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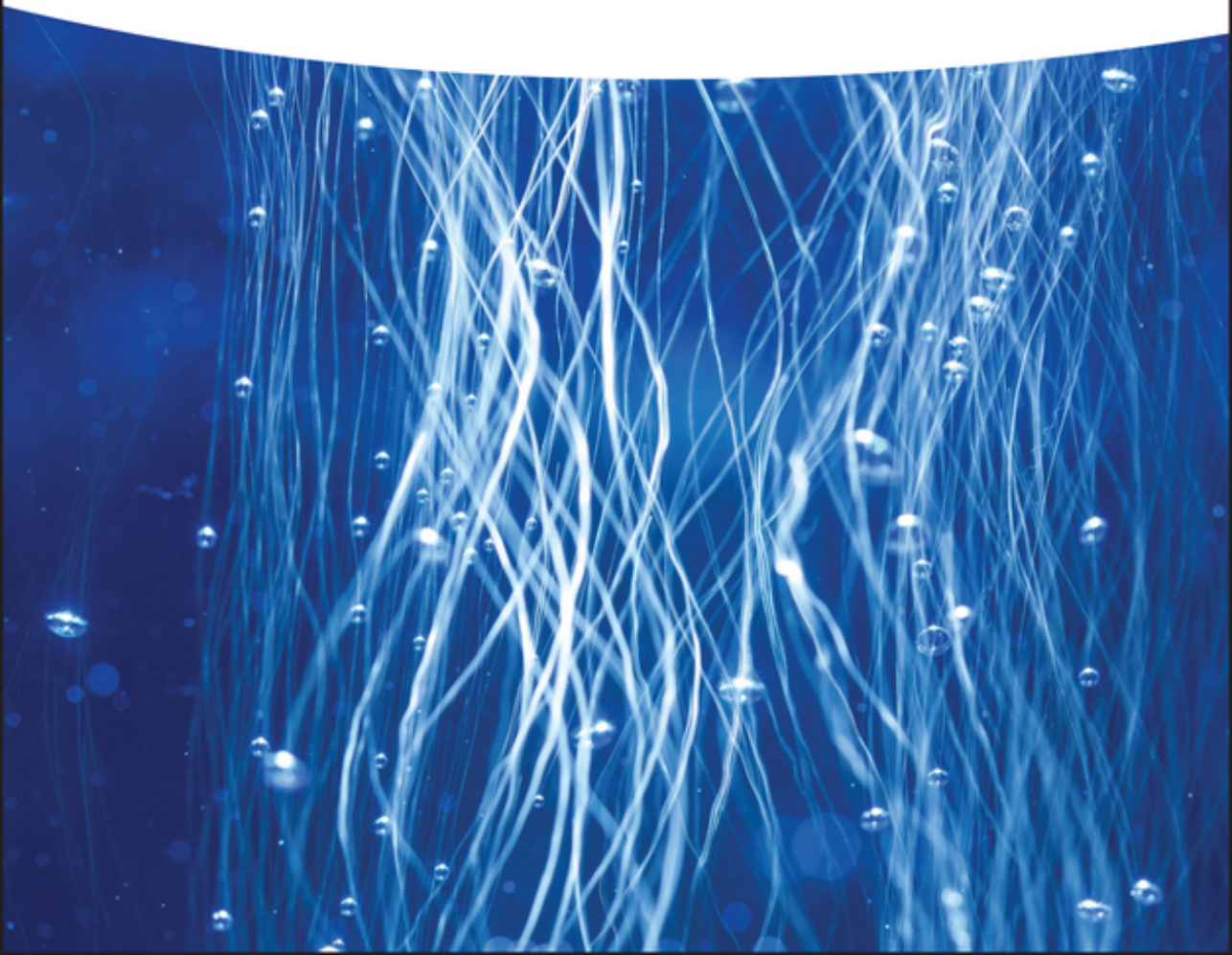
Edited by Vivek V. Ranade and Ranjeet P. Utikar

Multiphase Flows for Process Industries

Fundamentals and Applications

Volume 2



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Preface

We (VR and RU) started working together on multiphase flows when both of us were at National Chemical Laboratory (Industrial Flow Modelling Group, iFMg), Pune, India. Combined together, we have more than 50 years of experience in navigating through a wide range of multiphase flows encountered in chemical process industries. This experience and the challenges we faced in understanding and quantitatively simulating multiphase flows have motivated us to develop this book.

Multiphase flows and systems play a central role in overall performance and productivity of process industries. It is therefore essential to develop a thorough understanding and an ability to quantitatively simulate multiphase flows for enabling process innovations. Several excellent reviews, books, and comprehensive handbooks on multiphase flows are available. However, we felt that there is a need for a compiled resource that bridges the gap between theory and practice. The proposed book is aimed at filling this void.

This edited book builds further upon the earlier book of VR entitled *Computational Flow Modelling for Chemical Reactor Engineering* which was published couple of decades ago. That book was developed based on the flow modeling workshops conducted by VR and was mainly shaped by his personal experiences. Instead, in this book, we have invited key researchers and experts in multiphase processes as contributors and have drawn upon their vast experience for providing a unique resource on current state of the art in computational modeling of multiphase flows. The book elaborates specific issues encountered in various types of multiphase flows across the process industry. It intends to provide insight to tackle these issues and master multiphase flows. Industrial examples of process innovation enabled by this approach are included as well. The material in this book is arranged in two parts: fundamentals and applications for enabling process innovations. We hope that this book will stimulate further work in this very important area from an industrial as well as from a scientific point of view.

The intended users of this book are chemical and process engineers working in chemical and allied industries and industrial R&D laboratories as well as chemical engineering scientists/research students working on realizing process innovations and productivity enhancements. Enhancing resource efficiency and decarbonization via process innovations are global priorities of manufacturing sector. There is a significant excitement about digitalization, Industry 4.0, and their

impact on manufacturing in process industries. It has a potential to become the most transformative era for chemical manufacturing. High-fidelity computational models of multiphase reactors and systems are essential for realizing the potential of digitalization. The book will be useful for developing such high-fidelity models of multiphase systems. We have also included our thoughts on the role and potential of combining computational flow modeling with real-time data and machine learning for realizing digital twins of multiphase systems and thereby realizing significant productivity enhancements at the end.

We hope that the material included in this book will be useful in several different ways and at various stages of process innovations projects involving multiphase flows and systems. Some prior background in multiphase flows is assumed for readers. It may be used as a basic resource of methodologies for computational modeling of multiphase flow processes. The content may also be useful as a study material for an in-house course, or a companion book while solving practical problems in modeling of multiphase flows. We hope that this book will encourage chemical and process engineers to harness the potential of computational flow modeling in order to realize process innovations.

There are many people to thank who made this book possible. We would first like to thank all the contributors to this book. We are also grateful to many of our students, associates, colleagues, and collaborators with whom we worked on different research and industrial projects. Many of our colleagues and students have contributed to this book in different ways. VR would like to acknowledge Fluent Inc. and ANSYS for supporting our research at NCL and University of Limerick, respectively, via academic partnerships. We also wish to thank the editorial team at Wiley for their patience and understanding during the long process of developing this book.

Finally, VR wishes to acknowledge his wife Nanda and RU wishes to acknowledge his wife Manjushree for their patience, understanding, and enthusiastic support throughout this long and arduous book project.

October 2021, Limerick, Ireland — *Vivek V. Ranade*
Perth, Australia — *Ranjeet P. Utikar*

Part I

Introduction

1

Multiphase Flows and Process Industries

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Chemical and allied process industries are crucial for sustaining and enhancing quality of life as they touch lives of everyone, every day. These chemical and allied process industries help transform natural resources to useful things for ensuring well-being of everyone (see Figure 1.1). The primary mandate for the process industries (chemical, petrochemical, fertilizer, metallurgical, power, cement, and so on) is to add value to raw materials via physical, chemical, or biochemical transformations to realize products that meet customer requirements without compromising safety, environment, and economics. As almost all the processes relevant to the process industries involve flow of fluids in some way or the other, the innovative and competitive edge of any manufacturing industry rests on how well these flow processes are designed and operated.

In many industries, such as automotive or aerospace, flows involving just one phase (single-phase flow) are predominantly encountered. Reliable computational models are available to simulate such flows. The governing equations for the simulation of flow (the Navier–Stokes equations) and energy are well established, and the primary challenge is turbulence modeling and its influence on the transfer of mass, momentum, and energy. In those industries, flow models are used throughout the design cycle. However, a vast majority of the flows in process industries are multiphase in nature, that is, they involve more than one phases. A "phase" can be gas, liquid or solid (thermodynamic definition of state of the matter), or it can be different types of same thermodynamic phase (for example, two different sizes of solid particles may be defined as two different phases). Typically, in process industries each of these phases may contain several chemical components. These multiphase flows are characterized by complex interactions between the phases. Experimental techniques to quantify these interactions are limited. Consequently, computational models for these flows are not as well established as single-phase flows. Therefore, predicting and controlling the behavior of multiphase flow is challenging. Consequently, the computational models are not yet integrated with the design and optimization cycles

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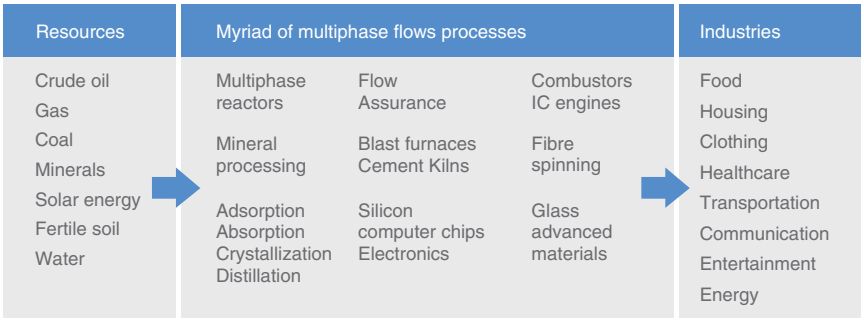

Figure 1.1 Multiphase flow processes connect natural resources and daily needs.

of process industries as they are in automotive and aerospace sectors. Despite this, the advances in both experimental characterization as well as computational modeling over the last couple of decades have provided process engineers unprecedented opportunities to understand and optimize multiphase flows in process industries.

This book is aimed at providing state of the art in commonly encountered multiphase flows in process industries. First part of the book covers fundamentals of multiphase flows including widely used experimental and computational methods for understanding multiphase flows. The second part is devoted to several examples from process industry covering a wide range of multiphase flows. The examples cover two phase flows (gas–liquid, solid–liquid, and gas–solid), three or more phases as well as multiphase flows with phase change. Finally, the book provides a direction on using the current advances in realizing efficient and optimized processes. Key aspects of process industry, role of multiphase flows in process industry, and overall organization of this book are briefly discussed in the following sections.

1.1 The Process Industry

The chemical and process industry faces its biggest challenges in rising raw material costs, depleting feedstocks, and stricter environmental regulations. These challenges also open up significant opportunities for innovation. It is essential to continuously focus on significant improvements in productivity via process innovations for conserving raw materials, catalysts, energy, and water. Enhancing resource efficiency and emphasis on deriving more value from less resources are becoming global priorities now. For example, Europe has set the goal of doubling its resource productivity by 2030 [1]. Improved productivity and resource efficiency will reduce costs, enhance competitiveness, promote jobs, growth, and resilience as well as realize environmental benefits by reducing carbon emissions. Resource efficiency and productivity are directly linked to carbon emissions and climate change. Almost all the major countries have pledged to make significant reductions in carbon emissions. For example, Europe has set an ambitious goal of becoming the first climate-neutral continent by 2050 [2]. Chemicals and materials play

crucial role in achieving these goals since they are essential for almost all human endeavors. Chemical industry provides products, materials, and technical solutions that improve resource efficiency throughout the value chain and across the economy. It is important that the manufacturing of these chemicals becomes resource-efficient. Multiphase systems, reactors, and processes are ubiquitous in process industry and therefore crucial for controlling overall resource efficiency and productivity of chemical and process industry.

Productivity of chemical and allied process industry may be measured in terms of variety of parameters such as:

- Atom economy (fraction of raw material being present in the product)
- Energy consumption per unit product
- Environmental and carbon footprint
- Product quality/cost
- Safety
- Spatial foot print
- Throughput per unit volume
- Waste generated per unit product
- Water consumption per unit product

Continuous improvement has been the cornerstone of the process industry and has resulted in significant advances in several process areas. For example, advances in materials, absorption, and regenerative heat recovery have tremendously improved the energy efficiency of sulfuric acid plants over recent years (see for example, [3]). Compared with a traditional double-catalyst double-absorption process cycle, where almost 40% low-level heat is wasted in acid cooling system, modern processes such as Monsanto Enviro-Chem's Heat Recovery System and Outokompu heat recovery system offer recovery of over 95% of the process heat as steam [4]. Recently, there has been significant effort to develop scalable technologies for the synthesis of carbon-neutral ammonia by conversion of intermittent energies (e.g. solar and wind) [5]. The new developments allow ammonia plants to behave like energy plants, a drastic shift from the traditional centralized, large-scale, capital- and energy-intensive Haber–Bosch process. It is imperative that major advances for the chemical and allied process industries will continue to emerge from catalysis, chemistry, and biological sciences. However, maximizing the benefits from these advances requires comparable advances in the design of chemical process equipment responsible for the chemical (and biological) transformations. A vast majority of such transformations involve multiphase flows, and therefore, there is an immense scope for enhancing and harnessing multiphase flow processes for realizing productivity enhancements.

