due to the complex, unsteady, multiphase fluid dynamics that occurs in these devices. The present paper sets out the basis of an new numerical model which can provide deeper insight into the fluid mechanics inside the twin orifice of pMDIs and is capable of predicting the mass flow rate together with the flow variables (pressure, velocity, vapour mass fraction, etc.). A key improvement offered by the proposed method is an account of propellant metastability. The findings of the model are compared with steady flow results reported by Fletcher (1975) and Clark (1991).

Introduction

Pressurized metered-dose inhalers (pMDIs) are the most common devices, around the world, for therapeutic aerosol delivery to the lungs in the treatment of asthma, bronchitis, cystic fibrosis and other pulmonary diseases. However, the mechanics of flow of propellant through the twin orifice of pMDIs is complex and poorly understood, involving a transient cavitating turbulent fluid that flashes into rapidly evaporating droplets. Although certain aspects of the flow in the twin orifice of pMDI are understood, an understanding of the detailed mechanics of the flow through the twin orifice of pMDI remains elusive due to the difficulty of performing experiments at the small length scales and short time scales. The existing empirical or semi-empirical models of flashing flow of propellants through twin orifice of pMDIs are based on modifications of the orifice flow equation along with thermodynamic equilibrium in the metering and expansion chambers (Fletcher (1975), Clark (1991). However, there are known limitations in the description of the physical processes and the models contain empirical correction factors in the predictions of mass flow rates and droplet diameter at the actuator nozzle exit. This may make it difficult to extrapolate the findings of these seminal works beyond the range of formulations and geometries for which the theory was developed. There would be clear benefits to the industry if an accurate generalized model for the flow of propellant mixtures were available for twin orifice systems, such as the pMDIs.

This paper presents a new numerical model, which includes an account of metastability or inhibited propellant evaporation and provides deeper insight into the fluid mechanics inside the twin orifice of pMDIs. It predicts the mass flow rate together with the flow variables (pressure, temperature, quality, void fraction, etc) inside the twin orifice of pMDI and can deal with pure propellants or propellant mixtures. The model is validated against the experimental results from Fletcher (1975) and Clark (1991).

Mathematical Modelling

The flow of propellant inside the twin orifice system is assumed to be in two phase metastable region, i.e. the propellant exists in three phases: metastable liquid, saturated liquid and vapour. The model uses the following assumptions:

- One dimensional steady state adiabatic flow.
- The fluid properties are assumed to be equal to those of the propellant (REFPROP v7.0, 2002).
- Kinematic equilibrium between the phases: liquid and vapour velocities are locally equal ($U_l = U_v = U$).
- The effect of surface tension is neglected: pressure of liquid and vapour phase are locally equal ($p_l = p_v = p$).
- The flow model is based on the one-dimensional conservation equations for mass, momentum and energy.

Metastability effects are included in the model using the Delayed Equilibrium Method (DEM) outlined by Feburie (1993) and Attou and Seynhaeve (1999). The basics of the method can be best understood by considering the conceptual two-orifice system sketched in Figure 1.

