Development of Discrete Population Balance Mixture Atomization Model

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Abstract
Eulerian mixture models of atomization of the type developed by Borghi and coworkers have been proposed to provide a unified description of primary and secondary atomization. These models represent the atomization process through a single evolution equation for a quantity proportional to the total droplet surface area. The present work extends mixture atomization models by using a discrete population balance approach to atomization. In this methodology the liquid phase is divided into a finite number of size classes and atomization is treated as a process of mass transfer from larger to smaller size classes. The balance laws associated with this concept are combined with an idealized description of the atomization process to create a set of governing equations. These equations are then employed to make predictions for atomizing jet flows. The predicted results are used to investigate the issue of the minimum number of size classes required for an accurate description of the atomization process.

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Introduction

Eulerian mixture models of liquid spray atomization have been proposed in [1-4] to provide a unified description of primary and secondary atomization without going into all the details of poorly understood aspects of atomization. These models represent the atomization process through a single evolution equation for a quantity proportional to the total droplet surface area.

The present work extends mixture spray atomization models by using a discrete population balance approach to atomization. In this methodology the liquid phase is divided into a finite number of drop size classes and atomization is treated as a process of mass transfer from larger to smaller size classes. The balance laws associated with this concept are combined with descriptions of the atomization process to create a set of governing equations. These equations are then employed to make predictions for atomizing liquid sprays. The predicted results are used to investigate the issue of atomization to create a set of laws associated with this concept are combined with transfer from larger to smaller size classes. The balance equations and atomization is treated as a process of mass.

In addition, it is shown that under certain circumstances an evolution equation for a single quantity characteristic of the drop size distribution somewhat analogous to those used in [1-4] can be derived from the formulation developed herein. This is done by following a suggestion made in [5] in a somewhat different context.

Governing Equations

For a system of M+1 phases, with the 0th phase being the gas and the other M phases being drop size classes, the respective mass and linear momentum balance laws for a mixture model of the atomizing system can be written as

$$\partial_t \rho + \nabla \cdot (\rho \vec{v}) = 0$$  \hspace{1cm} (1)

and

$$\rho D_i \vec{v} = \nabla \cdot \sigma + \vec{f}$$  \hspace{1cm} (2)

where

$$\rho = \sum_{i=0}^{M} \rho_i \phi_i,$$  \hspace{1cm} (3)

$$\vec{v} = \sum_{i=0}^{M} \left( \rho_i \phi_i \vec{v}_i / \rho \right),$$  \hspace{1cm} (4)

$$\vec{f} = \sum_{i=0}^{M} \vec{f}_i / \rho,$$  \hspace{1cm} (5)

and

$$\sigma = \sum_{i=0}^{M} (\sigma_i - \rho_i \phi_i \vec{u}_i \cdot \vec{u}_i)$$  \hspace{1cm} (6)

are the respective mixture density, mixture velocity, mixture body force, and mixture stress, t is time, $\vec{v}$ is the gradient operator, and $D_i = \partial_i + \vec{v} \cdot \nabla$ is the convective derivative. Here $\rho_i$ is the i’th phase true mass density, $\phi_i$ is the i’th phase volume fraction (ratio of i’th phase volume to mixture volume), $\vec{v}_i$ is the i’th phase velocity vector, $\sigma_i$ is the i’th phase body force, and $\vec{u}_i$ is the i’th phase diffusive velocity. The definition (6) of mixture stress is consistent with that suggested in [6] but is not the only possibility. An alternative employed in [7] is to treat the mixture stress as being the sum of the phasic stresses only and regard the sum of the terms involving diffusive velocities as determined separately. A discussion of possible definitions of mixture stress is given in [8]. The definition (6) is selected herein for consistency with [1-4].

