

COMPUTATIONAL STUDY OF HEAT AND MASS TRANSFER IN MULTI-PHASE FLUID FLOWS

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ABSTRACT

Multi-phase fluid flows and heat and mass transfer study are of great importance to many engineering practices such as chemical processing, energy systems, environmental control, and modern manufacturing. Multi-phase flows are complicated in interactions between liquid, gas and solid phases, which are affected by interfacial relationships, phase change, turbulence as well as transport. Computational methods are usually necessary when experimental research techniques fail to handle microscale behavior and transient processes. The paper provides an overview of available computational techniques in multi-phase flow modeling, such as the Volume of Fluid (VOF), Level Set, Phase Field, Eulerian Eulerian and Eulerian Lagrangian techniques. Transport equations of mass, momentum, energy and species transport have been addressed, as well as the computational methods of interface tracking and phase change modeling. The paper identifies specific progress in the field of numerical simulation and in high-performance computing and simulations aided by machine learning, which improve predictive performance and optimize industrial operations. The results of these computational studies can be used to achieve more accurate and efficient design, understanding and control of multi-phase systems.

Keywords: Multi-phase flow, Heat transfer, Mass transfer, Computational Fluid Dynamics (CFD), Volume of Fluid (VOF), Level Set Method

Introduction

Multi-phase fluid flows and the heat and mass transfer represent a very important field of research in the contemporary engineering sphere, and they find their application in chemical processing, energy systems, environmental engineering, and high-tech manufacture [1]. Multi-phase flows, i.e. liquid-gas or solid-liquid and liquid-liquid mixtures, are characterized by complicated interactions that are motivated by the dynamics at the interface, phase change, turbulent structures, and transport mechanisms [2]. Such interactions play a major role in the effectiveness, stability, and efficiency of many industrial processes such as boiling, condensation, particulate transport, drying, polymer processing, and combustion.

Conventional experimental studies of multi-phase flows are sometimes problematic because they are expensive, have measurement constraints, and it is hard to observe microscale interface processes in real-time [3]. Computational modeling and simulation have, therefore, been developed as effective in the analysis of heat and mass transfer in these systems. Recent developments in numerical schemes, including the Volume of Fluid (VOF), Level Set Method, Phase Field Method, Lattice Boltzmann Method (LBM), and multiphase Computational Fluid Dynamics (CFD) have allowed researchers to model the complex interfacial dynamics with more and more accuracy. These models enable the phase

boundaries to be visualized at a detailed level, prediction of the transport properties and even the process parameter to be analyzed in a controlled virtual environment [4-5].

Most recent studies have increased the accuracy of computational studies and their scalability through the combination of high-performance computing, machine learning-enabled turbulence modeling, and enhanced numerical algorithms [6]. The developments give more detailed information about the processes of heat and mass transfer, including evaporation, condensation, interfacial convection, breakup of droplets, bubble dynamics and diffusion of species [7]. The knowledge of these mechanisms is the key to maximizing engineering equipment such as heat exchangers, reactors, spray systems, fluidized beds, and renewable energy technologies [8].

With the growing complexity of the type of industrial systems and the necessity of providing sustainable and energy-efficient solutions, a specific computational study of heat and mass transfer in multi-phase fluid flows is timely and required [9]. The purpose of this paper is to investigate the controlling physics, computational methods, and computational simulation results, which are used to enhance predictive methods and design techniques in the case of multi-phase flow applications [10].

Problem Statement

Although the computational fluid dynamics have made tremendous progress, predicting the heat and mass transfer in multi-phase fluid flows remains a significant issue because it has complex interfacial interactions, phase change phenomena and nonlinear transport processes [11]. Current models have difficulty in representing the behavior of microscale interfaces, effects of turbulence and transient effects with enough accuracy resulting in uncertainties in engineering design and optimization of the processes [12]. Besides, multi-phase systems are hard, expensive, and even infeasible to experimentally validate, which also constrains the creation of effective predictive tools. Thus, it is of paramount importance that a thorough computational investigation is created that is able to simulate multi-phase heat and mass transfer with better precision, solve interfacial processes, and give conclusions that are useful in design and optimization of new industrial systems and thermal systems.

Significance of the study

Computational study of the heat and mass transfer in the multi-phase fluid flows is of great essence in the growth of scientific knowledge as well as industrial practice [13]. This study advances the construction of a more realistic predictive model by offering a deeper understanding of interfacial processes, phase change processes and transport processes to improve the efficiency, reliability and safety of systems either heat exchanger, chemical reactors, thermal energy storage reactor, or environmental fluid processes [14]. The results will assist the engineers and researchers to optimize operational parameters, cut down costs of experimentation, and the design of new thermal systems, which are better in performance. Besides, the research will contribute to the increasing need of using sustainable technologies, as it will make the use of energy and the stability of processes under multi-phase flow conditions easier to control [15].

