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Formulation of multiphase mixture models for fragmenting flows

Aditya Jayanthi, John Peddieson *

Department of Mechanical Engineering, Tennessee Tech University, Cookeville, TN 38505, USA

HIGHLIGHTS

- Formulation of multiphase mixture models of fragmentation is discussed.
- Consequences of specific constitutive choices are determined.
- Independence of large and small scale effects is investigated.
- Plug flow fragmentor closed form solutions are presented.

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ABSTRACT

The formulation of multiphase mixture models of fragmentation is discussed. It is demonstrated that choices of constitutive equations play a critical role in creating the independence of large and small scale effects exhibited by some models appearing in the literature. A model of this kind is used to make closed form plug flow fragmentor predictions which could be useful in the investigation of size class convergence.

1. Introduction

The work described herein was motivated by the papers of Vallet et al. [1], Demoulin et al. [2], Beheshti et al. [3], Lebas et al. [4], and Belhadef et al. [5] on the modeling of liquid atomization. These papers (in slightly different ways) all treated the gas/liquid mixture as a single fluid (mixture model) and postulated a single evolution equation to characterize the Sauter mean diameter (a composite drop size measure) of the atomizing liquid. These formulations were such that the large scale problem (determination of the mixture motion and the total liquid mass fraction) could be solved first and the results then used to solve the small scale problem (determination of the Sauter mean diameter distribution). This independence of large and small scale effects played a significant role in creating computationally efficient liquid atomization models that did not require a detailed knowledge of all the poorly understood aspects of the atomization process. Comparisons with experimental data appeared to be favorable. While the focus of [1–5] was on combustion related liquid atomization and based on specific special assumptions, the general methodology employed therein of using a mixture model is potentially applicable to a wide variety of convective fragmentation/agglomeration processes involving solid particles, liquid drops, or gas bubbles dispersed in a fluid. With this in mind, the present paper discusses issues related to the extension of the methodology of [1–5] by dividing the particle cloud into a finite number of size classes and treating fragmentation/agglomeration as a process of mass transfer between size classes. This modeling procedure can be called either a multiphase continuum mechanics approach or a discrete population balance approach. The former designation is selected herein for two reasons. First, the words "population balance" are often associated with the continuous population balance approach described by Ramkrishna [6]. Second, while multiphase continuum mechanics models can be derived from continuous population balance models, it is not necessary to do so. Instead they can be developed directly using only the principles of continuum mechanics. For these reasons the extensive literature on continuous population balance models and the discrete population balance and moment models that can be derived therefrom is not reviewed herein. For the sake of definiteness only the simplest case of isothermal pure fragmentation (mass transfer from larger to smaller size classes) is considered below.

* Corresponding author. Tel.: +1 931 372 3274.
E-mail addresses: aditya.amp@gmail.com (A. Jayanthi), jpeddieson@tntech.edu (J. Peddieson).

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There are a number of ways to implement a multiphase description of fragmentation ranging in complexity from mixture models (in which one velocity vector is sufficient to describe the overall mixture motion) to full multiphase models (in which each size class is assigned a separate velocity vector). A recent example of the application of the latter kind of model to liquid atomization is reported by Rayapati et al. [7], together with a brief taxonomy of multiphase models. Each type of model described in that taxonomy exhibits a unique combination of attributes such as ease of characterization, analytical complexity, computational intensity, and ability to capture physical phenomena. For example, mixture models involve less conservation equations than full multiphase models. For this reason the former are both less computationally intensive and able to capture less physical phenomena than the latter. The selection of a model for use in a given application involves tradeoffs between model attributes and requires engineering judgment. Information obtained through thorough study of all types of multiphase models is helpful in making model selection decisions. The present paper seeks to provide information of this kind by focusing on an extension (as indicated above) of the mixture formulation of [1–5] from a single evolution equation description to a multiphase description of fragmentation and the circumstances under which the independence of large scale and small scale effects exhibited by the models of [1–5] can be preserved in this process. While it is certainly not expected that mixture fragmentation models will be appropriate in all cases, the long history of successful application of mixture models to multiphase flow problems suggests that this subject is worthy of investigation.

In a multiphase fragmentation model the large scale problem remains the same as that described above while the small scale problem becomes that of determining the individual size class mass fractions (rather than the Sauter mean diameter). The independence of large and small scale effects exhibited by the models discussed in [1–5] is an inherent part of the formulations employed in those papers. It is often desirable to preserve this independence in multiphase fragmentation models (since it plays a significant role in producing computational efficiency) but it does not arise automatically therein. Instead, it must be created by specific choices of constitutive equations. Examples of this phenomenon will be discussed subsequently. Once constitutive choices creating independence of large and small effects are identified, their validity in specific applications must, of course, be addressed on a case-by-case basis.