In the present work, also for consistency with [1-4], the Newtonian constitutive equation

$$\sigma = -p \vec{l} + \mu (\nabla \vec{v} + (\nabla \vec{v})^T)$$  \hspace{1cm} (8)

for mixture stress will be employed where $\mu$ is an effective dynamic viscosity containing a turbulent contribution, p is the pressure, $\vec{l}$ is the unit tensor, and a superposed T denoted the transpose of a second order tensor. Substituting (8) into (2) produces

$$\rho D_i \vec{v} = -\nabla p + \vec{v} \cdot (\mu (\nabla \vec{v} + (\nabla \vec{v})^T)) + \vec{f}$$  \hspace{1cm} (9)

Mass balances for the individual phases can be written in terms of the respective i’th phase mass concentration

$$c_i = \rho_i \phi_i / \rho,$$  \hspace{1cm} (10)

and diffusive mass flux

$$\vec{j}_i = \rho_i \phi_i \vec{u}_i$$  \hspace{1cm} (11)

as

$$\rho D_i c_i = -\nabla \vec{j}_i + \sum_{j=0}^{M} s_{ij}$$  \hspace{1cm} (12)

The atomization mass transfer process involves only the drop size classes. Thus, the second term on the right hand side of (12) vanishes for the gas and its summation starts at unity for the drop size classes.

Following the work of [9-16] the source term in (12) will be written in the standard form
\[
\sum_{i=1}^{M} s_{ij} = \rho (-\Gamma_i c_i + \sum_{j=1}^{i} m_{ij} \Gamma_j c_j)
\]  
(13)

where \( \Gamma_i \) is the \( i \)'th drop size class atomization frequency (time rate of atomization) and \( m_{ij} \)'s are the volume distribution coefficients (fraction of \( j \)'th drop size class volume transferred to \( i \)'th drop size class per \( j \)'th drop size class atomization event). In writing (13) it is assumed that drop sizes are arranged in order of descending volume and that mass transfer is allowed only from larger to smaller drop size classes. Accounting for the latter while allowing for self atomization requires the sum in (13) to terminate at \( i \) rather than \( M \).

For consistency with [1-4] the gradient diffusion model

\[
\ddot{j}_i = -\rho D \nabla \bar{c}_i
\]  
(14)

is selected with \( D \) being a diffusion coefficient common to all phases and containing a turbulent component. Substituting (13) and (14) into (12) yields

\[
\rho D_t c_0 = \bar{\nabla} \cdot (\rho D \bar{\nabla} c_0)
\]  
(15)

for the gas and

\[
\rho D_t c_i = \bar{\nabla} \cdot (\rho D \bar{\nabla} c_i) + \rho (-\Gamma_i c_i + \sum_{j=1}^{i} m_{ij} \Gamma_j c_j)
\]  
(16)

for the drop size classes. Summing (16) over all drop size classes, adding (15) to the result, and taking account of the fact that all concentrations must add to unity leads to constraint

\[
\sum_{i=1}^{M} m_{ij} = 1
\]  
(17)

This can be interpreted as a statement of volume conservation associated with a single atomization event.

Defining the total liquid mass concentration as

\[
c = \sum_{i=1}^{M} c_i
\]  
(18)

summing (16) over all drop size classes, and using (17) leads to the liquid mass balance

\[
\rho D_t c = \bar{\nabla} \cdot (\rho D \bar{\nabla} c)
\]  
(19)

Equation (10) can be combined with the fact that all volume fractions must sum to unity to yield

\[
1/\rho = (1-c)/\rho_c + c/\rho_d
\]  
(20)

where \( \rho_c \) is the gas density and \( \rho_d \) is the liquid density.

Equations (1), (9), (19), and (20) together with the equations describing an appropriate turbulence model (which will not be discussed herein) constitute a determinate system of equations to solve for \( p, \bar{v}, \) and \( c \) without a knowledge of the atomization process (large scale problem in the terminology of [1-4]). Once these variables have been determined, (16) can be solved to characterize the atomization process (small scale problem in the terminology of [1-4]). This is an example of the independence of large scale phenomena from small scale phenomena discussed in [1-4]. It is important to note that this property is not a general characteristic of models of this kind but depends critically on the use of (6) and (14).