Computational Methods For Multi-Phase Fluid Flow Analysis

Multi-phase fluid flow analysis by computational models entails numerical techniques applied to model the behaviours among the various phases (e.g., liquid-gas, liquid-solid, or gas-solid systems) in which the heat and mass transfers are critical factors. The methods also seek to address the governing conservation equations with an accurate tracking or capture of moving interfaces and phase boundaries. The complexity of multi-phase systems leads to the computational methods assisting the visualization of interfacial dynamics, prediction of transport processes, and optimization of engineering tasks such as boiling, condensation, droplet breakup, bubble dynamics, and reactive flow.

Governing Equations for Multi-Phase Flow

Multi-phase flow governing equations are the basis of computational simulations and are mainly founded on the Navier Stokes equations, with the equations further extended to deal with multi-phase interactions. These are equations that explain the conservation of mass, momentum and energy at any stage taking into account the interfacial forces, changes in density and viscous forces. They give a mathematical basis to make forecast of fields of velocity, pressure distribution and temperature profiles of complex multi-phase systems. These equations allow the proper modeling of the processes of heat and mass transfer by adding phase change, surface tension and mass transfer source terms.

Continuity Equation

For an incompressible multi-phase flow:

$$\nabla \cdot \mathbf{u} = 0 \quad (1)$$

For compressible or varying-density flows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (2)$$

Momentum Equation

The momentum equation is used to explain the effects that forces, including pressure, viscous stresses, gravity, and surface tension have on the movement of the fluids in a multi-phase system. It controls the acceleration and velocity distribution of every stage, and is crucial in the interfacial prediction of behavior and dynamics of flow.

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot (\mu \nabla \mathbf{u}) + \rho \mathbf{g} + \mathbf{F}_\sigma \quad (3)$$

Energy Equation (for Heat Transfer)

The energy equation describes the variation in temperature of a multi-phase flow as a result of convection, conduction and phase-change processes. It is an important tool in determining the rate of heat-transfer and thermal interactions of various phases.

$$\rho c_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) = \nabla \cdot (k \nabla T) + S_T \quad (4)$$

Species Transport Equation (for Mass Transfer)

The species transport equation is an equation that defines the movement of various chemical species or components in a multi-phase system due to convection and diffusion. It plays a crucial role in the analysis of the mass transfer process including evaporation, dissolution, mixing, and chemical reactions.

$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_i) = \nabla \cdot (D_i \nabla Y_i) + R_i \quad (5)$$

Interfacial Momentum Exchange (Drag Force Model)

Used in Eulerian–Eulerian and Eulerian–Lagrangian methods:

$$F_D = \frac{1}{2} C_D \rho A_p |u - u_p| (u - u_p) \quad (6)$$

Surface Tension Force (Continuum Surface Force – CSF Model)

$$\mathbf{F}_\sigma = \sigma \kappa \nabla \alpha \quad (7)$$

Curvature equation:

$$\kappa = -\nabla \cdot \left(\frac{\nabla \alpha}{|\nabla \alpha|} \right) \quad (8)$$

Turbulence Modeling in Multiphase Flow (k-ε Model)

Turbulent kinetic energy (k):

$$\frac{\partial k}{\partial t} + u_i \frac{\partial k}{\partial x_i} = \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + P_k - \varepsilon \quad (9)$$

Computational Methods for Interface Tracking/Interaction

The flow simulations at multiple phases are based on the treatment of the interface between the phases. It has three large categories:

Volume of Fluid (VOF) Method

Volume of Fluid (VOF) method is a popular computational method of simulating multi-phase flows by tracing the volume fraction of a phase in a computational cell. It employs a scalar variable, α , with 0=200 of a cell being covered by the primary phase and 1=200 of a cell being covered by the secondary phase.

$$\frac{\partial \alpha}{\partial t} + \mathbf{u} \cdot \nabla \alpha = 0 \quad (10)$$

To determine the motion and deformation of interfaces between phases, the technique solves the advection equation of 2. VOF is also very effective in issues that apply to big interface deformations, including the rise of bubbles, formation of waves, and the breakages of droplets, but it is also associated with good mass conservation.