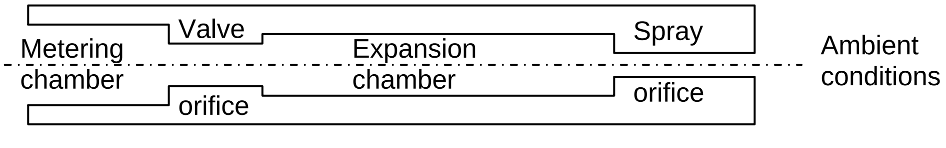

Figure 1: Two-orifice system

The present paper discusses steady state (i.e. continuous) discharge only. The fluid in the metering chamber enters the valve/upstream orifice in a known state. In the case studies reported here the propellant is saturated liquid, but the model is not limited to such flows. As the fluid enters the valve orifice, the saturated liquid is converted to metastable liquid due to the sudden pressure drop across the abrupt contraction. In the two-phase metastable state, the Delayed Equilibrium Model (DEM) proposed by Feburie et. al (1993) is used. According to this model, evaporation does not instantaneously produce a saturated mixture, but only a fraction *y* (the so-called vaporization index) of the propellant is transformed into saturated mixture, the other fraction *1-y* remains metastable liquid and is submitted to an isentropic evolution. In the flow direction *z* a conversion of metastable fluid into saturated fluid will take place, which is evaluated using a relaxation equation. The constant determining the rate of return to saturated conditions is dependent on the difference between the local pressure *p*, saturation pressure p_s at the fluid temperature, on the critical pressure p_c of the propellant. The relevant length scale is *P/A* where *A* is the cross-sectional area of the orifice or chamber and *P* is the perimeter length:

$$\frac{dy}{dz} = 0.02\frac{P}{A}(1-y)\left[\frac{p_s - p}{p_c - p_s}\right]^{0.25} \tag{1}$$

Evaluation of empirical coefficients

The friction factor is calculated from the Churchill's expression [cited by Lin et al. (1991)] using Dukler's viscosity model (Dukler et al. 1964). The pressure drop and recovery associated with a sudden contraction and sudden expansion for two-phase conditions is evaluated using equations given in ESDU reports (Report No. 05024 and 89012). The flow is critical when the propellant velocity reaches sonic velocity and the two phase mach number is unity. The sonic velocity is evaluated using the Attou and Seynhaeve (1999 a) equations. In case of choked flow at the exit of the spray orifice, discharge shock wave proposed by Escanes et al. (1995) is solved.

Numerical Solution

The numerical solution scheme subdivides the domain into N control volumes (CV). The method suggested by Escanes et al. (1995) is applied to generate a non-uniform grid for the valve and spray orifice and a uniform grid is generated for the expansion chamber. For each CV, a set of algebraic equations is obtained by the discretization of the governing equations. The values of the flow variables at the CV outlet section are obtained by solution of this set of equations, from the known values at the CV inlet section and the “current” mass flow rate. The solution procedure marches forward in the flow direction from the metering chamber to the spray orifice exit. At this point, the calculations are terminated and the computed discharge pressure is compared with the actual value. If the difference is greater than a preset tolerance the mass flow rate is adjusted and the solution procedure is restarted at the entrance of the tube until the calculated value agrees with the actual exit pressure.

Results and Discussion

In this section, two sample results obtained from the numerical procedure for spray orifice diameters of 350 μm and 479 μm, respectively, are compared with the experimental results of Fletcher (1975) and Clark (1991). Grid independence was achieved with the following numerical parameters: N (Total Number of Nodes) = 700 (Number of nodes in valve and spray orifices are 300 and the number of nodes in the expansion chamber are100). The conditions for the experimental results presented by Fletcher(1975) and Clark (1991) for the continuous flow through the twin orifice systems given in Table 1.

Table 1 Flow conditions

Nozzle	D_{vo} (μm)	L_{vo} (μm)	D_{so} (μm)	L_{so} (μm)	D_{ec} (mm)	L_{ec} (mm)	T_{in} (°C)	p_{dis} (bar)	Propellant
Fletcher	320	420	350	400	3.2	12.7	19.7	1.01325	R12/R11 (60%/40%)
Clark	420	542	479	1000	3.8	11	18	1.01325	R134a

The mass flow rates calculated for above cases are 2.789 Kg/h and 5.58 Kg/h against the experimental results 2.772 and 5.62 respectively, offering a relative discrepancy of 0.613% and -0.712%. The negative sign indicates over prediction of the mass flow rate against the experimental mass flow rate. The mass flow rates are also evaluated for all orifice combinations of Fletcher's thesis(1975). The evaluated mass flow rates were in good agreement with the experimental mass flow rates offering a relative discrepancy of -3.8% where as Fletcher's (1975) theoretical model under predicted the mass flow rates up to 14% for the orifice diameter ratio $D_{vo}/D_{so} \leq 1$