There are several examples where better understanding of multiphase flows has resulted in significant productivity enhancements. For example, understanding of the gas–solid flows has led to continuous evolution of pyrolysis technology from fixed-bed batch pyrolysis systems to fluidized bed and fast pyrolysis technologies that offer increased oil yield [6]. Similarly, development of fluidized bed and CFB reactors offers better heat management and improved process over packed bed reactors for

partial oxidation of butane to maleic anhydride [7]. Understanding and harnessing flow regimes have enabled development of a suite of micro-scale processes that offer order of magnitude increase in productivity over their large-scale counterparts [8]. Such performance enhancements and advances in process technologies have been achieved via thorough understanding of involved multiphase flow processes in a wide range of process equipment.

A wide variety of process equipment and operating protocols are used in practice. The driving force behind these different designs is to gain more control on the delivery of materials and energy. Any physical, chemical, or biochemical transformation process requires the addition or removal of different materials and energy. Efficient and effective design of process requires the delivery of materials and energy at the right places and at the right times by manipulating underlying fluid dynamics. Fluid dynamics controls the distribution of materials as well as the energy within the process vessel. The process of designing equipment can thus be described in four broad steps [9]:

- Step 1: Understand the process requirements and identify the desired fluid dynamic characteristics.
- Step 2: Evolve and evaluate the possible hardware configurations/operating protocols to achieve the desired fluid dynamic characteristics.
- Step 3: Develop quantitative relationships between the design and performance.
- Step 4: Optimize and fine tune the final process design.

The importance of fluid dynamics in all four steps is apparent. Most of the industrially relevant processes involve multiphase flows, and therefore a thorough understanding of multiphase flows is one of the critical "enabling technologies" to achieve desired control on delivery of materials and energy at the right time and at the right place. The deeper understanding of multiphase flows underpins process optimization, process systems engineering, and process intensification (PI) (see Figure 1.2).

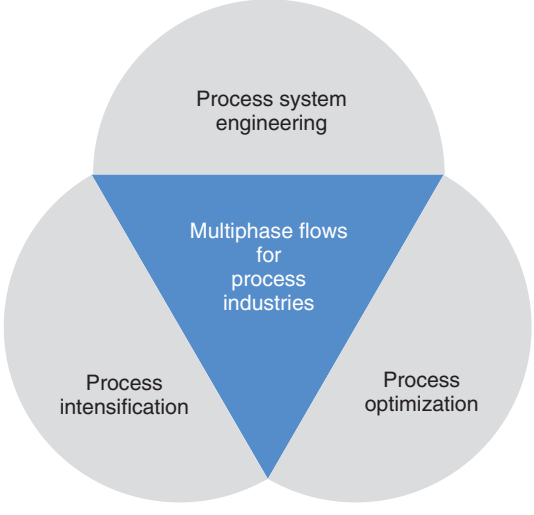

Figure 1.2 Multiphase flows are a key enabling technology for realizing sustainable process industry.

Advances in process optimization and process systems engineering were able to deliver sizable improvements in many processes, with more sophisticated integration of heating and coolant flows via process analysis as one example. Significant improvements in terms of cost/performance parameters were realized. Specific thrust on PI broadened these efforts by including development of better catalysts, routes, equipment, and advanced process control methods. PI may be broadly defined as the ability to obtain better results in terms of purity, conversion, and yield of the desired product by manipulating rates of relevant transport processes and chemical reactions so as to enhance overall performance (more throughput, better quality, less energy consumption, less waste, safer, etc.). Stankiewicz and Moulijn [10] have defined the modern interpretation of PI as "the development of novel apparatuses and techniques that are expected to bring dramatic improvements in manufacturing and processing, substantially decreasing equipment size, energy consumption, or waste production, and ultimately resulting in cheaper, sustainable technologies." This drive on PI in recent years has led to many new enhancements including multifunctional reactors/process equipment and new ways of significantly enhancing driving forces (such as use of nontraditional energy sources). Recently, Utikar and Ranade [11] have critically analyzed strategies for intensifying multiphase processes and have captured the suite of tools toward sustainable processes of twenty-first century as shown in Figure 1.3.

In recent years, the key drivers for realizing significant improvements in process industry are as follows:

- Circular economy: This involves prudent management of resources with careful analysis of social and environmental implications of manufacturing in present and future scenarios [12].
- Digitalization/industry 4.0: There is a significant excitement about the fourth industrial revolution – industry 4.0 and its impact on manufacturing in process

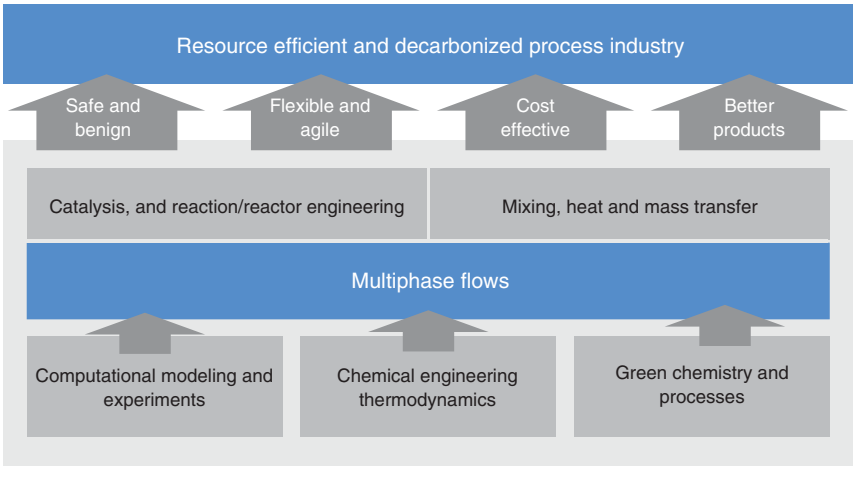

Figure 1.3 Suite of underlying science, enablers, and drivers of sustainable process industry.

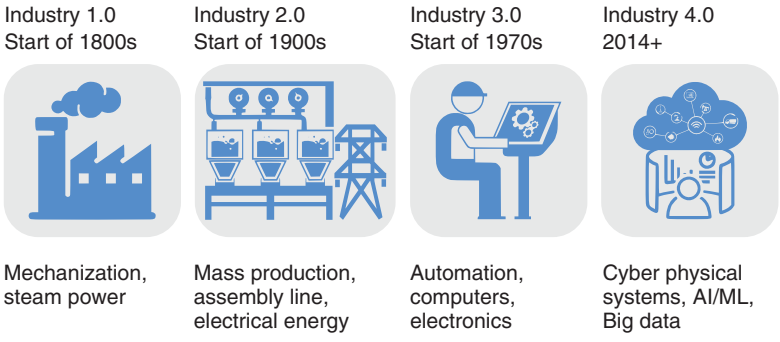

Figure 1.4 Progression of industrial technologies.

industries (see Figure 1.4). The goal here is to combine physical and digital technologies for significantly enhancing overall productivity of manufacturing. It is being argued as the most transformative era for chemical manufacturing [13].

- Product customization and distributed manufacturing: Personalized products are gaining significant attention in recent years. A recent white paper from the EPSRC has identified that small-scale, localized, high-speed, and automated manufacturing platforms are urgently needed, to realize personalized products [14]. The distributed manufacturing with a "factory in a box" approach will indeed be transformational for many sectors.

In all of these key drivers, it is important to have thorough understanding as well as comprehensive ability to simulate multiphase flow encountered in today's processes of relevance. Without such understanding and ability to quantitatively simulate multiphase processes, these envisaged transformations and productivity enhancements cannot be realized. For accelerating these transformations via cutting-edge research and to reduce the time of translating laboratory research and processes to practice as well as to reduce risk at the time of implementation, increased levels of quantitative understanding of science underpinning these processes are essential. Dudukovic [15] has elaborated this in detail and has succinctly brought out the need for quantitative understanding of the micro- to mesoscale (interactions of turbulent mixing with the kinetics, mass transfer, and heat transfer of multicomponent, multiphase systems), of meso- to reactor-scale (developments in computational fluid dynamics, CFD) models replacing ideal-flow models. Although CFD programs for multiphase systems are available, their application for reliable simulations of real-life processes is not straightforward, particularly for complex multiphase systems used in process industries (where processes such as heat transfer, mass transfer, mixing, phase change, and chemical reactions may occur simultaneously). It is therefore essential to critically analyze and understand the current state of the art on computational modeling of multiphase flows for realizing processes promoting circular economy and truly distributed manufacturing of new-age customizable products. In this book, we have made such an attempt. The following section briefly discusses key aspects of multiphase flows relevant to process industries.

1.2 Multiphase Flows

Process industry carries out desired transformations – physical, chemical, and biochemical transformations for creating products that meet customer needs without compromising safety, environment, and economics. Most of these transformations involve contacting different material streams, and therefore flow of materials (gases, liquids, and solids) is essential. Over the years, engineers have evolved several ingenious ways to achieve the desired flow and contact of materials. The desired flow of materials is achieved either by harnessing pressure, gravity, or surface forces or by employing rotating/moving elements. In several heat-transfer and mass-transfer equipment, fluids flow through conduits or in thin layers over solid surfaces to facilitate heat and mass transfer. A design engineer is often interested in finding out the characteristics of films/boundary layers and transport rates over different shapes. There are continuous attempts to evolve and develop new ways of optimizing the wall/conduit shapes so as to ensure maximum utilization of the supplied energy. Quantitative relationships between the throughput and operating flow regime, structures within the film, thickness of the film or boundary layer, pressure drop, wetted area, heat-transfer and mass transfer coefficients, and residence time distribution are needed for realizing best possible outcome from multiphase flow processes. Several flow processes use one or more moving elements to realize the desired fluid dynamics. The shape, size, number, and location of rotating/moving elements control the underlying fluid dynamics. For example, in stirred vessels, the design, number, location, and operating speed of the impeller profoundly affect the performance of the stirred vessel. In process equipment, several processes take place simultaneously (mixing, heat transfer, mass transfer, solid suspension, precipitation, agglomeration, breakage, and so on). The foremost expectation of a design engineer is, therefore, to clearly understand each of such processes and the interactions between these processes.

There are several ways of classifying these multiphase flows. The simplest, first layer classification is according to the presence of thermodynamic phases: gas–liquid, gas–solid, gas–liquid–solid, liquid–liquid, liquid–solid, and so on. Typical examples of these flows and equipment encountered in the process industry are given Table 1.1. In a gas–liquid flow, either the liquid, or the gas, or both, can be continuous. A continuous phase is a phase that occupies continuously connected regions of space. For example, in a bubble column, discrete gas bubbles pass through a continuous liquid. On the other hand, in a spray tower, dispersed liquid droplets move through a continuous gas phase. A dispersed phase occupies disconnected regions of space – for example, bubbles, drops, and particles. In case of oil and gas flow in a pipeline, a segregated flow might be observed in which the oil moves along the bottom of a pipe and the gas along the top. In this case, both phases are continuous. Similarly, liquid–liquid flow can also be either dispersed or continuous. Typical examples of process equipment are liquid–liquid extractor and oil–water transport. Gas–solid flows are usually a gas with suspended solid particles. The examples of such flow extend from fluidized beds to pneumatic transport. When the

Table 1.1 Examples of multiphase flows.

Type of flow	Illustrative flow conditions	Example of process equipment
Gas–liquid flow	Bubbly flows	Bubble column
	Separated flows	Falling film evaporator
	Gas-droplet flows	Mist eliminator
Liquid–liquid flow	Dispersed flow	Liquid–liquid extractor
	Slug flow	Micro-reactor, oil–water transport
Gas–solid flows	Gas–particle flows	Cyclone separator
	Pneumatic transport	Air conveying system
	Fluidized beds	Fluidized bed dryer
Liquid–solid flows	Slurry flows	Crystallizer
	Hydro-transport	Oil sands transport circuit
	Sediment transport	Thickener, Clarifier
Gas–liquid–solid (three-phase) flows	Bubbles in a slurry flow	Floatation
	Droplets/particles in gaseous flows	Spray scrubber
More than three phases	Gas–liquid–liquid–solid flows	Stirred multiphase reactor

flow is dominated by motion of particles, such as in case of rotary kiln, or flow in a storage silo, it is categorized as granular flow. Liquid–solid flows are also known as slurry flows. These flows involve transport of solid particles using liquid and cover a wide range of applications from crystallization to thickeners and clarifiers. Several process equipment such as trickle bed reactors, flotation systems, etc. encounter three-phase flows in which all gas, liquid, and solids are present.

For multiphase flow processes, several operating flow regimes may exist due to relative motion of the phases to each other. Flow regimes are defined based on characteristic structures or topological configuration of multiphase flows. Identification or realization of the desired flow regime is one of the crucial tasks of the design engineer. Each component of the classes can be grouped according to the flow regimes (topology of the flow). Broadly, the flow regimes are classified as dispersed flows, mixed flows, and separated flows [16]. In dispersed flows, all the phases, except one, exist as dispersed (discontinuous) particles flowing through the continuous fluid. Examples of this flow regime include bubbles in liquid, solid particles in gas or liquid, and liquid droplets in gas or other immiscible liquid. In separated flows, none of the phases exist as discontinuous particle form. All the phases flow in a semicontinuous mode with interface between different phases. Examples of this flow regime include film flow, annular flow, and jet flow. In mixed-flow regimes, dispersed particles and semicontinuous interface exist together. Examples of this regime include droplet annular flow (where liquid flows in the form of annular film over pipe as well as suspended droplets in the gas core), bubbly annular flow (where some gas bubbles flow through the annular liquid film), and slug flow. Separated or mixed-flow

regime may exist in trickle bed reactors, rotating packed beds, and other process equipment.

