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Constitutive equation for heat transfer caused by mass transfer

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HIGHLIGHTS

- A constitutive equation for enthalpy transfer due to mass transfer is proposed.
- The model is easily implemented in multiphase CFD software.
- Evaporating droplet simulations accurately predicted wet-bulb temperatures.
- Condensing water vapor simulations accurately predicted experimental data.

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ABSTRACT

This paper presents a constitutive equation for the thermal heat transfer associated by mass transfer, applicable to both Eulerian–Eulerian and Eulerian–Lagrangian multiphase computational fluid dynamic models. The proposed equation was incorporated into the open-source multiphase CFD code MFIX (https://mfix.netl.doe.gov) to demonstrate that the numerical predictions match experimental data for the limiting cases of evaporation and condensation. The application of the proposed equation to two cases of a reacting carbon particle yields physically consistent expressions for the heats of reaction.

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1. Introduction

Dispersed multiphase flows are ubiquitous in natural and engineered systems, such as volcanic flows consisting of solids and gas or CO_2 capture reactors where gas phase CO_2 reacts with suspended sorbent particles. They consist of bubbles or particles dispersed in a fluid, exchanging mass, momentum and energy and undergoing physicochemical changes. Multiphase computational fluid dynamics (CFD) models are widely used for describing such flows (e.g., Dufek and Bergantz, 2005; Guenther et al., 2002; Pannala et al., 2007). When mass is transferred between the phases because of physical or chemical changes, there is an accompanying transfer of energy. To the best of our knowledge, a general equation that accounts for such heat transfer is not well established, especially for cases when there are multiple chemical reactions. The objective of this paper is to postulate a constitutive equation for the heat transfer caused by interphase gas–solids mass transfer and to establish the validity of the formula analytically and numerically.

The constitutive equation we propose is applicable to Eulerian–Eulerian (e.g., Syamlal et al., 1993; Gidaspow, 1994) and Eulerian–Lagrangian (e.g., Musser, 2011; Garg et al., 2012) multiphase CFD models. Of the different types of such multiphase flows, the focus here is on particles or droplets suspended in a gas and undergoing physical and/or chemical changes resulting in mass transfer. In multiphase CFD, such a mixture is described by a (continuum) fluid phase interacting with discrete or continuum solids phases. The energy equations in such models include a term that accounts for the energy transfer accompanying interphase mass transfer. A constitutive equation is needed to close this term. Many cases within the literature either explicitly define a ‘heat of reaction’ for each reaction without addressing the interphase mass transfer term (e.g., Xue and Fox, 2014) or define a closure in terms of the specific reaction(s) of interest (e.g., Lathouwers and Bellan, 2001). Our intent is to establish a constitutive equation for a more general set of mass transfer conditions for dispersed multiphase flows and further to document these equations with sufficient clarity that can be more unambiguously coded into a CFD program.

In this paper we first postulate a constitutive equation for the heat transfer caused by mass transfer between gas and solids phases. Then four cases are used to establish the validity of the proposed equation: condensation, evaporation, a single heterogeneous chemical reaction,

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and multiple chemical reactions. In each case we demonstrate that the proposed equation reduces to the correct physically motivated equation. The closure term was also incorporated into the open-source CFD code MFIX (https://mfix.netl.doe.gov) to demonstrate that the numerical predictions match experimental data for the limiting cases of evaporation and condensation. Finally, the closure model is compared to other models found in the literature with respect to interphase enthalpy transfer.

2. Constitutive equation

The focus of this paper is in providing a closure for enthalpy transfer accompanying interphase mass transfer, however an overview of the energy equations are given for completeness. A simplified form of the gas phase energy equation as applied to gas–solids multiphase flows in terms of temperature is commonly written in a form similar to

$$\varepsilon_g \rho_g \overline{C}_{pg}\left[\frac{\partial T_g}{\partial t}+U_{gi}\frac{\partial T_g}{\partial x_i}\right] = -\frac{\partial q_{gi}}{\partial x_i}+\sum_m \gamma_{gm}(T_m-T_g)+\gamma_{Rg}\left(T_{Rg}^4-T_g^4\right)-H_g, \tag{1}$$

where ε_g, ρ_g, $\overline{C}_{pg}$, and T_g are the gas phase volume fraction, density, composite specific heat, and temperature. q_{gi} is the gas phase conductive heat flux, γ_{gm} is the convective heat transfer coefficient between the gas and mth solids phase at temperature T_m, γ_{Rg} is the gas phase radiative heat transfer coefficient, and T_{Rg} is the gas phase radiation temperature. This radiation model is an approximation used in the MFIX code. Further, the direct interaction of radiative heat transfer with mass transfer is not a component of the proposed constitutive equations and thus is not explicitly dependent on the particular approximation used for the radiation model. The last term on the right hand side is the total rate of enthalpy change for the gas phase due to chemical reactions and phase changes. The primary terms which are neglected from the gas phase energy equation are the convective derivative of pressure and viscous dissipation (e.g. Ahmadi et al., 2006; Ruggirello et al., 2012). For the relatively low speed flow (e.g. low Mach number) in a fluid–solid reactor system, these terms are expected to be small relative to the other heat transfer processes. Similarly, a simplified energy equation for the mth solids phase in a continuum solids model can be written as