Some fragmentation processes produce nearly continuous particle size spectra while others produce more discrete particle size spectra. In both cases the issue of size class convergence (estimating the minimum number of size classes needed to capture the essence of the fragmentation process) becomes important. While the authors intend to address this matter in detail elsewhere, two closed form solutions potentially useful for investigation of size class convergence are reported below. Each is based on a highly idealized fragmentation model and the assumption of plug flow. The corresponding configuration will be called a plug flow fragmentor herein, by analogy with the plug flow reactor well known from combustion modeling. When attempting to focus on size class convergence issues it is often helpful to simplify other aspects of the problem. Selection of a multiphase mixture (rather than a full multiphase) model is an example of one such simplification.

The remaining part of this paper is organized as follows. Section 2 discusses formulation issues. Section 3 presents closed form plug flow fragmentor solutions. Section 4 summarizes the foregoing work and reiterates important conclusions.

2. Formulation

There are two ways to produce a multiphase mixture model. One (used in [1–5]) is to directly postulate that the behavior of the multiphase system can be described with sufficient accuracy by the balance laws for a single material. The other is to begin with balance laws for the individual phases and derive from them the corresponding mixture balance laws. The latter approach seems more informative for the purpose of creating a multiphase mixture fragmentation model and some of its elements will be reviewed first. In this discussion the phases will be numbered 0 to M with phase 0 being a continuous fluid and phases 1 to M being clouds of particles (size classes).

The respective balance laws for mass and linear momentum of each phase can be written as

$$\partial_t\left(\rho_i\phi_i\right)+\vec{\nabla}\cdot\left(\rho_i\phi_i\vec{v}_i\right)=\sum_{j=0}^{M}s_{ij} \tag{1}$$

$$\partial_t\left(\rho_i\phi_i\vec{v}_i\right)+\vec{\nabla}\cdot\left(\rho_i\phi_i\vec{v}_i\vec{v}_i\right)=\vec{\nabla}\cdot\overline{\overline{\sigma}}_i+\vec{F}_i+\sum_{j=0}^{M}\vec{F}_{ij}+\sum_{j=0}^{M}s_{ij}\vec{v}_{ij} \tag{2}$$

where ρ_i is the i'th phase true mass density (i'th phase mass per unit of i'th phase volume), ϕ_i is the i'th phase volume fraction (i'th phase volume per unit of mixture volume), $\vec{v}_i$ is the i'th phase velocity vector, s_{ij} is the time rate at which mass is transferred from the j'th phase to i'th phase, $\overline{\overline{\sigma}}_i$ is the i'th phase stress tensor, $\vec{F}_i$ the i'th phase body force per unit volume, $\vec{F}_{ij}$ is the force per unit volume applied by the j'th phase to i'th phase, and $\vec{v}_{ij}$ is the velocity characterizing mass transfer between the i'th and j'th phases. In addition

$$\sum_{i=0}^{M}\phi_i=1 \tag{3}$$

and it will be assumed that

$$s_{ij}=-s_{ji},\qquad \vec{v}_{ij}=\vec{v}_{ji},\qquad \vec{F}_{ij}=-\vec{F}_{ji}. \tag{4}$$

The respective mixture density, velocity vector, and body force vector can be defined as

$$\rho=\sum_{i=0}^{M}\rho_i\phi_i, \tag{5}$$

$$\vec{v}=\sum_{i=0}^{M}\rho_i\phi_i\vec{v}_i/\rho, \tag{6}$$

and

$$\vec{F}=\sum_{i=0}^{M}\vec{F}_i. \tag{7}$$

Summing Eqs. (1) and (2) over i and using Eqs. (4)–(7) yields the respective mixture mass and linear momentum balances

$$\partial_t\rho+\vec{\nabla}\cdot(\rho\vec{v})=0 \tag{8}$$

and

$$\partial_t(\rho\vec{v})+\vec{\nabla}\cdot\sum_{i=0}^{M}(\rho_i\phi_i\vec{v}_i\vec{v}_i)=\vec{\nabla}\cdot\sum_{i=0}^{M}\overline{\overline{\sigma}}_i+\vec{F}. \tag{9}$$

Eliminating $\vec{v}_i$ in favor of the i'th phase diffusive velocity

$$\vec{u}_i=\vec{v}_i-\vec{v} \tag{10}$$