Occurrence of various flow regimes highlights the importance of various subprocesses and their interactions over a wide range of time and length scales. Understanding of these interactions is a key to mastering multiphase flows. Conventionally, various dimensionless numbers are used to quantify relative importance of different subprocesses. Some of the key dimensionless numbers for multiphase flows are as follows:

$$\text{Reynolds number} = Re = \frac{\text{Inertial force}}{\text{Viscous force}} = \frac{LV\rho}{\mu}$$

$$\text{Froude number} = Fr = \frac{\text{Inertial force}}{\text{Gravity force}} = \frac{V^2}{gL}$$

$$\text{Weber number} = We = \frac{\text{Inertial force}}{\text{Surface force}} = \frac{LV^2\rho}{\sigma}$$

$$\text{Eotvos number} = Eo = \frac{\text{Buoyancy force}}{\text{Surface force}} = \frac{\Delta\rho g L^2}{\sigma}$$

Additional dimensionless numbers may be written as a combination of these. For example,

$$\text{Capillary number} = Ca = \frac{\text{Viscous force}}{\text{Surface force}} = \frac{\mu V}{\sigma} = \frac{We}{Re}$$

where L and V are characteristic length scale and velocity scale; ρ, σ, and μ are density, surface (or interfacial) tension, and viscosity of characteristic phase(s). Meaningful choice of these characteristic properties as well as length and velocity scale depends on the type of multiphase flow under consideration. These dimensionless numbers are often used to define and correlate key characteristics of multiphase flows.

Some of the commonly encountered multiphase flows and their flow regimes in process industries are realized by using pressure, gravity, or surface forces or by employing rotating/moving elements and are shown schematically in Figure 1.5. In process equipment handling solids, solid particles may be suspended within a continuous phase. Depending on the properties of fluid and solid particles, geometrical configuration of process equipment and operating flow rates of gas and solid phases, several different subregimes of dispersed flows may exist (ranging from dense bed – bubbling bed – fast fluidized bed to pneumatic transport). In all these flow regimes; the relative importance of fluid–particle, particle–particle, and particle–wall interaction is different.

For many gas–liquid or gas–liquid–solid processes, liquid phase is a continuous phase in which gas bubbles and solid particles are dispersed (bubble columns, multiphase stirred tanks, and so on). Bubble columns may also exhibit different subregimes, namely homogeneous bubbly flow, churn-turbulent flow, and slug flow depending on the geometry, operating conditions such as flow rates, pressure, temperature, and physical properties of individual phases. The characteristics of these regimes are quite different from each other, and each regime may require specialized models and boundary conditions. When there is further increase in gas

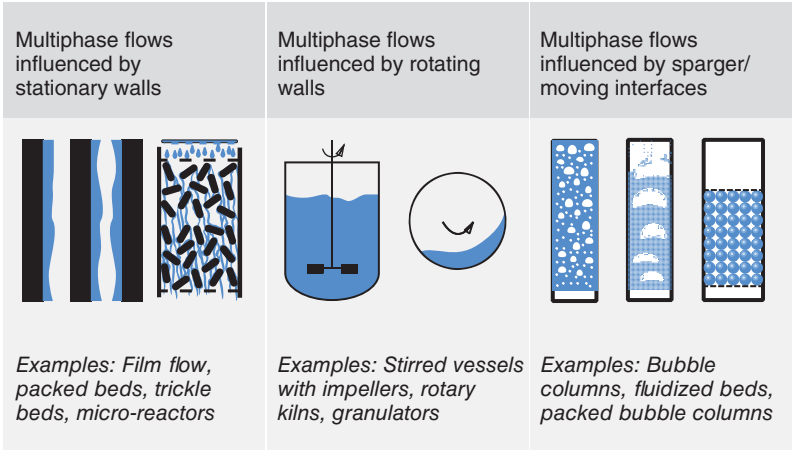

Figure 1.5 Different types of multiphase flows.

flow rate, in some cases, frothing may occur. Beyond frothing, further increase in gas flow rate may make gas as a continuous phase with liquid drops dispersed in it. When an additional flow-modifying element, such as rotating impeller in stirred tanks, is present, one may have to use different classification for the flow regimes. Other special types of process equipment may have different flow regimes specific to those particular configurations. For example, in trickle bed reactor, liquid and gas flow through a packed bed of solid particles. Gas and liquid phases maintain a free interface and flow over solid particles. Several flow regimes may occur in such trickle bed reactors. All these examples of different types of multiphase flows highlight importance of various subprocesses and their interactions over a wide range of spatiotemporal scales.

Dispersed multiphase flows are inherently unsteady. Interaction between the hardware configuration (distributor design, internals, etc.), operating conditions (flow rates, phase fractions, temperature), physical properties of all of the phases, and flow regime and resulting flow needs to be known. Even small-scale hardware details may have a dramatic influence on the resulting flow structure. The role of the size distribution of dispersed-phase particles on the operability and performance needs to be known. Interface phenomena also play a significant role. It is, therefore, of paramount importance to develop understanding and predictive tools for understanding multiphase flow processes for developing process technologies and industries.

Most of the multiphase flow processes involve subprocesses with interactions over a wide range of spatiotemporal scales. For example, in flows through packed beds, complex structure of porous medium comprising macro-pores existing between pellets or packed solid particles and micro-pores within the porous solid particles and its interaction with various phases flowing through the bed determine the operating regime and other key characteristics. Several issues such as isotropy of the porous medium, initial distribution of gases, characteristics of solid particles, ratio of characteristic length scale of solid particle and that of reactor, and so on influence the flow within such packed beds.

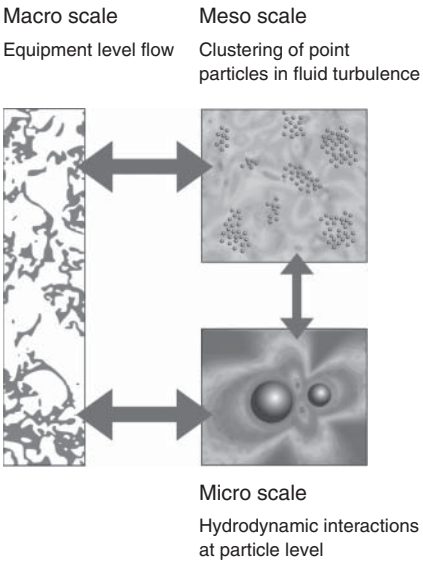

Figure 1.6 Interdependency of micro- and macro-scales.

Processes occurring on different scales influence each other and govern overall behavior of multiphase flow processes (see a schematic shown in Figure 1.6).

The idea of a hierarchy of multiple scales controlling variety of processes is not new. However, in early studies, the subprocesses on multiple scales were usually analyzed in a sequential mode (onion structure, Vlachos [17]): the smaller (finer) scales are analyzed first and information is passed to the larger scale. More often than not this is a one-way information traffic paradigm. These analysis and models based on these were rather simple and could provide tools to understand multiphase flow processes. Building simple models reflecting the essentials of complex processes was the trademark of the profession of chemical engineering. However, with the spectacular computational science and technology, it is now being expected that computational models will realize virtual process engineering, which will replace an experience-and-experiment-simplified models process engineering. It is expected that computing will enable next wave of process innovations and facilitate new age, sustainable process industries.

If this dream of virtual process engineering is to be realized, it is essential to develop a thorough understanding and accurate computational models of industrially relevant multiphase flow processes. The only way to realize this is via better understanding of various subprocesses occurring on multiple scales, which underpin such multiphase flow processes. It is customary to organize interactions over a wide range of scales into three broad groups of scales, namely micro-scales, meso-scales, and macro-scales. Obviously, the groupings depend on the objective under consideration, and it exhibits a fractal character: for every objective under consideration, one may organize scales into these three broad groupings. Meso-scales refer to the intermediate scales, which interact to shape the global behavior of the system [18]. Reasonable description of the structures at such scales is a bottleneck for reliable and accurate modeling of global behaviors. Therefore, ability of process engineers to accurately simulate multiphase flow

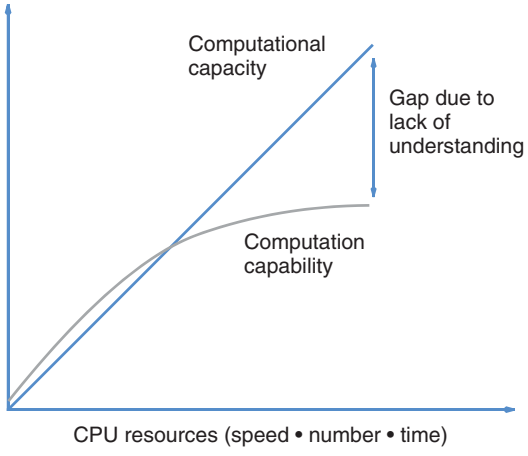

Figure 1.7 Divergence between computational capability and computer capacity.

processes has not kept the tremendous pace of increase in computing ability (see Figure 1.7).

In order to harness the advances in computing capability to the fullest extent and realize virtual process engineering, it is essential to develop comprehensive "multi-scale" understanding and models of multiphase flows. This requires assimilation of available empirical information and experimental data, use of recent advances in experimental techniques to improve our understanding and generate new experimental data for validation of computational models and judicious development of computational models to simulate multiphase flows. This book attempts to provide a platform to achieve this.

Several excellent resources on multiphase flows are available. Without going back before 2000, here we cite some examples of these resources. The book by Ranade [19, 20] provides an excellent basis for developing and applying computational flow models to simulated reactors and equipment of interest to process industries. Worner [21] provides a very compact introduction to multiphase flows and computational models. The handbook of Michaelides et al. [22] covers details of various numerical approaches for modeling multiphase flows – including direct numerical simulations (DNSs), lattice Boltzmann methods, immerse boundary methods, and probability distribution function–based models. Widely used Euler–Euler and Euler–Lagrange models for variety of multiphase flows are included as well. The handbook also covers models for cavitation, boiling, and condensation. Detailed modeling of collisions, aggregation, breakup, and wall impact are included. Brennen [23] provides extensive discussion and models on cavitation in addition to other aspects of multiphase flows. In their comprehensive review, Joshi and Nandakumar [24] have presented key aspects of computational modeling of multiphase flows. Their focus was on developing a rational methodology for mapping a large design space with the help of validated, high-fidelity models. More information on computational techniques may be found in Yeoh and Tu [25]. Wider and more general information about the multiphase flow processes may be found in Michaelides et al. [22] and Yadigaroglu and Hewitt [26]. Though these and many

other references cited therein provide significant and useful information about multiphase flows, specific aspects of multiphase flows relevant to process industries and their applications to enable process innovations are the unique focus of this book. Overall organization of the book is discussed in the following section.

1.3 Organization of This Book

The information in this book is organized to enable process innovations via understanding of multiphase flow processes. The material in this book is organized mainly in two parts. The first part presents fundamental aspects of multiphase flows in three chapters. Different types of multiphase flows and different flow regimes are discussed in Chapter 2. Over the years, significant information on multiphase flows has been accumulated. Chapter 2 synthesizes this information and presents it in a form useful to develop better understanding of different spatiotemporal scales associated with different multiphase flows. Empirical and semiempirical correlations available in the published literature are critically reviewed to facilitate estimation of key characteristics. A large variety of simplified models of multiphase flows such as drift flux models and other lower-order one-dimensional models are discussed. The relationship between lower-order models and detailed computational fluid dynamics–based models is discussed.

In recent years, there have been tremendous advances in experimental techniques. These advances have opened up entirely new ways of looking at multiphase flows and allow insights into micro-, meso-, and macro-scale characteristics of variety of multiphase flows. It is essential to use these state-of-the-art experimental techniques to generate high-quality experimental data to validate various submodels representing various scales of multiphase flow processes. Overall process of verification and validation of computational models is shown in Figure 1.8.

Conventional modeling approaches rely on using experimental data for calibration and validation purposes. Unfortunately, no systematic framework is available for calibrating multiphase flow models. There are several published studies that claim to validate computational models by comparing macroscopic results (such as

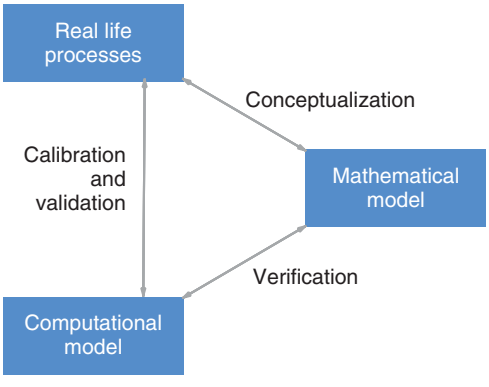

Figure 1.8 Verification and validation of mathematical and computational models.

conversion and selectivity profiles while simulating multiphase reactors) without independently validating submodels or without fully discussing sensitivity and values of the adjustable parameters used in the computational model. Such studies, though may be useful to achieve specific goals pertaining to the considered case, have limited generality and use from the perspective of virtual process engineering. Several excellent reviews on experimental techniques are available which may be used for selecting appropriate measurement techniques for obtaining data relevant for validating computational models. Some of the older reviews (e.g. Joshi et al. [27]) or books (e.g. Chaouki et al. [28]) provide excellent summary of the techniques useful for obtaining quantitative data. Powell [29] has discussed five non-invasive measurement techniques for multiphase systems. The detailed discussion on advances in experimental techniques relevant to multiphase systems may be found in recent reviews by Refs. [30–36]. These recent advances in experimental techniques provide unprecedented opportunity to develop systematic insights and database for possible calibration and validation of various submodels of different relevant scales in multiphase flows. This chapter presents key experimental techniques relevant to multiphase flows that are broadly grouped into three types (i) flow imaging and visualization, (ii) velocimetry techniques, and (iii) tomography and radiography techniques. The chapter also discusses characterization of multiphase flows in pilot and commercial units. Possibility of using real-time data for calibrating computational models and thereby realizing high-fidelity models is briefly discussed in the last chapter of the book.