Figure 2 (a and b) and Figure 3 (a and b) show the distribution of flow variables across the twin orifice system for Fletcher and Clarks cases respectively. The sudden pressure drop (Figure 2a and Figure 3a) at the inlet is due to abrupt contraction at the entrance of the valve orifice. Then the pressure decreases across the valve orifice. The pressure almost remains constant inside the expansion chamber. Large pressure drop at the entrance of the

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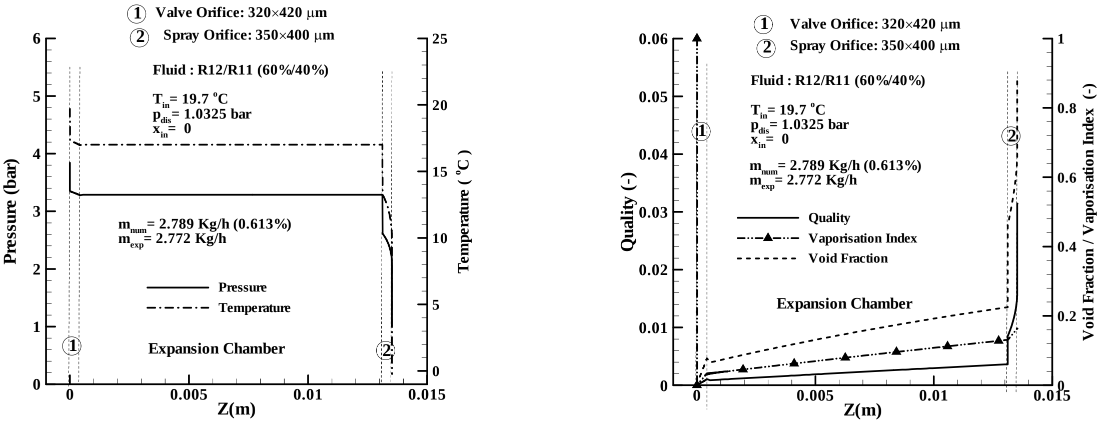
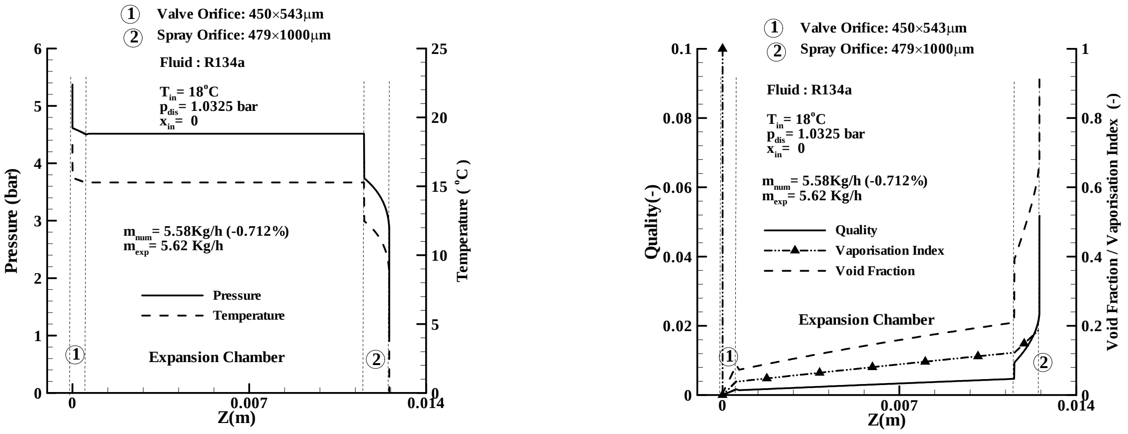


(a) Pressure and Temperature Distribution (b) Quality and Void fraction Distribution

Figure 2 Distribution of flow variables across the twin orifice system for the Fletcher’s nozzle



(a) Pressure and Temperature Distribution (b) Quality and Void fraction Distribution

