



Brief communication

Crossing trajectories and phase change in Eulerian–Eulerian models of disperse multiphase flows



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ABSTRACT

We analyze the representation in Eulerian–Eulerian models of disperse multiphase flows of phase change phenomena (such as particle drying or vapor condensation) occurring at the saturation temperature. The usually-employed model, whereby the heat transferred among the phases drives the phase change, leads to physically incorrect results (*viz.* the presence of liquid at a temperature above the boiling point) as illustrated in this paper for the drying of solid particles. An efficient correction is proposed and verified in two canonical configurations (1D dilute flow and 2D horizontal channel with gravitational phase segregation). An application to a realistic bubbling fluidized bed is included as Supplementary Material.

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Introduction

Disperse multiphase flows involving phase change are commonplace in many industrial applications in the fields of nuclear engineering, chemical engineering, food manufacturing, or energy. Eulerian–Lagrangian models are often used to solve, using Computational Fluid Dynamics (CFD), such flows when the computational cost of tracking each individual particle (or parcel of identical particles) is affordable; this is usually the case for pulverized-coal or oil combustion in burner-fired boilers, among other problems. On the other hand, Eulerian–Eulerian (or multi-fluid) approaches are often chosen as the framework for the simulation of devices involving complex flow patterns and a large number of discrete particles, because they offer a good compromise between accuracy and computational cost (see *e.g.* van Wachem *et al.*, 2001).

Eulerian–Eulerian models represent all the phases as interpenetrating continua that share the available space. A set of macroscopic (or mesoscopic) balance equations for mass, momentum and energy is obtained for each phase by applying some sort of averaging to the motion equations of the fluid particles in each (separately considered) phase (Ishii and Hibiki, 2011). As a result each phase is characterized by a single set of (averaged) fields

(such as velocity, temperature, species mass fraction, density or diameter). The phase averaging procedure leads to the loss of information. Closure relationships for evaluating the interaction among phases (such as momentum or mass transfer) must be provided. Additionally, for granular phases, constitutive relations (*e.g.*, for solid viscosity) are usually obtained from the kinetic theory of granular flows (Gidaspow, 1994).

A known shortcoming of standard multi-fluid models is the inability to handle the crossing of particle trajectories, since the velocity at the crossing location is as single, averaged one for each phase (see Fig. 1 in de Chaisemartin *et al.*, 2009 for illustration). The multi-fluid multi-velocity approach, based on (high order) node quadrature methods of moments, where each node has its own velocity, is an advanced Eulerian model able to capture crossing trajectories (de Chaisemartin *et al.*, 2009; Desjardins *et al.*, 2008).

We analyze in this article the performance of Eulerian–Eulerian algorithms for problems with interphase heat and mass transfer (such as, for instance, the drying of solid particles), where mass exchange occurs when the phase temperature reaches the saturation point (*e.g.*, boiling temperature). At this point, it is considered that all the heat transferred to the disperse phase is used in the phase-change process, and its temperature remains constant until the liquid phase is consumed. In a widely used model, the mass transfer rate is calculated as a ratio between interphase heat transfer rate and the latent heat. In the Eulerian framework, this approach has been used by a number of authors in a variety of applications. Some examples are the modeling of an evaporating

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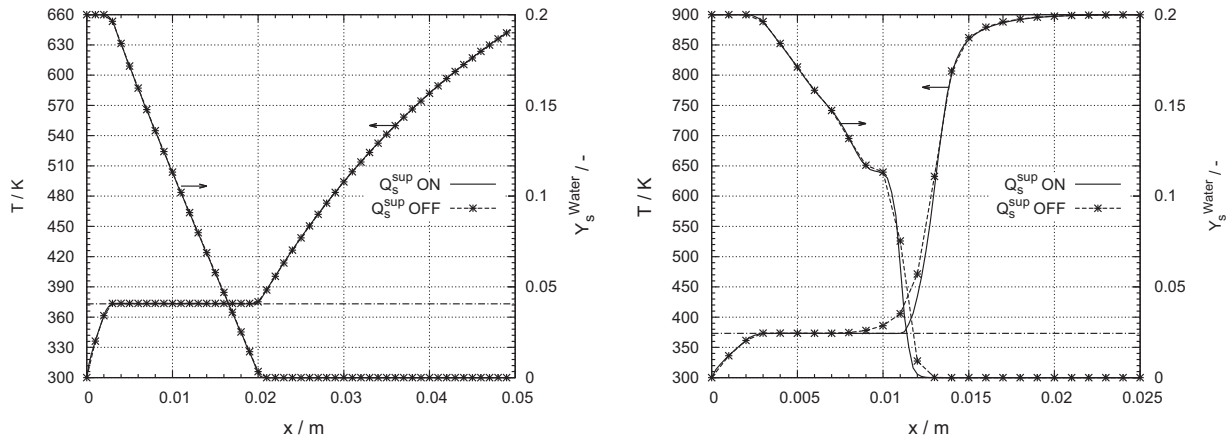


Fig. 1. 1D flow with particle drying: Spatial evolution of the solid-phase temperature and water mass fraction at the steady state (left) and at an intermediate time (right), obtained with (Q_s^{sup} ON) and without (Q_s^{sup} OFF) the correction proposed in this paper.

spray (Li et al., 2010); an in-tube evaporator (Morales-Ruiz et al., 2012); the simulation of the gas–liquid flow of crude oil inside petrochemical fired-heater pipes (Fontoura et al., 2013); the modeling of subcooled boiling flows (Yeoh and Tu, 2006); or the simulation of coal gasification in a fluidized bed (Fueyo et al., 1995; Vicente et al., 2003).