The theoretical and numerical basis of computational flow modeling (CFM) is described in detail in Chapter 3. Three major tasks involved in CFD, namely mathematical modeling of fluid flows, numerical solution of model equations, and computer implementation of numerical techniques, are discussed. The discussion on mathematical modeling of fluid flows has been divided into two subsections: dense gas–solid flows and gas–liquid or gas–liquid–solid flows. Basic governing equations (of mass, momentum, and energy), ways of analysis, and possible simplifications of these equations are discussed. In most of the cases, industrial processes are operated under turbulent flow regime. Introduction to turbulence and various approaches (DNS, large eddy simulations (LES), and Reynolds averaged Navier–Stokes (RANS) equations simulations) for modeling turbulent flows are discussed. The Euler–Euler and Euler–Lagrange approaches for modeling multiphase flows are discussed in detail with special emphasis on dispersed multiphase flows. For relatively denser multiphase flows, where DNS becomes impractical to use, the Eulerian–Lagrangian approach is commonly used. This approach is routinely used for the design of coal-fired burners, cyclones, electrostatic precipitators, mist eliminators, and so on. For dense dispersed-phase flows, the Eulerian–Eulerian approach is used, in which appropriate closure models are needed. The approach requires extensive modeling efforts and potentially may be applied to the simulation of complex industrial multiphase equipment consisting of a large number of dispersed particles. Current multiphase CFD models are still not in a position to make "a priori" quantitative predictions of interphase transport rates. For simulating complex multiphase flows, often it is necessary to use multiple modeling

approaches for developing the adequate understanding of the flow processes under consideration. Numerical solution of model equations and effective simulation strategies are discussed as well. Guidelines for making appropriate selection of available techniques based on the objective at hand are discussed. Practical ways of estimating errors in numerical solution of model equations are discussed.

Chapters 2 and 3 constitute the first part of this book. These fundamentals – flow regimes, lower-order models, experimental techniques, and computational flow models, provide insights and ability to quantitatively predict multiphase flows used in practice. Applications of these for simulating industrially relevant multiphase flows are discussed in the second part of the book comprising Chapters 4–10. The second part of the book discusses overall methodology of using insights, experimental data, and computational flow models of multiphase flows for enabling process innovations. The necessity of using hierarchy of modeling tools and establishing clear relationship between process innovation objectives and computational flow model is illustrated with the help of examples. Importance of physical understanding of the system for facilitating rational simplification of problem, formulation of appropriate boundary conditions, and identification of key issues is emphasized. The information discussed in Part 1 is used to evolve a systematic methodology for enabling process innovations. The methodology is illustrated with the help of some practical examples.

The discussion in this part is organized as per different types of multiphase flows. A separate chapter is devoted to major types of multiphase flows, namely gas–solid flows, gas–liquid (–solid) flows, liquid–liquid flows, flows through packed beds, and multiphase flows with phase change. Recent work on modeling these complex multiphase flows is critically reviewed. The modeling approaches and the flow results obtained therefrom are evaluated from the point of view of their application to process improvements/intensification. Limitations of the current state of knowledge in describing complex underlying physics of some of the flows relevant for process innovations are discussed. Despite such limitations, suggestions are made for making the best use of these computational flow models for stimulating process innovations.

Gas–liquid and gas–liquid–solid flows and process equipment are discussed in Chapter 4. Besides ubiquitous stirred reactors and bubble column reactors, other relatively recent contactors such as spinning disc reactors and oscillatory baffle reactors are also discussed. Key separation equipment such as tray distillation columns and packed columns are also discussed. Emphasis is on how understanding of multiphase flows influences process design, optimization, and innovations. In Chapter 5, liquid–liquid processes and reactors are discussed. Liquid–liquid extractions are widely used in many commercial processes. Key aspects governing liquid–liquid extraction processes such as mixing, dispersion of liquid phase into other, mass transfer, and reactions are discussed. Besides conventional extraction equipment, development of novel contactors is also discussed. Some comments on future development such as computer-assisted properties prediction, liquid–liquid equilibrium calculation as well as numerical simulation of the multiphase-flow regime with mass transfer and chemical transformations are also included.

The chapter provides useful suggestions for harnessing models and successfully applying liquid–liquid processes in practice.

Gas–solid processes are discussed in Chapter 6. Several industrially important processes such as oil refining, mineral processing, polymerization, gasification, and pyrolysis use gas–solid flows. Such gas–solid flows involve multiple scales ranging from characteristic turbulence scales–particle scales–large flow structures–equipment scale. Gas–solid flows have been extensively investigated experimentally as well as computationally and large body of published studies are available in open literature. This chapter briefly reviews and discusses the modeling of gas–solid flows with the help of four case studies. The presented case studies illustrate the use of experimental measurements and computational modeling of gas–solid flows for enabling process innovations. Solid–liquid flows are discussed in Chapter 7. Like multiple applications of gas–solid flows, several applications handling solid particles involve the presence of liquid. Solid–liquid flows occur in, for example, paints, suspensions, ceramic, paper pulp, food processing to mining processes. Several liquid-phase chemical transformations use solid catalysts. Different types of process equipment are used for processing solid–liquid systems such as stirred tanks, slurry columns, and trickle bed reactors. This chapter discusses applications ranging from slurry transport, particle separation via cyclones, stirred tanks, and liquid–solid fluidized beds. A few application examples are discussed to bring out importance and usefulness of modeling of multiphase flows. The discussion will be useful to select appropriate modeling approach and provides useful suggestions for applications.

Process involving three or more phases is discussed in Chapter 8. Various examples that demonstrate use of computational models to three-phase processes are presented. The capability of multiscale phenomenological models and CFD models to simulate influence of local hydrodynamics on reactor performance is illustrated. Examples covering multiphase bubble columns, stirred tanks, and ejector jet reactors are discussed. Need for adapting a multiscale approach is highlighted. Chapter 9 covers modeling and applications of trickle bed reactors. A stage-wise approach for modeling complex flows and reactions in trickle bed reactors is presented. The last chapter of Part 2 (Chapter 10) discusses key issues pertaining to multiphase flows with phase change. Additional complexities imposed by phase changes such as boiling, cavitation, evaporation, crystallization, and melting are briefly discussed. Ways of extending multiphase models discussed in earlier chapters for simulating flows with phase change are discussed. Some illustrative case studies are presented to bring out key issues and strategies for addressing them.

In the last chapter of the book (Chapter 11), the current state of the art on multiphase flow modeling is reviewed. A need for developing better multiscale models and multilayer models is emphasized. Need to develop appropriate verification, validation, and model calibration practices is discussed. The lessons learnt from our experience of applying CFM to complex multiphase systems are briefly summarized. Some comments on selecting right level of complexity and modeling approach are included.

The role and potential of recent trend of developing specialized vertical application tools are discussed. General-purpose modeling tools have limitations and may become unmanageable code or difficult to support if attempt is made to expand the application horizons of monolithic code. There is an increasing trend to use such general-purpose codes (either commercial or open source) as basic computing engines over which a dedicated vertical application is developed. The vertical application includes possibility of integrating experimental data, correlations, and other semiempirical models along with the rigorous multiscale models to develop easy-to-use and easy-to-deploy tools for catalyzing process innovations. Such application-specific focused tools to facilitate engineering decision-making provide computing infrastructure to integrate and assimilate different modeling technologies and experimental data and may eventually act as expert systems.

Availability of noninvasive sensors, data processing, advances in multiphase flow modeling and machine learning may open up opportunities for developing high-fidelity computational models by combining real-time data, computational flow models, and physics-based machine learning. The role and potential of combining computational flow modeling with real-time data and machine learning for realizing digital twins of multiphase systems and thereby realizing significant productivity enhancements are discussed at the end. We hope that this book provides a framework and useful guidelines for enabling process innovations via deeper understanding and accurate modeling of multiphase flows.

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Part II

Fundamentals of Multiphase Flows

2

Multiphase Flows: Flow Regimes, Lower Order Models, and Correlations

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2.1 Introduction

Chapter 1 has clearly brought out the crucial importance of the knowledge of flow, temperature, and concentration fields in process equipment. Such a knowledge is needed for complex geometries and multiphase flows which may be laminar or turbulent. Such knowledge is obtained by solving governing equations (statements of conservation of mass, momentum, energy, and species). During the past 100 years, methods are being developed for solving the governing equations. Initial period heavily depended on extreme simplifications in governing equations and supplement the poor knowledge of flows by experimented data collected on laboratory and pilot scales. It remained always the desire of the researchers/design engineers to know the behavior of any designed equipment a priori before it comes to actual operations. Figure 2.1 shows the methodology used to describe the relationship between the physical world and the simulation/conceptual world. The phenomena observed in the physical world are modeled mathematically, and the solution to the mathematical models is obtained to predict the physical phenomena under consideration. Various models depending upon the requirement of resolution in spatial domain are utilized for solving the conservation equations describing the system behavior. Feedback plays an important role in such simulations; hence, experimental data from the physical world are of utmost importance. After comparing the predictions of the mathematical models with actual experimental data, the models and its parameters are varied to have a better prediction.

These models have been developed over a century. Joshi and Nandakumar [1] have summarized a large number of innovations (Table 2.1) in the development of a variety of chemical processes, as well as analytical/computational tools used for understanding their performance. Most of these designs were enabled through extensive pilot-scale experimentation and the development of specific

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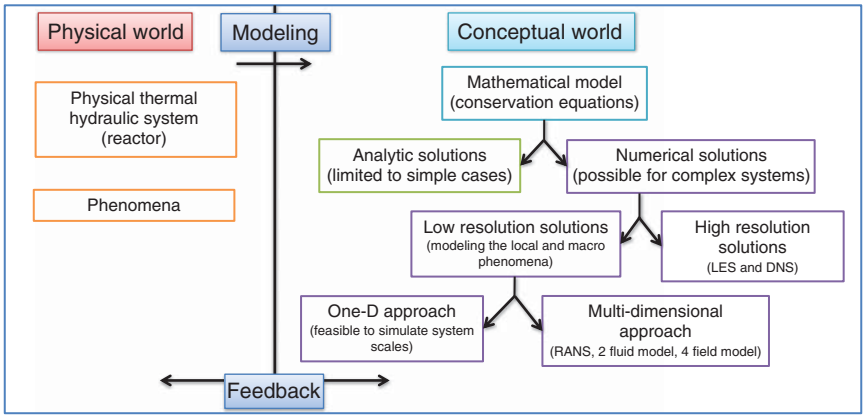

Figure 2.1 Relationship between physical world and conceptual world.

empirical correlations for such performance measures as height equivalent of theoretical plate, plate efficiency, mass, and heat transfer coefficients. Such empiricism has several limitations: (i) the empirical correlation is valid over a range of parameters within which the correlation is proposed; (ii) it assumes some sort of lumped/homogeneous behavior inside process vessels and ignores the macro- and microscale heterogeneities, such as phase fractions, mean and turbulent velocity fields, turbulent kinetic energy, and energy dissipation rates; (iii) the flow pattern in the vicinity of bubble (drop or particle) may get modified by small amounts of adventitious surface active impurities, the concentration of which cannot be measured with the present status of instrumentation; (iv) a separate empirical correlation is typically needed for each design parameter and piece of equipment; (v) model fluids, such as air, water, sand, and glass beads, are used for the data collection on the pilot scale, thus making it difficult to preserve kinematic, dynamic, and geometric similarities between the pilot and field scale processes; and (vi) empirical correlations assume unique dependency of the design parameter on the geometrical parameters or physical properties. For understanding this point, let us consider simple Dittus–Boelter correlation for heat transfer in pipe flow which is given by,

$$\frac{h_w}{k} = 0.023\left(\frac{\rho UD}{\mu}\right)^{0.8}\left(\frac{\mu c_p}{k}\right)^{1/3}\left(\frac{\mu}{\mu_w}\right)^{0.14} \tag{2.1}$$

The above correlation suggests $h_w \propto \mu^{-0.33}$, irrespective of the range of other parameters such as D, U, ρ, k, etc. In reality (particularly in three-dimensional turbulent multiphase flow system), such unique relationship does not hold and they depend on geometrical details during scale-up and the physical properties which are different from those covered in the laboratory.

In modern times, such empiricism is giving way to systematic innovations in process design. These innovations typically begin with the discovery of a chemical in a bench-scale experiment by a chemist. The transition from a bench-scale batch process to a plant-scale continuous process occurs through the ingenuity of an

Table 2.1 Chronological stages of development of process equipment [1].