Figure 3 Distribution of flow variables across the twin orifice system for the Clark’ s nozzle

spray orifice is due to rapid fluid acceleration and abrupt contraction at the entrance to the spray orifice. The pressure of the propellant, drops along the spray orifice due to the frictional and acceleration effects. The large pressure drop at the exit plane of the spray orifice indicates that the flow is choked at the exit. As the fluid inside the twin orifice system is in two phase metastable state, the temperature of the superheated liquid has been assumed constant (Feburie et al.,1993) and therefore, two temperatures has to be distinguished, the superheated liquid temperature (T_{lm}) and the saturation liquid or gas temperature (T_{equil}). For this reason, an averaged temperature has been defined as:

$$T = \frac{T_{equil} + T_{lm}}{2} \qquad (2)$$

From the above figures, it can be seen that the temperature has similar profile of that of pressure.

Figure 2b and Figure 3b show the distribution of quality, vaporisation index and void fraction along the twin orifice system. The quality increases inside the valve orifice due to start of vapour formation. It increases gradually inside the expansion chamber. The sudden increase in the quality at the inlet of the spray orifice is due to abrupt contraction Then the quality increases non-linearly inside the spray orifice as more metastable liquid gets converted into saturated mixture. It increases rapidly at the exit as the flow reaches to the critical condition. From the Figure 2b and Figure 3b, it is seen that y = 1 at the inlet, i.e. propellant is saturated. As expected, y is much smaller than 1 in the valve and spray orifice indicating that the evaporation process cannot keep pace with the rapid changes in the flow. It should also be noted that y varies between 0.07 and 0.17 in the expansion chamber. This indicates that, in spite of the considerable residence time of the fluid inside the expansion chamber, it remains in a metastable state that is far from the thermodynamic equilibrium state assumed by Fletcher and Clark. The void fraction has same profile as that of quality. From the above figures, it is clear that very rapid acceleration of mixture take place at the exit of the spray orifice, where the sudden and very large pressure drop takes place. This is expected to play a major role in the flash atomisation and subsequent formation of aerosol droplets.

The distinctive elements of the current model are: (i) an account to metastability pointing to non-homogeneous conditions in the expansion chamber and propellant evaporation inside the valve and spray orifices, (ii) the resolution of distributions of pressure and quality/void fraction etc. inside the valve and spray orifice. Fletcher (1975) assumed thermodynamic equilibrium conditions in the expansion chamber neglecting the metastability. Clark (1991) also assumed equilibrium conditions in the expansion chamber and applied a correction for metastability in the expansion chamber in an ultimately unsuccessful attempt to account for the discrepancies between theoretically predicted and experimentally measured pressure and temperatures.

Figure 2b and Figure 3b show that the quality increases slowly in the expansion chamber and significantly inside the valve orifice, expansion chamber and the spray orifice. This challenges the accuracy of the assumptions made in previous models of homogeneous conditions in the expansion chamber and frozen flow inside the valve orifice and spray orifice. The relaxation equation used to trace metastability has a strong track record of applications is steam-water flows (Feburie et al.,1993) and has been well validated for the flow of propellants through long capillary tubes (Garcia-Valladares et al.,2002a and 2002b). A further advantage of the current solution procedure is the absence of semi-empirical coefficients that require case-by-case adjustment.

Conclusions

A delayed equilibrium model for propellant two-phase flow inside the twin orifice has been developed using the steady-state, one-dimensional governing equations (continuity, momentum and energy) and correlations given by Feburie et al. (1993) to evaluate the vaporisation index in a two-phase metastable region. The findings of the model were compared with steady flow results reported by Fletcher (1975) and Clark (1991) and showed excellent agreement with these experiments. The new numerical model presented here provides deeper insight into the events taking place inside the twin orifice system which forms the basis of pMDIs. A key improvement offered by the proposed method is its account of propellant metastability or inhibited evaporation, which has the potential to alter the atomisation conditions at the actuator orifice considerably. Furthermore, the numerical formulation of the method enables the computation of the distributions of pressure, velocity and vapour content along the orifice axis. Such detailed information of the flow conditions would be necessary for the prediction of surface generation and flow regime change in the actuator orifice of pMDI's, which themselves are essential steps towards the development of improved atomisation models.

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