We report that such a model provides unphysical solutions when used in an Eulerian–Eulerian framework. Specifically, particles with superheated water (i.e., particles that are heated beyond the saturation temperature before the phase change has finished) are present in the flow. We attribute this behavior to the mixing of particles with different thermal and compositional histories, a phenomenon akin to the crossing-trajectories one for momentum. An efficient remedy is proposed for preventing this undesirable effect.

The nature of the problem

The standard mass transfer submodel in Eulerian–Eulerian models

Eulerian–Eulerian models for multicomponent (or multispecies) and multiphase flows with mass and heat transfer postulate balance equations for the conservation of mass, momentum, and energy for each phase. A complete set of equations is included as [Supplementary Material](#) to this paper; such set is representative of the equations typically employed in Eulerian–Eulerian, and it is also the one used in the calculations presented below. (The [Supplementary Material](#) annex contains also a full nomenclature list.)

Of particular relevance to the present paper are the equations of mass and energy conservation, and these will be singled out below.

The remainder of this paper will refer to granular flows made of n (wet) solid phases (denoted with the subscript s) and a gas phase (subscript g); the closure relations provided here and in the [Supplementary Material](#) are valid for this kind of multiphase flow. Nevertheless, the correction for the mass transfer model proposed in this work can be readily adapted for use with other correlations for the interphase mass transfer.

The heat transfer between the solid and gas phases is proportional to the phase temperature through a convection coefficient, f_{gs}^h , which in turn depends on the dimensionless Nusselt number Nu_{gs} :

$$\dot{Q}_{sg} = r_s r_g f_{gs}^h (T_s - T_g); \quad f_{gs}^h = 6k_g \text{Nu}_{sg} / d_s^2 \quad (1)$$

where d_s is the particle diameter.

Traditional phase-change models assume that the transfer of a species α (e.g., water during particle drying) from the disperse to

the continuous phase occurs at its saturation temperature. At this temperature, all the heat transfer is used for the phase change, and the disperse-phase temperature remains constant until the process is complete.

According to this model, the mass transfer rate due to vaporization of a component α from the solid phase to the gas phase $\dot{m}_{sg}^{\text{vap},\alpha}$ is governed by the interphase heat transfer \dot{Q}_{sg} (Eq. 1):

$$\dot{m}_{sg}^{\text{vap},\alpha} = \frac{\dot{Q}_{sg}}{L_{sg}^{\alpha}} = \frac{r_s r_g f_{gs}^h (T_s - T_g)}{L_{sg}^{\alpha}} \quad (2)$$

Here, L_{sg}^{α} is the specific latent heat, or energy required for the phase change of a mass unit of species α .

(Phase condensation, the reverse process by which a species α is transferred from the gas to the solid phase releasing heat, can be modeled in an analogous way. In this case, the proposed approach will prevent the appearance of artificially supercooled phases.)

This usually-employed model will be referred to below as the standard model.

Improved mass transfer submodel

It will shown below that the use of Eq. 2 for evaluating the mass transfer rate fails to hold the phase temperature at the saturation point while there is still liquid in the particle. The reason for the unphysical behavior is related to the Eulerian treatment of disperse phases: particles with different temperature and mass histories are averaged in a cell, and the result is a phase with inconsistent average properties. For example, wet particles at the boiling temperature can be mixed with completely dry particles at greater temperature. The result would be a wet phase with temperatures above the boiling point (a “numerically superheated” phase). We propose that a properly formulated Eulerian approach for the phase-change process should account for the extra energy available in superheated phases, in the form of sensible enthalpy. This extra energy can be evaluated at each cell as:

$$\Delta Q_s^{\text{sup},\alpha} = r_s \rho_s C_{p_s} (T_s - T_{\text{sat}}^{\alpha}) \Delta V \quad (3)$$

where T_{sat} is the saturation temperature and ΔV is the cell volume. Thus, the total mass transfer rate due to evaporation is corrected by the amount:

$$\Delta m_{sg}^{\text{sup},\alpha} = \frac{\Delta Q_s^{\text{sup},\alpha}}{L_{sg}^{\alpha}} = \frac{r_s \rho_s C_{p_s} (T_s - T_{\text{sat}}^{\alpha}) \Delta V}{L_{sg}^{\alpha}} \quad (4)$$

For unsteady solvers and time-marching ones, the correction can be viewed as an additional mass-transfer rate:

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