Stages	Achievements	Tools and techniques
5000 BCE to 1900	Extraction of metals, edible and nonedible oils, natural materials, and their medicinal formulations; making of paper and cloth, pigments, fermentation, food processing, and a variety of construction materials	Apprenticeship-based incremental evolutionary design; design by analogy (if it works in one place, it may work in similar circumstances)
1901–1950	Evolution of the concepts of unit operations, e.g. distillation, absorption, extraction, crystallization, and adsorption; started with George Davis [2]	Algebraic equations as models; graphical methods for nonlinear problems, nomograms; data from pilot plants used in design
1901–1950	Evolution of the concepts of unit processes [3], e.g. oxidation, hydrogenation, alkylation, acylation, nitration, sulfonation, esterification, hydrolysis, carbonylation, ammonolysis, and ozonolysis	Procedures were established for predicting physicochemical properties, phase equilibria, and reaction equilibria; measurement of kinetics of single-phase reaction and lumped kinetics of multiple reactions
1920–1950	Large-scale processing of petroleum crude and petrochemicals led to the development of a variety of tray designs; catalytic cracking was introduced together with the large-scale use of fluidized and circulating fluidized beds; gasoline desulfurization and other catalytic processes saw the development of fixed bed catalytic reactors, pressure swing absorption, simulated moving bed chromatography, and bubble columns for fermentation to give antibiotics	Innovations of reactors and processes happened on laboratory scale followed by validation on pilot scale; several multiphase reactor designs were first commercialized, and subsequent attempts were made to understand their hydrodynamics
1930–2000	Development of theories of heat and mass and momentum transfer, including their analogies, eddy viscosity models, and surface renewal; theories of Higbie [4] and Danckwerts [5]; theories of similitude, modeling, and dimensional analysis with a large number of correlations involving *Re*, *Pr*, *Sc*, *Nu*, and *Sh* were developed	Mathematical models (differential equations) as unifying force became dominant; empirical correlations on the equipment scale with data from pilot plants provided the parameters in the models; development of tools such as ASPEN and HYSIS became possible with the advent of computer
1980 to current	Fundamental understanding of the following: (i) chemical kinetics on the basis of molecular mechanisms; (ii) detailed flow profiles, k–ϵ profile, energy spectra, and other turbulence parameters could be determined; (iii) bubble/drop size distributions, cluster size distribution and dynamics, and flow structures and their impact on transparent phenomena could be understood; and (iv) interface transport mechanisms could be determined	High-performance computing and high-fidelity measurements provided deep insight into transport and reaction processes; density functional theory; molecular dynamics; experimental fluid dynamics; in situ kinetic measurements; computational fluid dynamics; discrete particle modeling; population balance models

Source: Joshi and Nandakumar [1].

experienced chemical process design engineer via several pilot-scale experiments to ensure that process efficiency and safety are maintained.

Often multiphase flow is involved at every step of the way, and it is currently the least understood phenomena. So, process design has remained an art, and hefty design margins are introduced to combat the uncertainties in the process design methodology. Walas's classic 1970 book devoted to the subject of Chemical Process Equipment: Selection and Design have gone through three editions, the latest of which was published in 2012 [6, 7]. It is clear from this work that the design process is still guided by a combination of rules of thumb (evolving from experience), design by analogy (a philosophy that if it worked in one scenario, it might work in a similar scenario), established principles (i.e. ASPEN type of lumped parameter models that result in algebraic equations), data (encapsulating information and experience from pilot-scale experiments), and experience of the designer. Clearly, at the design stage, a large number of degrees of freedom are available, exercised at present in an ad hoc manner, but which could be used to explore a large design space in a systematic manner to develop future plant designs that are energy efficient and environmentally benign, if only the right tools and design objectives are developed. A substantially resolved flow field on the equipment scale as well as the dispersed phase scale (in the vicinity of individual bubbles, drops, or particles) will avoid the heuristic interdependencies and empiricisms of design correlations developed based only on input/output and gross geometrical parameters.

2.2 Modeling of Multiphase Flows

Multiphase flow systems form important part in all industrial equipment designs. The equipment designed for multiphase flows essentially operates in bubbly flows to annular flow regimes. For designing of multiphase flow systems, it is important to first identify the flow regime of operation so that the model's applicability could be ensured. These systems are often designed with a lot of care in terms of margins. For instance, the primary heat transport system of a Boiling Water Reactor (BWR), which is sometimes over designed and makes the system economically very costly. One of the reasons is limited understanding of the complex behavior of systems. Computational Fluid Dynamics (CFD) can play a vital role in designing and optimization of design margins of such two-phase flow systems. These simulations are essentially multidimensional in nature and require hefty computational resources. However, in the absence of large computational power, lower order models are continued to being used, which also provides some judgment for design engineers. Sections 2.2 to 2.9 discuss the chronological development of these lower order models and their mathematical formulations.

This chapter is concerned with the chronological developments in understanding lower order models for different regimes of operation of multiphase flows. This chapter is particularly devoted to the various stages of developments prior

to the emergence of CFD, and these will be referred to as lower order models. The knowledge so gained during all the stages was employed for the design of multiphase process equipment. Obviously, the lower order models had limitations, and the need for CFD was felt (which has been dealt in detail in Chapter 4). At this stage, it was thought desirable to take a stock of the strengths and limitations of lower order models, expectations, and realizations of CFD.

2.3 Chronological Development of Mathematical Models

Two-phase flow provides better opportunities for the process designers of any industry in terms of enhanced mixing and heat transfer and in turn better economical product at end. Key to design efficient products always lies in the better understanding of the physics of flow and its modeling. Mathematical modeling of any physical phenomena is essential to have insights in it. In very primitive days of designing of two-phase flow systems, zero-dimensional models were used. Those models essentially provide mass and energy conservation without any movement of the fluid. Transient mass and energy equations are solved for a static system under consideration. These models are able to handle the mixing and heat transfer and chemical reaction problems inside a chamber for instance. Still mass and energy balances are solved for designing the thermal hydraulic systems like heat exchangers. These models utilize the empirical correlations for calculations of the interaction coefficients like heat transfer coefficient. For resolving the fluid flow issues in two-phase flows, homogeneous flow models are the next developments in the series. These models solve three-conservation equations for mass (scalar), momentum (vector), and energy (scalar) also known as effective property models. The fluid properties are evaluated based on the average void fraction estimated empirically. The models are able to solve many engineering problems in homogeneous flow regimes particularly in multiphase flows with low voidages. However, due to the assumption of zero slip at the interface in the two-phase flow systems, these models have limitations. Further refinement in this sequence is drift flux model proposed by Zuber and Findlay [8]. They accounted for the slip between the phases by providing extra equation for slip in term of drift velocity. These models included the non-uniformity of voidages along with continuous and dispersed phase velocities in transverse directions. It is a notable engineering effort to analyze two-phase flow at competitive computational cost. In 1980s, Ishii proposed one-D two-fluid model for two-phase flows [9]. The model utilizes averaged NS equations for two-phase flow. It was a breakthrough at that time. The model became very popular and reliable, and it was used for analysis in many system codes like RELAP and CATHARE. These codes still are preferred and used for reactor safety calculations. In addition to these one-D models, parallel developments were happening for multidimensional models. Drew proposed the three-dimensional model for two-phase

flows with phase change [10]. The model proposed by them requires large numbers of closures for modeling the interphase transfer mechanisms like interfacial forces and heat transfer. Still, the situation is the same to this date with large number of empirical correlations forms the part of the three-dimensional modeling of two-phase flow. These correlations are either obtained from analytical theory, experiment, or by direct numerical simulations (DNS). Considering the topology of the multiphase flows, broadly three methods exist for CFD simulations viz field average model, interface tracking models, and entity tracking models (Figure 2.2). While field average models treat the multiphase flows equivalent to an average flow based on the weighted void parameters, the interface tracking or entity tracking models resolve the interfaces separating the flows or the flow field of the dispersed phase like bubbles in the bubble flows and water drops in the mist flows. Later, models require enormous computational capacities. With increasing computational capacities, high-resolution simulations interface tracking or entity tracking (LES and DNS) has also become feasible. These simulations are useful for microscale understanding of the phenomena. Owing to the computational cost-effectiveness, one-dimensional field averaging models are vastly used for system scale simulations. In the subsequent sections (Sections 2.2 to 2.9), comprehensive details of these models and their development are explained with examples.

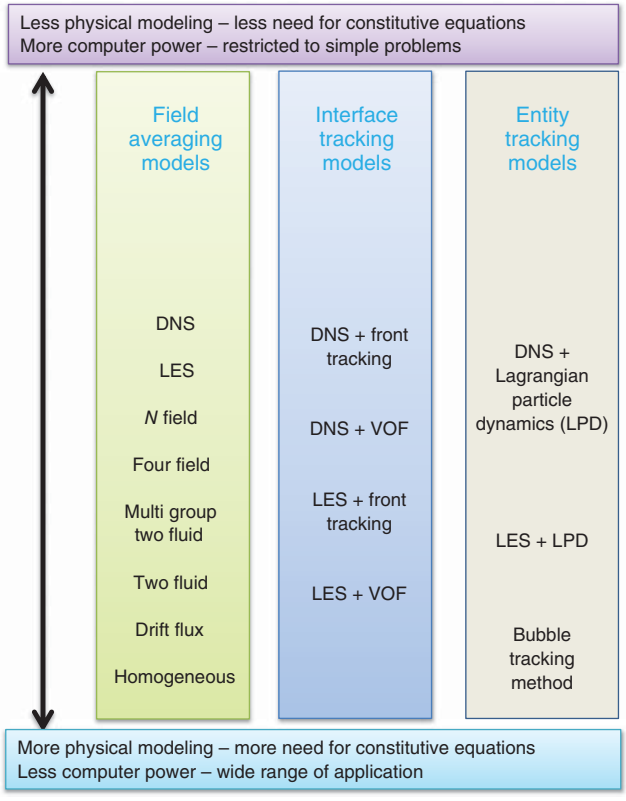

Figure 2.2 Various models for multiphase flows.

2.4 Zero-Dimensional Two-Equation Model

This model solves the mass and energy conservation for a static system under consideration, e.g. mass and energy balances for a vessel. It does not solve the momentum equation. Only an open thermodynamic system is considered with mass and energy balance. Transient analysis of cooling of a sphere is a typical example. Besides, mixing of the two streams with different temperatures inside a stirred vessel is also an example that can be handled with zero-D model.

Figure 2.3 shows a typical system that can be analyzed with zero-dimensional model. Two streams with mass flow rate m_1 and m_2 and enthalpy with h_1 and h_2 enter a tank and get mixed inside the tank with the help of an agitator. Here, one can find out the temperature and enthalpy of the mixer coming out from the tank.

Mass conservation for the tank gives:

$$m_1 + m_2 = m_3 \tag{2.2}$$

And, energy balance gives:

$$m_1 h_1 + m_2 h_2 + W_{\text{stirrer}} = m_3 h_3 \tag{2.3}$$

2.5 Homogeneous Equilibrium Model

Homogeneous equilibrium model treats multiphase phase flow as well mixed flow of the two or more phases with no slip at interface along with thermodynamic equilibrium. Here, the phases move with the same velocity. The phases exist only at the same temperature (they are at the saturation temperature for the prevailing pressure). The governing equations for one-dimensional area averaged equation can be obtained from the classical integral approach using the Reynolds Transport Theorem. In this case, all the phases (here, a case for two phases has been considered) are assumed to be well distributed in the entire cross section of the pipe so that the mixture of the two-fluids can be assumed to be a single fluid with averaged properties. This model does not assume variation of holdup within cross section due to its one-dimensional nature.

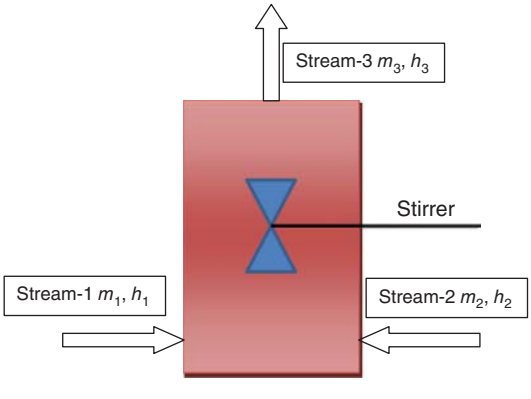

Figure 2.3 Zero-dimensional system example.

For instance, the conservation of mass for a gas liquid system is written as:

$$\frac{\partial(\overline{\rho}_m A)}{\partial t} + \frac{\partial(\overline{\rho}_m \overline{u}_m A)}{\partial z} = 0 \tag{2.4}$$

$$\overline{\rho}_m = \rho_L \overline{\alpha}_L + \rho_G \overline{\alpha}_G \tag{2.5}$$

In homogeneous no-slip model, as both phases are well dispersed (at every point as it is idealized), the average velocity of both the phases would be same as the mixture velocity and hence the slip s, defined as

$$s = {}^{\overline{u}_G}\!/_{\overline{u}_L} = \frac{x}{1-x}\frac{\rho_L}{\rho_G}\frac{1-\alpha_G}{\alpha_G} = 1 \tag{2.6}$$

For HEM

$$\alpha_G = \frac{1}{1 + \frac{1-x}{x}\frac{\rho_G}{\rho_L}} = \beta = \frac{Q_G}{Q} \tag{2.7}$$

Here, β is known as volumetric holdup.