Volume of Fluid (VOF) — Mixture Density & Viscosity

$$\rho = \alpha \rho_1 + (1 - \alpha) \rho_2 \quad (11)$$

$$\mu = \alpha \mu_1 + (1 - \alpha) \mu_2 \quad (12)$$

These are essential to calculate properties in mixed cells.

Level Set Method

Uses a signed distance function ϕ :

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0 \quad (13)$$

$$\kappa = \nabla \cdot \left(\frac{\nabla \phi}{|\nabla \phi|} \right) \quad (14)$$

The Level Set method is a computer algorithm that is well suited to modeling smooth and continuous interfaces between phases and can therefore be applied in simulating irregular interfacial profiles like droplets, bubbles, and interface merging and interface splitting. The technique gives correct curvature computation and permits accurate tracing of interface movement by modeling the interface as a signed distance function. Level Set is however less effective at the conservation of mass as compared to the Volume of Fluid (VOF) method, and may cause small yet compounding errors in the phase volume with time. In spite of this shortcoming, its capacity to cope with smooth interface dynamics renders it a useful multi-phase flow simulation tool, when interface precision counts.

Phase Field Method (Cahn–Hilliard Model)

Interface represented by an order parameter ψ :

$$\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi = M \nabla^2 \left(\frac{\partial F}{\partial \psi} \right) \quad (15)$$

$$\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi = M \nabla^2 (\lambda(\psi^3 - \psi) - \epsilon^2 \nabla^2 \psi) \quad (16)$$

Phase Field technique is very useful in the modeling of micro-scale interface physics, and it offers a thermodynamically consistent method to model a diffuse interface between two phases. It is the interface that is simulated in an order parameter in such a way that interfacial effects like surface tension, phase separation and thin-layer dynamics can be studied in detail. This technique is especially appropriate when undergoing a phase change, such as boiling, condensation and droplet coalescence, poised where precise resolution of interface behaviour is highly necessary. The Phase Field technique is useful in multi-phase flow analysis by providing accurate prediction of heat and mass transfer in the micro-scale by solving small scale interactions.

Eulerian–Eulerian Method

Treats each phase as an interpenetrating continuum.

$$\frac{\partial(\alpha_k \rho_k)}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) = 0 \quad (17)$$

Used for fluidized beds, slurry flows, gas–liquid reactors.

Eulerian–Lagrangian Method

The Eulerian Lagrangian method is an intermediate method of computation, where the continuous fluid phase is computed on a fixed Eulerian grid, but discrete particles, droplets, or bubbles are solved by a

Lagrangian method. This enables the complexity modeling of the particle-fluid interactions such as momentum, heat, and mass exchange between the phases. The method can also be used to accurately solve more complicated dispersed phase flows, including sprays, aerosols, and bubbly flows by taking the advantages of both Eulerian and Lagrangian representation. It is specifically useful in tracking the trajectories, residence times and interfacial impacts of discrete bodies inside a continuous media, rendering it important to engineering operations in combustion, cooling and chemical processing.

$$m_p \frac{d\mathbf{v}_p}{dt} = \sum \mathbf{F} \quad (18)$$

Used for sprays, aerosol transport, droplet dynamics.

Computational Studies on Heat and Mass Transfer in Multi-Phase Flows

Computational heat and mass transfer in multi-phase flows concentrate on the interaction of the various phases, e.g., liquids, gases or solids, by their interactions among themselves either thermally or chemically. These experiments give us information on the distribution of temperature, species concentration, phase change behavior, interfacial motion and transport mechanisms which are hard to measure in experiments. With the aid of computational fluid dynamics (CFD), scholars study such processes as boiling, condensation, droplet evaporation, bubble growth, and interfacial diffusion, which aid in predicting the performance of a system in an industrial application.

Heat Transfer Modeling in Multi-Phase Flows

Multi-phase flows modeling Heat transfer In multi-phase flows, modeling of heat transfer is used to analyse the transport of energy by conduction, convection and by exchange of phase change between distinct fluid phases and is considered to be fundamental in the study of thermal interactions between fluid phases. In computational simulations, the generalized energy equation is the equation that is applied to describe how temperature changes with time and space taking into consideration the effects of fluid movement, thermal conductivity, and release or absorption of latent heat when there is a change of phase such as boiling or condensation. The method facilitates forecasting of temperature dynamics, heat flux and thermal efficiencies in multi-phase systems of complex geometry to give vital information that helps optimize the industrial processes, develop cost effective heat exchangers and enhance energy management in applications where liquids, gases or particle phases are involved.