Characterization of the atomization process is an important research area in and of itself and no attempt will be made herein to make a contribution thereto. Instead, a simple idealized model consistent with previous publications such as [9] and [13-16] will be employed. In this model the atomization frequency is represented by the separable form

\[
\Gamma_i = \Gamma_0 \gamma_i \Gamma_1
\]  
(21)

with \( \Gamma_0 \) being a constant having the dimensions of inverse time; \( \gamma \) being a dimensionless function of position, flow conditions, etc.; and \( \Gamma_i \) being a dimensionless function of drop volume \( x_i \). Other elements of the model will be introduced subsequently as needed.

Global Drop Size Measures

It is of interest to identify global drop size measures. Two such measures, the Sauter mean volume (SMV) and the average volume (AV), will be presented in this section.

The SMV is defined by

\[
x/x_1 = \left\{ \frac{c/\sum_{i=1}^{M} (c_i (x_1/x_i)^{1/3})^3}{\sum_{i=1}^{M} N_i x_1 / (\sum_{i=1}^{M} N_i x_i^{2/3})^3 / x_1} \right\}
\]  
(22)

where

\[
N_i = \rho c_i / \rho_l x_i
\]  
(23)

is the number density of \( i \)'th phase. A spherical drop having the SMV would have the Sauter mean diameter.

The AV is defined by

\[
x/x_1 = \left\{ c/\sum_{i=1}^{M} (c_i x_1 / x_i) \right\} \left( \sum_{i=1}^{M} N_i x_1 / (\sum_{i=1}^{M} N_i) / x_1 \right)
\]  
(24)

This definition is motivated by a desire to make contact with [5].

Some atomization models have a vanishing smallest drop size class (\( x_0 = 0 \)). This creates an ambiguity in (22) and (24) because \( N_M \) is finite and \( c_M =
\[ \rho \Delta x M N_M/\rho = 0 \] simultaneously. Thus, the concentration forms of (22) and (24) become indeterminate. The number density form of (22) shows that the summation actually ends at \( i = M - 1 \), resolving the indeterminacy in the concentration form so that either can be used. The indeterminacy in the concentration form of (24) cannot be resolved and the number density form must be used. Based on these observations it can be inferred that a completed atomization process will result in an SMV and AV of \( x_M \) for a finite \( x_M \) or an SMV of \( x_{M-1} \) and an AV of zero for a vanishing \( x_M \).

It is now desired to develop a single evolution equation for a quantity related to AV. This will be done using an approach similar to that first reported in [5] in the context of a continuous population balance model.

It is convenient to combine (23) and the concentration form of (24) into

\[ X = c/\sum_{i=1}^{M}(\rho_i N_i/\rho) = 1/S \] (25)

and (16) and (23) into

\[ \rho D_t (\rho_i N_i/\rho) = \vec{\nabla} \cdot (\rho D \vec{\nabla} (\rho_i N_i/\rho)) + \rho(\vec{c}_i (\rho_i N_i/\rho)) \sum_{j=1}^{i} n_{ij} \Gamma_i(\rho_i N_i/\rho) \] (26)

where

\[ n_{ij} = m_{ij} x_i/x_i \] (27)

are the number exchange coefficients (number of j’th size class drops transferred to i’th drop size class per j’th drop size class atomization event). Summing (26) over all drop sizes and assuming that the atomization model satisfies Kolmogorov’s hypothesis (number of drops formed from an atomization event of any drop size class is independent of that size class) results in

\[ \rho D_t \sum_{i=1}^{M}(\rho_i N_i/\rho) = \vec{\nabla} \cdot (\rho D \vec{\nabla} \sum_{i=1}^{M}(\rho_i N_i/\rho)) + \rho(n-1) \sum_{i=1}^{M} \Gamma_i(\rho_i N_i/\rho) \] (28)

where

\[ n = \sum_{i=1}^{M} n_{ij} \] (29)

is the number of drops produced due to single atomization event (same for all drop size classes).

Let

\[ \hat{\Gamma}_i = (x_1 - x_M)/(x_1 - x_M) \] (30)

which reflects the common phenomenology that atomization frequency decreases with decreasing drop size and ensures that the atomization frequency of smallest drop size class vanishes (as it must). Then substituting (25) into (28) and using (19) and (21) leads to

\[ \rho D_t S = \vec{\nabla} \cdot (\rho D \vec{\nabla} S) + \rho \Gamma_y (n-1) (1-x_M S)/(x_1 - x_M) \] (31)

which is the desired single evolution equation for the inverse of AV. This equation becomes determinate once the solution to the large scale problem is known. In this case the evolution equation is not postulated but derived from the discrete population balance equations.