The conservation of momentum for the fluid is given as,

$$\frac{\partial(\overline{\rho}_m A \overline{u}_m)}{\partial t} + \frac{\partial\left(\overline{\rho}_m \overline{u}_m^2 A\right)}{\partial z} = -A\frac{\partial p}{\partial z} - \tau_w P_{\text{hyd}} - \overline{\rho}_m A g \tag{2.8}$$

where P_{hyd} is the hydraulic perimeter and τ_w is the perimeter-averaged wall shear stress. In case of steady adiabatic flows with constant gas and liquid densities, the mass balance equation reduces to the condition that the mixture velocity does not vary for a uniform pipe diameter. Thus, the velocity and holdup do not vary along the length of the pipe. However, it should be clear that an expression to close the wall shear stress is required to obtain a solution for the variation of pressure. This is the first encounter of requirement of a two-phase closure model. This is normally done by using the concept of a two-phase multiplier, ϕ^2, which is a multiplication factor required for the estimation of the two-phase pressure gradient, if a suitable single-phase pressure gradient can be computed. This classic approach was given by Lockhart and Martinelli [11]. Many variants have come into play, and four types of two-phase multipliers $\phi_L^2, \phi_{LO}^2, \phi_G^2, \phi_{GO}^2$ are seen in the literature. ϕ_{LO}^2 is discussed here in the chapter. In this case, the two-phase shear stress is computed by multiplying the single-phase shear stress obtained by assuming the entire mass of two-phase flowing as single-phase liquid. The value of wall shear stress for the single-phase case referred above, τ_{wLO} may be expressed as,

$$\tau_{wLO} = f_{LO}\frac{\rho_L \overline{u}_{LO}^2}{2} = f_{LO}\frac{G^2}{2\rho_L} \tag{2.9}$$

where G is the total mass flux obtained by dividing the total mass flow rate by the area of the pipe. The closing relation used for the friction factor f_{LO} in pipes is,

$$f_{LO} = CRe_{LO}^{-n} \quad \text{and} \quad Re_{LO} = \frac{\rho_L \overline{u}_m d_{\text{hyd}}}{\mu_L} \tag{2.10}$$

where μ_L is the viscosity of the liquid and d_{hyd} is the hydraulic diameter. The values for C and n are (typically) 16 and 1 or 0.079 and 0.25, respectively, for Re below or

above 1500. Finally, under the assumption that the wall shear stress in two-phase flow would be similar to single-phase flow except for the use of homogeneous mixture properties, the two-phase multiplier can be shown to be

$$\frac{\tau_{w\text{-2phase}}}{\tau_{wLO}} = \phi_{LO}^2 = \frac{\rho_L}{\rho_m}\left(\frac{\mu_L}{\mu_m}\right)^{-n} \tag{2.11}$$

Often, the viscosity term is neglected as the predictions do not vary too much from the experimental data. Thus, system of equations is closed for adiabatic flows.

In the case of diabatic flows wherein phase change occurs (as in boiler tubes), the simplified (neglecting viscous dissipation) conservation of energy per unit length of the pipe can be written as,

$$\frac{\partial(\overline{\rho}_m A\overline{h}_m)}{\partial t} + \frac{\partial(\overline{\rho}_m A\overline{u}_m\overline{h}_m)}{\partial z} = q'_w \tag{2.12}$$

where $\overline{h}_m$ is the specific enthalpy (mass flow weighted average across the flow area) of the mixture and q'_w is the heat generated per unit length at the wall. In the case of no-slip flows with thermodynamic equilibrium, it can be shown that

$$\overline{\rho}_m = \frac{1}{\overline{v}_m} = \frac{1}{\overline{v}_L + \overline{x}_{\text{eq}}(\overline{v}_G - \overline{v}_L)} \tag{2.13}$$

where v represents the specific volume and $\overline{x}_{\text{eq}}$ represents the thermodynamic equilibrium quality. The equation of state for the specific enthalpy of mixture is taken as the thermodynamic definition,

$$\overline{h}_m = h_L + \overline{x}_{\text{eq}}(h_G - h_L) \tag{2.14}$$

In case of no-slip equilibrium flows that the thermodynamic equilibrium quality $\overline{x}_{\text{eq}}$ is same as the flow quality $\overline{x}$ defined as,

$$\overline{x} = {}^{\dot{m}_G}/_{(\dot{m}_G+\dot{m}_L)} \tag{2.15}$$

$$\overline{x}_{\text{eq}} = \overline{x} = \frac{1}{1 + (\rho_L/\rho_G)(\overline{\alpha}_L/\overline{\alpha}_G)} \tag{2.16}$$

In case of two-phase flows,

$$\overline{\alpha}_L + \overline{\alpha}_G = 1 \tag{2.17}$$

Thus, we are having a closed system of equations for diabatic flows, and we can solve for $\overline{u}_m$, ρ_m, $\overline{h}_m$, and p variations along the length.

2.6 Drift Flux Model

In the homogeneous flow model, the two-phase mixture is treated as a pseudo fluid with average properties. Both the phases are assumed to be moving with same velocities with no slip. Hence, the next level of complexity starts with the introduction of slip. The motivation stems from the fact that homogeneous model can only be applied to extremely dispersed flows, which are probably valid for

dispersed bubble flows with very small bubble diameters. Even for bubbly flows, it would be unreasonable to assume that the bubbles and liquid flows at the same velocity with no slip. Generally, in two-phase flows, the average gas velocity is higher than that for the liquid. The effect of slip or gas moving faster than the liquid can be accounted for in many ways. The most successful and simplest procedure for this purpose is the drift flux model [8]. However, this model essentially utilizes only three conservation equations but along with those the drift flux model includes one additional equation of drift for accounting slip between the phases so it can be called four-equation model.

The bubble distribution in the two-phase flows across the cross section is not uniform implying that there will be a variation of local gas and liquid holdup in the cross section. At this stage, it is important to note that this model has been primarily designed for bubbly and slug flows, where the dispersed phase is the gas and the continuous phase is the liquid. The variation of local holdup demands the holdup or void weighted averages for properties and field variables as introduced by Zuber and Findlay [8]. For any general variable F, the void weighted average $\langle\langle F\rangle\rangle$ can be obtained by,

$$\langle\langle F\rangle\rangle = \frac{\int_A F\alpha_G \mathrm{d}A}{\int_A \alpha_G \mathrm{d}A} \tag{2.18}$$

The local point values of the void can be measured experimentally by using conductance probe and proper time averaging. The need for void weighting arises from the fact that these can be prescribed by knowing the superficial quantities. For example, the void weighted gas velocity is nothing but the volumetric flow of gas (Q_G) as shown below,

$$\int_{AG} u_G \alpha_G \mathrm{d}A = Q_G \tag{2.19}$$

The relative velocity between the phases can be expressed as:

$$u_{GL} = u_G - u_L \tag{2.20}$$

The drift flux is defined as:

$$j_{GL} = \alpha_G \alpha_L u_{GL} = \alpha_G \alpha_L (u_G - u_L) \tag{2.21}$$

And, total volumetric flux is given by:

$$j = \frac{Q}{A} = \frac{Q_G + Q_L}{A} = \frac{A_G u_G + A_L u_L}{A} = \alpha_G u_G + \alpha_L u_L = j_G + j_L \tag{2.22}$$

Then, from Eqs. (2.21) and (2.22)

$$j_G = j_{GL} + \alpha_G j \tag{2.23}$$

Dividing Eq. (2.23) by α_G and taking weighted average over area, we get

$$\frac{j_G}{\overline{\alpha}_G} = \langle u_G\rangle = \frac{\langle \alpha_G j\rangle}{\langle \alpha_G\rangle\langle j\rangle}\langle j\rangle + \frac{\langle j_{GL}\rangle}{\langle \alpha_G\rangle} = C_0\langle j\rangle + \langle u_{Gj}\rangle \tag{2.24}$$

Again dividing Eq. (2.24) by $\langle j \rangle$

$$\frac{\langle u_G \rangle}{\langle j \rangle} = \frac{\langle j_G \rangle}{\langle j \rangle \langle \alpha_G \rangle} = C_0 + \frac{\langle u_{Gj} \rangle}{\langle j \rangle}$$

$$\frac{\langle \beta \rangle}{\langle \alpha_G \rangle} = C_0 + \frac{\langle u_{Gj} \rangle}{\langle j \rangle}$$

$$\langle \alpha_G \rangle = \frac{\langle \beta \rangle}{C_0 + \frac{\langle u_{Gj} \rangle}{\langle j \rangle}} = \overline{\alpha}_G = \frac{\beta}{C_0 + \frac{\overline{u}_{Gj}}{j}} \tag{2.25}$$

From Eq. (2.25), it is clear that if there is no homogeneous flow and slip velocity is zero, then $\overline{\alpha}_G = \beta$. Here, C_0 is an empirical factor correcting the one-dimensional homogeneous theory to account for the variation of concentration and velocity profiles across the channel in actual case. In the above equation, j_G and j_L are the volume fluxes of gas and liquid, respectively. Thus, the mean drift velocity can be measured, if the local void fraction is measured and averaged and the volumetric flow of gas and liquid is known.

The governing equations for the drift flux model written per unit volume of the pipe are given below. The mixture mass balance can be obtained by adding the mass balance for the gas and liquid phases.

$$\frac{\partial \overline{\rho}_m}{\partial t} + \frac{\partial \overline{\rho_m u_m}}{\partial z} = 0 \tag{2.26}$$

Instead of writing in void weighted quantity, if we write the equation in simple area weighted quantity, the same can be written as,

$$\frac{\partial (\rho_G \overline{\alpha}_G + \rho_L \overline{\alpha}_L)}{\partial t} + \frac{\partial (\rho_G \overline{\alpha_G u_G} + \rho_L \overline{\alpha_L u_L})}{\partial z} = 0 \tag{2.27}$$

It may be noted that the density of the two phases individually can be assumed to be a constant and hence is not inside the averaging operator. To relate the average of the product to the product of the averages, in general, a covariance distribution parameter $C_{x,y}$ is defined as,

$$C_{x,y} = \frac{\overline{xy}}{\overline{x} \cdot \overline{y}} \tag{2.28}$$

This parameter has to be closed empirically using profile assumptions. The value of this parameter for turbulent flows is close to 1 and can be neglected in most cases. Thus, if we ignore this parameter, the mass balance equation can be written as,

$$\frac{\partial (\rho_G \overline{\alpha}_G + \rho_L \overline{\alpha}_L)}{\partial t} + \frac{\partial (\rho_G \overline{\alpha}_G \overline{u}_G + \rho_L \overline{\alpha}_L \overline{u}_L)}{\partial z} = \frac{\partial \overline{\rho}_m}{\partial t} + \frac{\partial \overline{\rho_m u_m}}{\partial z} = 0 \tag{2.29}$$

The vapor mass equation is given by,

$$\frac{\partial (\rho_G \overline{\alpha}_G)}{\partial t} + \frac{\partial (\rho_G \overline{\alpha}_G \overline{u}_G)}{\partial z} = \Gamma_G \tag{2.30}$$

where Γ_G is the mass of vapor generated per unit length of the pipe. It is specified for adiabatic flows or computed using energy equation for diabatic flows.

The momentum equation for the drift flux model can be written as,

$$\frac{\partial(\overline{\rho_m u_m})}{\partial t} + \frac{\partial\left(\overline{\rho_m u_m{}^2}\right)}{\partial z} = -\frac{\partial p}{\partial z} - f_m \frac{\overline{\rho}_m \overline{u}_m |\overline{u}_m|}{2d_{\text{hyd}}} - \frac{\partial}{\partial z}\left(\frac{\overline{\alpha}_G \rho_G \rho_L \overline{u}_{Gj}^2}{\overline{\alpha}_L \overline{\rho}_m}\right) - \overline{\rho}_m g \tag{2.31}$$

If the covariance distribution parameters are ignored, then the equation becomes,

$$\frac{\partial(\overline{\rho}_m \overline{u}_m)}{\partial t} + \frac{\partial\left(\overline{\rho}_m \overline{u}_m{}^2\right)}{\partial z} = -\frac{\partial p}{\partial z} - f_m \frac{\overline{\rho}_m \overline{u}_m |\overline{u}_m|}{2d_{\text{hyd}}} - \frac{\partial}{\partial z}\left(\frac{\overline{\alpha}_G \rho_G \rho_L \overline{u}_{Gj}^2}{\overline{\alpha}_L \overline{\rho}_m}\right) - \overline{\rho}_m g \tag{2.32}$$

In the above equation, a new term using the mean drift velocity, $\overline{u}_{Gj}$ (the relative velocity with which the gas moves faster than the mixture velocity), has been introduced following the work of Zuber and Findlay, and is given by Eq. (2.25) [8].

The above parameter can also be experimentally obtained by locally measuring the velocity of the phases and void. Thus, in drift flux model, in addition to the wall shear stress closure in the form of a friction factor f_m, we need an additional closure that involves two additional empirical parameters. Further, as these parameters are not universal and are flow regime-dependent, methods for predicting flow regimes become necessary.

2.7 One-Dimensional Five-Equation Models

It is basically a Two-Fluid Partial Non-equilibrium model. Here, usually, we solve two mass and two momentum equations for the two phases and one mixture energy balance equation, hence called five-equation model. Other formulations are also possible that includes either mixture mass or mixture momentum equation instead of mixture energy equation. For two-fluid model, we need to solve for six variables, while in five-equation model only five conservation equations are used. In such case, we solve one variable for the mixture, viz temperature of the mixture or velocity of the mixture. Table 2.2 shows various combinations for five-equation models:

2.8 One-Dimensional Six-Equation Two-Phase Flow Models: Axial Variation of Field Variables

2.8.1 Mathematical Formulations

This model was developed in late 1970s by Ishii and coworkers (for instance, Ishii [9]). This is generally a four-equation model for adiabatic flows and six-equation model for diabatic flows. In this case, equations for mass, momentum, and energy conservations are solved for each phase. While the governing conservation equations are simple, the closure equations required for closing the mathematical model are

Table 2.2 Various combinations of governing equations for five equation model.