$$\varepsilon_m \rho_m \overline{C}_{pm}\left[\frac{\partial T_m}{\partial t}+U_{mi}\frac{\partial T_g}{\partial x_i}\right] = -\frac{\partial q_{mi}}{\partial x_i}-\gamma_{gm}(T_m-T_g)+\gamma_{Rm}\left(T_{Rm}^4-T_m^4\right)-H_m \tag{2}$$

where ε_m, ρ_m, $\overline{C}_{pm}$, and T_m are the mth solids phase volume fraction, density, composite specific heat, and temperature. γ_{Rm} and T_{Rm} are the radiative heat transfer coefficient and radiation temperature for the solid. Again, the last term on the right hand side is the total rate of enthalpy change for the mth solids due to chemical reactions and phase changes. Any viscous dissipation of heat due to the gas–solid drag is neglected because the slip-velocity and in turn, the heat transfer associated with this process, is relatively small for operating regimes of interest. Additional details for the gas and solids energy equations are available in Syamlal and Pannala (2011).

The mth solids phase's rate of enthalpy change due to chemical reactions and phase changes for P simultaneous reactions can be written as

$$H_m = \sum_p^P \left(\xi_{gmp} + \sum_{n=1}^{N_m} h_{mn}(T_m)R_{mnp}\right) \tag{3}$$

where N_m is the number of species comprising the mth solids phase, $h_{mn}(T_m)$ is the specific enthalpy of the mth particle's nth species evaluated at the particle's temperature, and R_{mnp} is the rate of formation (or destruction) of the mth solids phases' nth species resulting from the pth reaction. ξ_{gmp} is the enthalpy transfer attributed to mass transfer between the mth solids and gas phases for the pth reaction. Similarly, the gas phase rate of enthalpy change due to chemical reactions and phase changes for P simultaneous reactions can be written as

$$H_g = \sum_p^P \left(\sum_{m=0}^{M}\left(-\xi_{gmp} + \sum_{n=1}^{N_g} h_{gn}(T_g)R_{gmnp}\right)\right). \tag{4}$$

where M is the total number of phases, $h_{gn}(T_g)$ is the specific enthalpy of the nth gas phase species evaluated at the gas phase temperature. R_{gmnp} is the rate of formation (or destruction) of the nth gas phase species attributed to the pth reaction between the gas and mth phase. The case of $m=0$ represents homogeneous gas phase reactions whereby ξ_{g0p} is zero. This is done to prevent introducing additional terms and nomenclature. Observe that the ξ_{gmp} terms cancel when the gas and solids phase energy equations are added. Therefore, the constitutive equation for ξ_{gmp} does not affect the overall energy balance, but it may have a significant effect on both the particle and gas temperatures and in turn, on chemical reaction rates.

We propose the following constitutive equation for ξ_{gmp} to account for enthalpy transfer caused by mass transfer,

$$\xi_{gmp} = \sum_{n=1}^{N_g} h_{gn}(T_{gm})R_{gmnp}. \tag{5}$$

The temperature at which the specific enthalpy is evaluated, T_{gm}, is identified explicitly and given by

$$T_{gm} = \begin{cases} T_g \text{ for } R_{\text{gmnp}} \le 0 \text{ (i.e., consumption of } n\text{th gas species)} \\ T_m \text{ for } R_{\text{gmnp}} > 0 \text{ (i.e., formation of } n\text{th gas species)} \end{cases}. \tag{6}$$

This constitutive equation makes the physically reasonable assumption that a chemical species transferred from a source phase to a destination phase reaches the destination phase with its specific enthalpy calculated at the temperature of the source phase.

The above closure model is applicable to general multiphase flow energy equation formulations and is not restricted to the energy equations given by (1) and (2). Any differences can be attributed to variations in the definitions used for the phase specific 'rates of enthalpy change due to chemical reactions and phase changes', Eqs. (3) and (4). The temperature form of the energy equations are employed here because this is the form implemented in MFIX which was used in the testing of the proposed closure. Likewise, the proposed closure model is equally applicable to Eulerian–Eulerian and Eulerian–Lagrangian models. The Eulerian solids model was selected for this discussion to avoid confusion arising from the differing frames of reference (i.e., per volume as opposed to per particle (Musser, 2011)).

To the best of our knowledge, the general model for ξ_{gmp} defined by Eqs. (5) and (6) has not been reported in the literature as further discussed in Section 5. Furthermore, the equation can be easily incorporated into any multiphase CFD program. The proposed compact equation eliminates the need for a CFD practitioner to define this term for each specific instance of a physical and/or chemical change in a multiphase system. In the next section, we show that this compact equation correctly captures physically reasonable behavior for different mass transfer cases.

3. Validation of the constitutive equation

In this section we present four cases with gas–solids mass transfer and show that the model (Eqs. (5) and (6)) gives physically expected results. Each case assumes without loss of generality that