**Thin Layer Equations**

It is now desired to discuss the thin layer forms of the governing equations derived previously applicable. Consider an axisymmetric steady flow in the absence of body forces described by cylindrical polar coordinates \( r \) and \( z \) with the z axis being the axis of symmetry. Let the transverse \( r \) velocity component be denoted by \( u \), the axial \( z \) velocity component be denoted by \( w \), and the axial pressure gradient be denoted by \( P \). Carrying out the standard boundary layer order of magnitude analysis on equations (1), (9), (19), (16), and (31) leads to

\[ \partial_z (r^\delta u) + \partial_r (r^\delta pw) = 0 \] (32)

\[ \rho (u \partial_z w + w \partial_z w) = -P + \partial_z (r^\delta \mu \partial_z w)/r^\delta \] (33)

\[ \rho (u \partial_r c + w \partial_z c) = \partial_r (r^\delta \rho D \partial_r c)/r^\delta \] (34)

\[ \rho (u \partial_r c_1 + w \partial_z c_1) = \partial_r (r^\delta \rho D \partial_r c_1)/r^\delta + \rho(\vec{c}_1 + \sum_{j=1}^{M} m_{ij} \vec{c}_j) \] (35)

and

\[ \rho (u \partial_z S + w \partial_z S) = \partial_r (r^\delta \rho D \partial_r S)/r^\delta + \rho \Gamma_y (n-1) (1-x_M S)/(x_1 - x_M) \] (36)

with \( \delta = 1 \). Equations (32-36) also contain the corresponding governing equations for steady flow in a plane thin layer, which can be recovered by setting \( \delta = 0 \). These equations apply to all thin layer flows (ducts, jets, wakes, boundary layers, etc.). For liquid thin jet spray atomization \( P \) is a known quantity. First (20), (32), (33), and (34) (large scale problem) can be solved for \( u, w, \) and \( c \). Then (35) (one version of small scale problem) can be solved to determine the \( c_j \)’s and (36) (another version of small scale problem) can be solved to determine \( S \) for atomization models obeying Kolmogorov’s hypothesis.

**Analytical Solution**

Numerical solutions for jet spray atomization have been reported in [1-4]. Instead of presenting more solutions of this kind, attention will be focused herein on a special atomization model which leads to closed form solutions.
Let
\[ \gamma = w/w_o \]  
\hfill (37)

(\(w_o\) being a velocity characteristic of the nozzle exit conditions). Substituting (37) and the separable form
\[ c_i(r, z) = c(r, z)g_i(z) \]  
\hfill (38)

into (35) and defining the dimensionless axial coordinate
\[ \xi = \Gamma_0 z/w_0 \]  
\hfill (39)

measuring distance downstream from the nozzle exit leads to
\[ g'_i = -\bar{f}_i g_i + \sum_{j=1}^{i-1} m_{ij} \bar{f}_j g_j \]  
\hfill (40)

where a superposed prime denotes differentiation with respect to \(\xi\). These equations have a form similar to Reid’s grinding equations [17] except that the summation in the grinding equations stops at \(i - 1\). Nevertheless the solution presented in [17] (referred herein as Reid’s solution) can be extended to this case by rewriting (40) as
\[ g'_i = -\beta_i g_i + \sum_{j=1}^{i-1} m_{ij} \bar{f}_j g_j \]  
\hfill (41)

Where
\[ \beta_i = \bar{f}_i (1 - m_{ii}) \]  
\hfill (42)