Five equation models			
Two-fluid partial non-equilibrium 2 – Mass phase balance 2 – Momentum phase balance 1 – Mixture energy balance	$T_L = T_{\text{SAT}}$ or $T_G = T_{\text{SAT}}$	2 – Phase wall friction 1 – Mixture heat flux friction 1 – Interfacial mass 1 – Interfacial momentum	$\overline{\alpha}_G, p, u_L, u_G, T_L$, or T_G
Two-fluid partial non-equilibrium 1 – Mixture mass balance 2 – Momentum phase balance 2 – Energy phase balance	$T_L = T_{\text{SAT}}$ or $T_G = T_{\text{SAT}}$	2 – Phase wall friction 2 – Phase heat flux friction 1 – Interfacial mass 1 – Interfacial momentum 1 – Interfacial energy	$\overline{\alpha}_G, p, u_L, u_G, T_L$, or T_G
Slip or drift non-equilibrium 2 – Mass Phase balance 1 – Mixture momentum balance 2 – Energy phase balance	Slip or drift velocity	1 – Mixture wall friction 2 – Phase heat flux friction 1 – Interfacial mass 1 – Interfacial energy 1 – Slip velocity or drift flux	$\overline{\alpha}_G, p, u_m, T_L, T_G$
Homogeneous non-equilibrium 2 – Mass phase balance 1 – Mixture momentum balance 2 – Energy phase balance	Equal velocity $u_L = u_G = \overline{u}_m$	1 – Mixture wall friction 2 – Phase heat flux friction 1 – Interfacial mass 1 – Interfacial energy	$\overline{\alpha}_G, p, u_m, T_L, T_G$

quite complex and no universal agreement exists for closure laws. The mass balance for each phase per unit volume around an arbitrary point in the flow domain is given by,

$$\frac{\partial}{\partial t}(\alpha_G \rho_G) + \frac{\partial}{\partial x}(\alpha_G \rho_G u_G) = \Gamma_G \tag{2.33}$$

$$\frac{\partial}{\partial t}(\alpha_L \rho_L) + \frac{\partial}{\partial x}(\alpha_L \rho_L u_L) \quad = \Gamma_L \tag{2.34}$$

In the above equations, Γ_G and Γ_L are the mass source of vapor and liquid per unit volume of the pipe. As the interface can store no mass, the interface conditions would demand,

$$\Gamma_G = -\Gamma_L \tag{2.35}$$

Similarly, the momentum equations for the two phases are:

$$\frac{\partial}{\partial t}(\alpha_G \rho_G u_G) + \frac{\partial}{\partial x}(\alpha_G \rho_G u_G u_G) = -\alpha_G \frac{\partial p}{\partial x} - p\frac{\partial \alpha_G}{\partial x} + \alpha_G \rho_G g + F_G^{\text{VM}} + F_G^i + F_G^W + \Gamma_G u_G \tag{2.36}$$

$$\frac{\partial}{\partial t}(\alpha_L \rho_L u_L) + \frac{\partial}{\partial x}(\alpha_L \rho_L u_L u_L) = -\alpha_L \frac{\partial p}{\partial x} - p\frac{\partial \alpha_L}{\partial x} + \alpha_L \rho_L g + F_L^{\mathrm{VM}} + F_L^i + F_L^W + \Gamma_L u_L \tag{2.37}$$

In the above equations, the convective term on the left-hand side has been written after simplifying to the primitive form and taking the velocity inside the derivative. On the right-hand side, the force terms sequentially are the pressure term, body force term, virtual mass, interfacial friction term, wall friction term, and interfacial momentum transfer term due to mass transfer.

Energy equation for gas and liquid phases can be written as

$$\frac{\partial}{\partial t}(\alpha_G \rho_G h_G) + \frac{\partial}{\partial x}(\alpha_G \rho_G u_G h_G) = -\alpha_G \left(\frac{\partial p}{\partial t} + u_G \frac{\partial p}{\partial x}\right) + Q_G^W + Q_G^i + \Gamma_G h_G^* \tag{2.38}$$

$$\frac{\partial}{\partial t}(\alpha_L \rho_L h_L) + \frac{\partial}{\partial x}(\alpha_L \rho_L u_L h_L) = -\alpha_L \left(\frac{\partial p}{\partial t} + u_L \frac{\partial p}{\partial x}\right) + Q_L^W + Q_L^i + \Gamma_L h_L^* \tag{2.39}$$

The first and second terms on LHS are accumulation and convective term which has been written after simplifying to the primitive form and taking the velocity inside the derivative. On the right-hand side, the energy terms sequentially are the work done by pressure, wall heat transfer, interfacial energy transfer term, and heat transfer due to mass transfer.

Here, in this mathematical formulation, the numbers of unknowns are 7, while equations are 6 in numbers, so we have to solve one additional equation that establishes the relation between density and pressure (equation of state).

2.8.2 Closure

2.8.2.1 Regime Maps and Criteria for Transition

The six-equation model requires closures for interfacial friction, wall friction, added mass, and energy equation closures, which depend upon the flow regime. Figure 2.4 shows flow regime map for vertical gas–liquid two-phase flows.

The flow regimes depend on the boiling regime, void fraction, and the mixture velocity. Major flow regimes that are encountered for adiabatic vertical flows are bubbly, slug, and annular flow. Various correlations exist to evaluate the transition conditions from one flow regime to the other based on the void fraction.

2.8.2.2 Momentum Closure

Momentum equation depicted by Eqs. (2.36) and (2.37) requires closures for virtual mass force (F_G^{VM}), interfacial friction force (generally known as drag force, F_G^i, F_L^i), and wall friction force (F_G^W, F_L^W). Empirical models are used for closing these terms in the momentum equations. Various models based on the flow regimes are used for calculating the drag coefficient eventually for calculations of the drag force. Similarly, empirical model for virtual mass coefficient is used for virtual mass force, and two-phase friction multiplier approach is used for evaluation of wall friction factor and pressure drop due to wall friction. Various models used for momentum closures are discussed below.

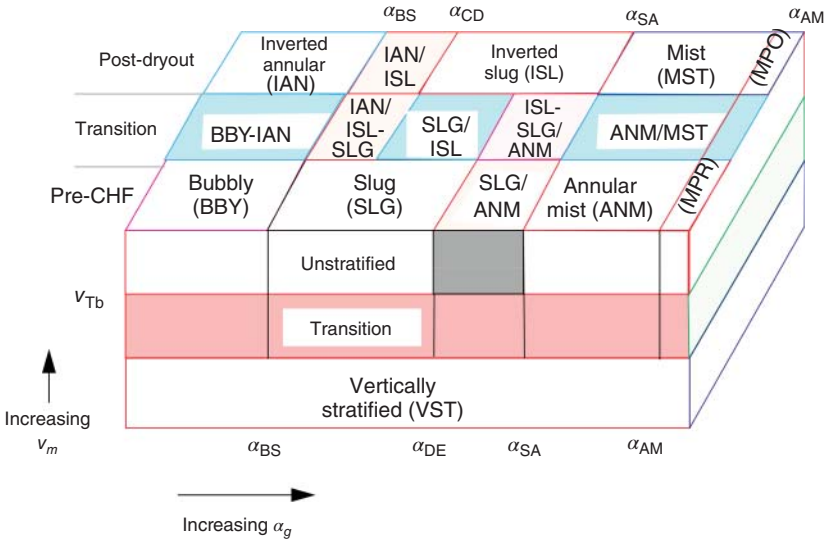

Figure 2.4 Schematic of the flow regime map for vertical flows (RELAP/MOD3.2 Code Manual [12]). Source: RELAP5 Development Team [12].

2.8.2.2.1 Wall Friction

The wall friction model is based on a two-phase multiplier approach in which the two-phase multiplier is calculated from the modified Baroczy correlation [13]. The individual phasic wall friction components are calculated by apportioning the two-phase friction between the phases using a technique developed by Chisholm from the Lockhart–Martinelli Model [11, 14, 15]. The Colebrook–White correlation, 1937, is used to compute the Darcy, 1857 and Weisbach friction factor, 1845, [16–18].

The *modified Baroczy correlation* is expressed as

$$\phi_L{}^2 = 1 + \frac{C}{\chi} + \frac{1}{\chi^2} \tag{2.40}$$

$$\phi_G{}^2 = 1 + C\chi + \chi^2 \tag{2.41}$$

Here, C is the correlation coefficient. The term is expressed as

$$2 \le C < \{-2 + f_1(G) f_2(\Lambda, G)\} \tag{2.42}$$

where,

$$f_1(G) = 28 - 0.3\sqrt{G} \tag{2.43}$$

$$f_2(\Lambda, G) = \exp\left[-\frac{(\log_{10}\Lambda + 2.5)^2}{2.4 - G(10^{-4})}\right] \tag{2.44}$$

where, $\Lambda = \frac{\rho_G}{\rho_L}\left(\frac{\mu_L}{\mu_G}\right)^2$

The *Lockhart–Martinelli Model* computes the overall friction pressure drop in terms of the liquid-alone wall friction pressure drop [11]

$$\left(\frac{dP}{dz}\right)_{2\phi} = \phi_L{}^2\left(\frac{dP}{dz}\right)_L \tag{2.45}$$

Or the vapor-alone wall friction pressure drop

$$\left(\frac{\mathrm{d}P}{\mathrm{d}z}\right)_{2\phi} = \phi_G{}^2\left(\frac{\mathrm{d}P}{\mathrm{d}z}\right)_G \tag{2.46}$$

Here, ϕ_L and ϕ_G are the liquid-alone and vapor-alone two-phase Darcy [17] and Weisbach [18] friction multipliers, respectively.

The phasic wall-friction gradients are expressed in Eqs. (2.47) and (2.49).

$$\left(\frac{\mathrm{d}P}{\mathrm{d}z}\right)_L = \frac{f_L L G_L{}^2}{2D\rho_L A^2} \tag{2.47}$$

$$\left(\frac{\mathrm{d}P}{\mathrm{d}z}\right)_G = \frac{f_G L G_G{}^2}{2D\rho_G A^2} \tag{2.48}$$

The Lockhart–Martinelli Ratio, 1949, is defined as [11]

$$\chi^2 = \frac{\left(\frac{\mathrm{d}P}{\mathrm{d}z}\right)_L}{\left(\frac{\mathrm{d}P}{\mathrm{d}z}\right)_G} = \frac{\phi_G{}^2}{\phi_L{}^2} \tag{2.49}$$

The turbulent friction factor is given by the *Zigrang–Sylvester approximation, 1982*, to the *Colebrook–White correlation, 1937*, expressed as [16, 19]

$$\frac{1}{\sqrt{f_T}} = -2\log_{10}\left\{\frac{\epsilon/D}{3.7} + \frac{2.51}{Re}\left[1.14 - 2\log_{10}\left(\frac{\epsilon}{D} - \frac{21.25}{Re^{0.9}}\right)\right]\right\} \tag{2.50}$$

2.8.2.2.2 Interphase Friction

Two different models can be used for the calculation of interphase friction force, namely the Drift Flux model and the Drag Coefficient method.

The *Drift flux model* can be used in the bubbly and slug flow regimes for vertical flow.

The interfacial force is given in terms of the phasic velocities as

$$F_i = C_i|C_1 u_G - C_0 u_L|(C_1 u_G - C_0 u_L) \tag{2.51}$$

Here, u_G and u_L are the individual phasic velocities and

$$C_i = \frac{\alpha_L \alpha_G{}^3(\rho_L - \rho_G)g}{u_{Gj}{}^2} \tag{2.52}$$

$$C_1 = \frac{1 - \alpha_G C_0}{1 - \alpha_G} \tag{2.53}$$

The global interfacial friction coefficient is given as

$$\mathrm{FI} = \frac{\left(\frac{F_G^i}{\alpha_G\rho_G} + \frac{F_L^i}{\alpha_L\rho_L}\right)}{\rho_m(C_1 u_G - C_0 u_L)} \tag{2.54}$$

The drift flux correlation used is proposed by Chexal–Lellouche [20]. As per the correlation, the distribution parameter C_0 is given as

$$C_0 = F_r C_{0v} + (1 - F_r)C_{0h} \tag{2.55}$$

The Drift Velocity is given as

$$u_{Gj} = F_r u_{Gjv} + (1 - F_r)u_{Gjh} \tag{2.56}$$

Here, C_{0v} and C_{0h} are the distribution parameters for vertical and horizontal flows, respectively. F_r is the flow orientation parameter, and u_{Gjv} and u_{Gjh} are the drift velocities for vertical and horizontal flows, respectively.

The *Drag Coefficient method* is used in all flow regimes except for bubbly and slug flows in vertical components. The constitutive relation for the frictional force on a body moving relative to a fluid is given by

$$F_D = \frac{1}{2}\rho u^2 C_D A \tag{2.57}$$

Expressing the frictional force for a group of bodies moving relative to a fluid in terms of the frictional force for each body leads to the following constitutive relation for the frictional force per unit volume of fluid

$$F_i = \frac{1}{8}\rho_L |u_G - u_L|(u_G - u_L) C_d S_F a_i \tag{2.58}$$

Here, S_F = Shape Factor.

Using this, the global friction factor is calculated using

$$\text{FI} = \frac{\left(\frac{F_{iG}}{\alpha_G \rho_G} + \frac{F_{iL}}{\alpha_L \rho_L}\right)}{\rho_m (u_G - u_L)} \tag{2.59}$$

2.8.2.3 Energy Closure

Energy equations (Eqs. (2.38) and (2.39)) also contain the terms which requires empirical closures. Those closures also depend upon the flow regime and boiling regime of the flow. Various wall heat transfer coefficient correlations are used for heat transfer calculations under different flow regimes. Heat transfer models used in system codes employ several well-known correlations depending upon the type of flow and the heat transfer geometry involved. Various models of heat transfer are as follows:

Dittus–Boelter correlation, 1930: It is used in case of turbulent forced convective heat transfer [21]. It takes the form

$$Nu = 0.023 \cdot Re^{0.8} Pr^n \tag{2.60}$$

The physical properties are evaluated at bulk fluid temperature. Value of n is taken as 0.4 for heating and 0.3 for cooling.