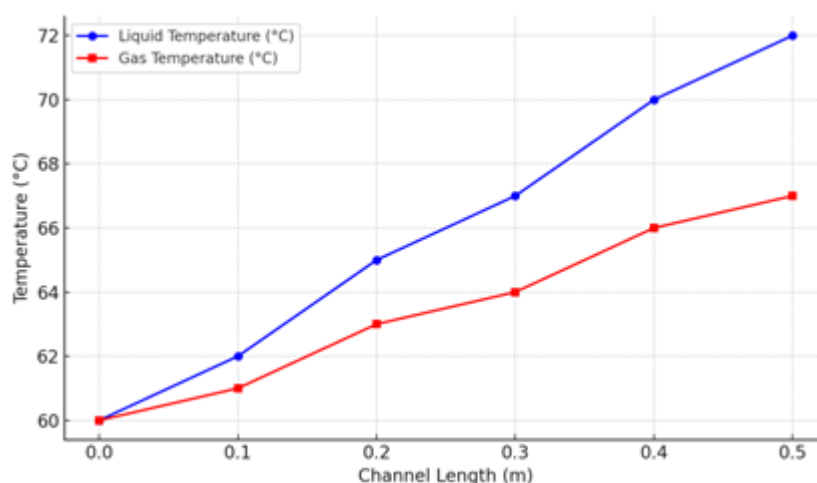


Figure 1: Temperature Distribution along Two Phase Flow Channel

$$\rho c_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) = \nabla \cdot (k \nabla T) + S_T \quad (19)$$

where

- S_T = source term representing latent heat during processes like boiling and condensation.

Phase Change Modeling Example (Boiling):

Latent heat source term:

$$S_T = \dot{m} h_{fg} \quad (20)$$

Mass Transfer Modeling in Multi-Phase Systems

Transport of species is important to evaporation, diffusion and dissolution. The equation of transport of the species is:

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_i) = \nabla \cdot (D_i \nabla Y_i) + R_i \quad (21)$$

Multi-phase systems are dependent on species transport since it controls such important processes as evaporation, dissolution, diffusion, and mixing of phases. It determines the motion of various species under concentration gradient and fluid flow which has a direct impact on interfacial mass exchange. These mechanisms can only be accurately modeled in order to predict reaction rates, phase-change behavior, and concentration distribution. In computational simulation, the species transport equation is popular to describe these effects.

Interfacial Mass Transfer Example:

Mass transfer across interfaces is expressed by:

$$\dot{m} = k_L (C^* - C) \quad (22)$$

Used for evaporation, absorption, or gas-liquid reactions.

Multi-Phase Heat & Mass Transfer: Computational Approaches

The manner in which microprocessors are used to analyze the multi-phase heat and mass transfer process is based on numerous numerical techniques which render the intricate interaction between fluid phases, interfaces, and transport processes. On large scale interfaces Simulation of bubble interaction, wave propagation and large interface deformations techniques like the Volume of Fluid (VOF) method are popularized to trace phase fractions, and the Level Set method to offer a smooth and accurate representation of interfaces, thus it is applied across a wide range of study of condensation, droplet merging and interfacial curvature influences. The Phase Field method provides a thermodynamically consistent model of phase-change processes such as boiling, melting, and evaporation through the solution of diffuse interfaces and to micro-scale thermal interactions. In the case of dispersed phase systems, the Eulerian-Eulerian method considers each phase as an interpenetrating continuum, and can be used to simulate dense gas-solid, gas-liquid, or slurry flows with effective heat and mass transport. Meanwhile, the Eulerian-Lagrangian methods follow single droplets, bubbles or particles within a continuous fluid field, and are thus useful in studying spray cooling, aerosol transport, and the exchange of heat between particles and fluids. Combined with experimental techniques, these computational

techniques offer highly effective tools to understand interfacial heat flux, mass diffusion, phase change, and multi-scale transport processes in multi-phase systems of complex types.

Conclusion

Computer based studies of heat and mass transfer in multi-phase fluid flows give invaluable information on interfacial behavior, phase change processes, and transport processes which are difficult to experimentally measure. The complex flow behaviors that can be accurately simulated using advanced numerical methods include droplet and bubble dynamics, evaporation, condensation, and species diffusion using advanced numerical techniques including VOF, Level Set, Phase Field, Eulerian-Eulerian, and Eulerian-Lagrangian methods. The accuracy and scalability of these simulations has been increased by the combination of high-performance computing and better numerical algorithms and is used to design and optimize industrial systems, including heat exchangers, reactors, and fluidized beds. All in all, the computational methods allow to gain deeper insight into the multi-phase heat and mass transfer, lower the expenses of the experiments, as well as create the systems of thermal transfer that will be energy-efficient and performance-based.

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