The appropriate extension of the closed form solution given in [17] to (41) is
\[ g_i = \sum_{k=1}^{i} A_{ik} \exp(-\beta_i \xi) \]  
\hfill (43)

with the coefficients appearing in (43) being given by the recurrence relations
\[ A_{ik} = \begin{cases} \sum_{j=1}^{i-1} m_{ij} \bar{f}_j A_{jk} / (\beta_i - \beta_k) & \text{for } k \neq i \\ g_{i0} - \sum_{j=1}^{i-1} A_{ij} & \text{for } k = i \end{cases} \]  
\hfill (44)

and \(g_{i0}\) being the value of \(g_i\) at \(\xi = 0\). In the present model spray atomization is initiated by having all liquid in the largest size class at the nozzle exit. Thus
\[ g_{i0} = \begin{cases} 1 & \text{for } i = 1 \\ 0 & \text{otherwise} \end{cases} \]  
\hfill (45)

Substituting (38) into the mass concentration form of (22) yields
\[ x/x_1 = (1/\sum_{i=1}^{M} (g_i(x_1/x_i)^{1/3}))^3 \]  
\hfill (46)

Thus, in this special case, SMV is independent of radial position in the spray and can be determined in closed form without any information about large scale features of the flow field.

Up until this point the developments in this section are independent of the specific form of \(\bar{f}_i\). However the closed form solution for AV to be presented in the next paragraph is possible only when (30) is applicable.

Substituting (37) into (36) and using (39) reveals that \(S\) is independent of \(r\) and governed by
\[ S' = (n - 1)(1 - x_M S)/(x_1 - x_M) \]  
\hfill (47)

which must be solved subject to the initial condition
\[ S(0) = 1/x_1 \]  
\hfill (48)

This produces the closed form solutions for AV
\[ X/x_1 = 1/(x_1/x_M + (1 - x_1/x_M) \exp(-(n - 1)x_M \xi/(x_1 - x_M))) \]  
\hfill (49)

for \(x_M \neq 0\) and
\[ X/x_1 = 1/(1 + (n - 1)\xi) \]  
\hfill (50)

for \(x_M = 0\). Like SMV, AV is independent of radial position in the spray and can be determined in closed form without any information about large scale features of the flow field in this special case.

In thin layers \(w \gg u\) and \(w\) can be thought of as a measure of the kinetic energy of the flow. Thus, the atomization frequencies being proportional to the axial velocity are indicative of a mechanism in which atomization increases with increasing kinetic energy. This is certainly plausible, but no attempt will be made herein to relate such a mechanism to any specific atomization process. For the purposes of the present work the important point is that this mechanism facilitates the development of a closed form solution for SMV. This, in turn, creates the possibility of investigating size class convergence (number of drop size classes needed to achieve an accurate solution) without extensive numerical computation. That issue is important no matter what atomization model is used.

**Results and Discussion**

It should be noted that, for a given atomization model, (41) and (47) contains no parameters. Thus the results to be discussed in this section have certain universality. A complete atomization model is required to make these equations fully determinate. The model selected herein consists of (30), (37), and...
These volume distribution coefficients are based on the work of [18]. The authors of this paper started with a continuous population balance model having the properties that each atomization event produced two drops and all combinations of resulting drop sizes were equally likely and then discretized the model using a fixed pivot technique to obtain the equivalent of (51). Satisfaction of (17) requires that \( x_M \) be zero. When this is true the model satisfies Kolmogorov’s hypothesis (with \( n=2 \)) and the summation in (46) terminates at \( M-1 \) (to eliminate the ambiguity as discussed earlier). Because (30) and (51) involve only ratios of drop sizes, the largest size can be taken to be unity without loss of generality.

Equation (51) is correct for any distribution of drop sizes. The issue of optimizing non-uniform size distributions in order to minimize the number of size classes required to obtain an accurate solution is of current interest but will not be addressed here. Instead, a uniform size distribution (sometimes called arithmetic) is used to avoid biasing size class convergence studies. Some typical results pertinent to this matter are presented in Figures 1-6. As indicated earlier, all these predictions are independent of the specifics of the atomizing liquid jet configuration because of the special atomization model employed herein.

The most straightforward procedure is to use an arithmetic progression of drop sizes in the entire size range between \( x_M = 0 \) and \( x_1 = 1 \). Figures 1 and 2 are based on this approach.

Figure 1 depicts four representative normalized centerline drop size class mass fraction (i mass per liquid mass) axial distributions. As indicated by (38), each curve describes the ratio of a drop size class concentration to total liquid concentration normalized with its maximum value (to facilitate plotting on a single drawing). The mass transfer from large to smaller size classes due to atomization is clearly illustrated. The atomization process can be seen to be essentially complete as almost all the liquid has been transferred into the smallest non-zero drop size class.

Figure 2 presents typical SMV axial distributions. It can be observed that size class convergence is achieved in the depicted region. However, the fact that the smallest drop size decreases with \( M \) causes the SMV value reached at the completion of atomization to decrease with \( M \). This dependence on \( M \) decreases as \( M \) increases and is slight for the largest values of \( M \) shown in Figure 2.

Because of the phenomenon mentioned in the last paragraph, a lack of size class convergence will always be observed at a sufficiently long distance from the nozzle exit. Other calculations (not presented here) show that this is not unique to the atomization model employed herein, but is typical of a wide variety of models. This indicates that one must be careful in defining the concept of size class convergence. It can be shown that one way to define this concept unambiguously is to create a situation in which \( x_{M-2} \) and \( x_{M-1} \) are held constant as \( M \) is increased. Fixing \( x_{M-1} \) insures that the SMV at the end of atomization is independent of \( M \). Fixing \( x_{M-2} \) insures that the largest relaxation length (which controls the distance from the nozzle required to complete atomization) is independent of \( M \). Figures 3-5 are based on the approach described above with an arithmetic progression of drop sizes being used between \( x_{M-2} \) and \( x_1 = 1 \).

Figure 3 is similar to Figure 1 with the maximum distance from the nozzle being used in both to facilitate comparison. The atomization behavior is qualitatively similar in both cases but the process depicted in Figure 3 proceeds much more slowly with only 40% of the liquid being transferred into the smallest non-zero drop size class in the depicted domain. This is an example of the influence of size distribution on predictions based on the same atomization model.

Figure 4 depicts typical SMV axial variations. It can be seen that SMV is approaching the final value of \( x_{M-1} \) for all values of \( M \) in this case (see inset) and, therefore it is possible to define size class convergence unambiguously. Size class convergence appears to be reached in this case for \( M=17 \). Convergence was regarded as being achieved when SMV predictions associated with a given \( M \) differed from those associated with \( M-1 \) by 1% or less at all distances from the nozzle. Figure 5 presents the axial error variations corresponding to Figure 4.

Figure 6 shows the axial variation of the AV based on (50) (since \( x_M = 0 \) for this atomization model). As discussed earlier, this atomization model satisfies Kolmogorov’s hypothesis for all distributions of drop sizes. Thus, Figure 6 can be compared directly with both Figures 2 and 4. In both cases it can be seen that AV is smaller than SMV. Predictions made with several other atomization models (not presented here) show that this is a general result.

**Conclusion**

In the foregoing a mixture model of liquid spray atomization was extended to include a discrete population balance approach to atomization. It was shown that the use of specific constitutive equations for diffusive mass flux and mixture stress allowed the separation of small scale and large scale features observed by previous authors. It was demonstrated that for thin layer
configurations the use of a special atomization model in which the atomization frequencies are proportional to the axial velocity allows certain closed form predictions of universal applicability to be made using a slight extension of Reid’s grinding solution.

Some specific universal results were presented graphically and those pertaining to SMV distributions were used to investigate the issue of size class convergence. It was found that this concept could be defined unambiguously only for certain versions of the atomization model employed.

References
Figure 1. Normalized drop size class liquid mass fraction axial distributions (M = 11)

Figure 2. Normalized SMV axial distributions
**Figure 3.** Normalized drop size class liquid mass fraction axial distributions ($M = 11, x_{M-2} = 0.02, x_{M-1} = 0.01$)

**Figure 4.** Normalized SMV axial distributions ($x_{M-2} = 0.02, x_{M-1} = 0.01$)
Figure 5. Normalized SMV axial error distributions ($x_{M-2} = 0.02, x_{M-1} = 0.01$)

Figure 6. Normalized AV axial distribution