Sellars–Tribus–Klein correlation, 1956: It is used in case of laminar forced convective heat transfer and is an exact solution of the fully developed laminar flow in a tube with uniform wall heat flux and constant thermal properties [22]. The solution takes the form

$$Nu = 4.36 \tag{2.61}$$

Churchill–Chu correlation, 1975: It is used in case of natural convective heat transfer if the connecting hydraulic cell is vertical [23]. The correlation has the form

$$Nu = \left\{ 0.825 + \frac{0.387 (Ra_L)^{\frac{1}{6}}}{\left[1 + \left(\frac{0.492}{Pr}\right)^{\frac{9}{16}}\right]^{\frac{8}{27}}} \right\}^2 \tag{2.62}$$

Nusselt correlation, 1916: It is used in case of condensation heat transfer involving inclined or vertical surfaces [24]. The expression has the form

$$h_c = 0.725\left[\frac{\rho_L(\rho_{L-}\rho_g)gh_{fg}(k_L)^3}{\mu_L L(T_{\mathrm{SAT}} - T_w)}\right]^{\frac{1}{4}} \tag{2.63}$$

Shah correlation, 1979: This is accepted as the most verified predictive general technique available [25]. The correlation takes the form

$$h_c = h_{sf}\left(1 + \frac{3.8}{Z^{0.95}}\right) \tag{2.64}$$

where,

$$Z = \left(\frac{1}{\bar{x}_{\mathrm{eq}}} - 1\right)^{0.8} {p_{\mathrm{red}}}^{0.8}$$

$$h_{sf} = h_{DB}(1 - \bar{x}_{\mathrm{eq}})^{0.8}$$

Chato correlation, 1962: It is used in case of condensation heat transfer involving horizontal surfaces, although it has given satisfactory results up to an inclination of 37° [26]. It takes the form

$$h_c = F\left(\frac{g\rho_L(\rho_L - \rho_G)h_{fgb}{k_L}^3}{d_{\mathrm{hyd}}\mu_L(T_{\mathrm{sppb}} - T_w)}\right)^{\frac{1}{4}} \tag{2.65}$$

Here, F = Liquid level correction term.

Chen correlation, 1966: The Chen correlation is used in cases involving nucleate boiling [27]. The correlation is expressed as

$$q'' = h_{\mathrm{mac}}(T_w - T_{\mathrm{spt}})F + h_{\mathrm{mic}}(T_w - T_{\mathrm{spt}})S \tag{2.66}$$

h_{mac} is calculated using the Dittus–Boelter correlation. The total convective heat transfer is given by h_{mac} times the temperature difference and the Reynolds Number Factor F.

h_{mic} is calculated using the Forster–Zuber equation, given as

$$h_{\mathrm{mic}} = 0.001\,22\left(\frac{{k_L}^{0.79}{c_{pL}}^{0.45}{\rho_L}^{0.49}g^{0.25}}{\sigma^{0.5}{\mu_L}^{0.29}{h_{fg}}^{0.24}{\rho_G}^{0.24}}\right)\Delta{T_w}^{0.24}\Delta P^{0.75} \tag{2.67}$$

The total boiling heat transfer is given by h_{mic} times the temperature difference and the Suppression Factor S, which is the ratio of effective superheat to wall superheat. It accounts for decreased boiling heat transfer because the effective superheat across the boundary layer is less than the superheat based on a wall temperature. Here, $\Delta T_w = T_w - T_{\mathrm{spt}}$ = wall superheat over saturation and ΔP = Pressure based on wall temperature minus total pressure.

2.8.3 Software (RELAP5)

Since the development of the two-fluid model, a large number of codes have been developed based on the two-fluid model. Various scales of an engineering system that includes system scale to micro scales are shown in Figure 2.5. Most of the time it is not possible to simulate the 3-D behaviour of whole plant under consideration. In such a situation, one-dimensional models are very useful, which give overall behaviour rather performance behaviour of the whole plant. There exist many such models and software. RELAP5 (Reactor Excursion and Leak Analysis Program), CATHARE, and TRACE are the few to name [12, 28, 29]. These codes are best estimate codes being used in nuclear industry for plant simulation under accidental conditions. RELAP is the series of codes start developing during mid-1960s, and RELAP5 mod 3 is the fully developed code based on the two fluid six equation mathematical model. The RELAP5 series of codes have been developed at the Idaho National Laboratory (INL) under sponsorship of the U.S. Department of Energy, the U.S. Nuclear Regulatory Commission, members of the International Code Assessment and Applications Program (ICAP), members of the Code Applications and Maintenance Program (CAMP), and members of the International RELAP5

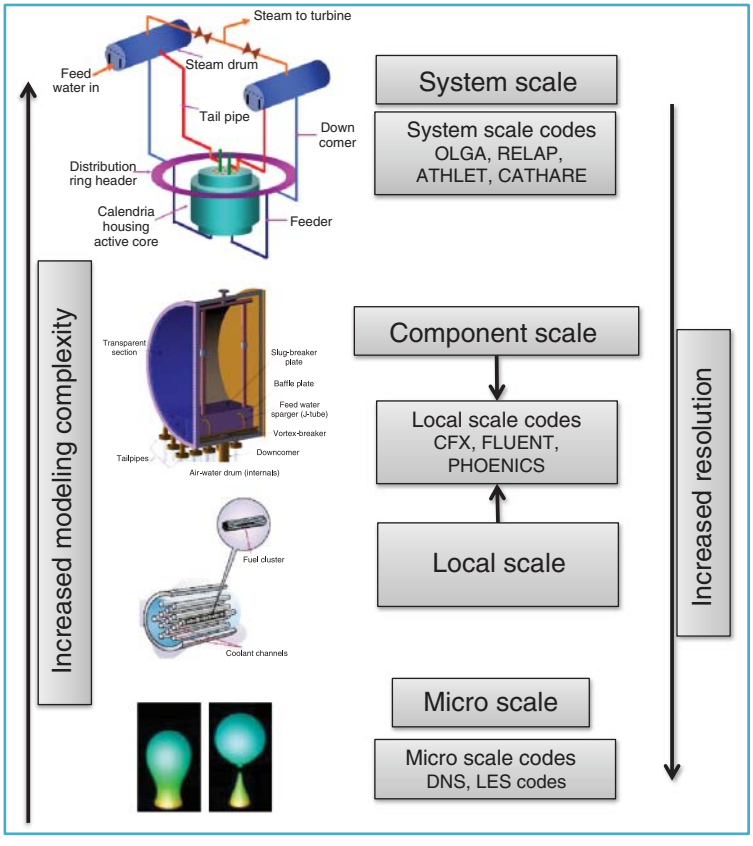

Figure 2.5 Various scales for mathematical modeling and computer codes.

Users Group (IRUG). Specific applications of the code include simulations of transients in light water reactor (LWR) systems such as loss of coolant, anticipated transients without scram (ATWS), and operational transients such as loss of feed water, loss of offsite power, station blackout, and turbine trip.

RELAP5 is a highly generic code that, in addition to calculating the behavior of a reactor coolant system during a transient, can be used for simulation of a wide variety of hydraulic and thermal transients in both nuclear and non-nuclear systems involving mixtures of vapor, liquid, non-condensable gases, and non-volatile solute. It is based on a non-homogeneous and non-equilibrium model for the two-phase system that is solved by a fast, partially implicit numerical scheme to permit economical calculation of system transients.

The code includes many generic component models from which general systems can be simulated. The component models include pumps, valves, pipes, heat releasing or absorbing structures, reactor kinetics, electric heaters, jet pumps, turbines, compressors, separators, annuli, pressurizers, feed-water heaters, ECC mixers, accumulators, and control system components. In addition, special process models are included for effects such as form loss, flow at an abrupt area change, branching, choked flow, boron tracking, and non-condensable gas transport.

The RELAP5/Mod 3.2 hydrodynamic model is a one-dimensional, transient, two-fluid model for flow of a two-phase steam–water mixture that can contain non-condensable components in the steam phase and/or a soluble component in the water phase. The RELAP5/Mod 3.2 thermal-hydraulic model solves eight field equations for eight primary dependent variables. The primary dependent variables are pressure, phasic-specific internal energies, vapor volume fraction (void fraction) (αg), phasic velocities, non-condensable quality, and boron density. The independent variables are time and distance.

The difference equations in RELAP5/Mod 3.2 are based on the concept of a control volume (or mesh cell) in which mass and energy are conserved by equating accumulation to the rate of mass and energy in through the cell boundaries minus the rate of mass and energy out through the cell boundaries plus the source terms. This model results in defining mass and energy volume average properties and requiring knowledge of velocities at the volume boundaries. The velocities at boundaries are most conveniently defined through the use of momentum control volumes (cells) centered on the mass and energy cell boundaries. This approach results in a numerical scheme having a staggered spatial mesh. The scalar properties (pressure, energies, and void fraction) of the flow are defined at cell centers, and vector quantities (velocities) are defined on the cell boundaries.

A semi-implicit numerical solution scheme is employed, based on replacing the system of differential equations with a system of finite difference equations partially implicit in time. The semi-implicit numerical solution scheme uses a direct sparse matrix solution technique for time step advancement. The method has a material Courant time step stability limit.

The constitutive relations in RELAP5/Mod 3.2 include models for defining flow regimes and flow-regime-related models for interphase drag and shear, the coefficient of virtual mass, wall friction, wall heat transfer, interphase heat, and mass transfer.

The phasic interfacial friction force calculations in RELAP5/Mod 3.2 are done using two different models: the drift flux method and the drag coefficient method. The constitutive models are flow-regime-dependent. The drift flux approach is used in the bubbly and slug flow regimes for vertical flow. It specifies the distribution coefficient and the vapor drift velocity. The drag coefficient method is used in all flow regimes except for bubbly and slug flows in vertical components. This model uses correlations for drag coefficients and for the computation of the interfacial area density.

The wall friction calculations are based on a two-phase multiplier approach, in which the two-phase multiplier is calculated from the Heat Transfer and Fluid Flow Service (HTFS), 1972 modified Baroczy correlation, 1965 [13, 30]. The individual phasic wall friction components are calculated by apportioning the two-phase friction between the phases using a technique derived by Chisholm, 1973, from the Lockhart–Martinelli model, 1949 [11, 15]. The partitioning model is based on the assumption that the frictional pressure drop may be calculated using a quasi-steady form of the momentum equation. Table 2.3 shows various empirical models incorporated in RELAP5 and uncertainty associated with the models.

Table 2.3 Various models and associated uncertainties.

Sl. no.	Model	Uncertainty (%)
1.	Heat transfer	
	I. Dittus–Boelter correlation [21]	±25
	II. Sellars–Tribus–Klein correlation [22]	±10
	III. Churchill–Chu correlation [23]	±12.5
	IV. Nusselt correlation [24]	±7.2
	V. Shah correlation [25]	±25.1
	VI. Chato correlation [26]	±16
	VII. Chen correlation [27]	±11.6
2.	Wall friction	
	I. Colebrook–White correlation with Zigrang–Sylvester approximation [16]	±0.5
	II. Lockhart–Martinelli correlation [11]	±25.61
	III. HTFS modified–Baroczy correlation [13, 30]	±21.2
3.	Interphase friction	
	I. Chexal–Lellouche correlation (drift flux model)	±15.25
	II. Drag coefficient method [12]	±30
4.	Choking flow [12]	±5
5.	Abrupt area change [12]	N/A
6.	Counter current flow limitation [12]	±8.7
7.	Modified energy term [12]	N/A
8.	Stratification [12]	±20
9.	Thermal front tracking [12]	±13–19

2.8.4 Application and Validation of Various One-D Models and CFD

One-D models have been applied for predictions of the boiling two-phase flows inside a tube. These models are validated against the experimental data of Bartolomei and Chanturiya, at 4.5 MPa [31]. The experimental setup presented by the authors consists of a 2 m long heated tube (stainless steel tube; 5 mm thick) with an inner diameter of 15.4 mm (Figure 2.6) operating at a constant wall heat flux of 570 kW/m^2 (one of the cases). The mass flow rate of water at a pressure of 4.5 MPa amounts to 900 kg/s m^2 with inlet sub-cool temperature set at 59 K. Table 2.4 shows boundary conditions for the case under consideration.

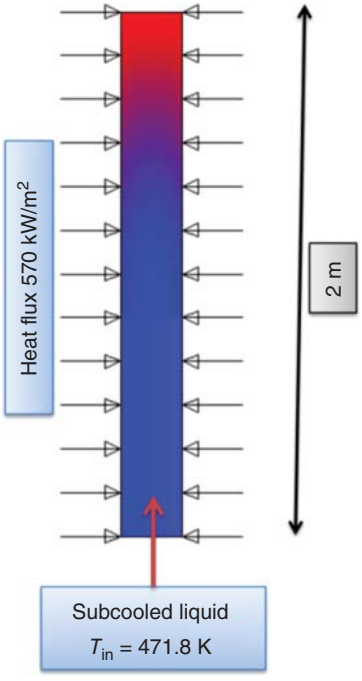

Figure 2.6 Bartolomei and Chanturiya experiment details. Source: Bartolomei and Chanturiya [31].

Table 2.4 Boundary conditions for Bartolomei and Chanturiya experiment [31].

Wall boiling model		**Non-equilibrium RPI boiling model**
Boundary conditions		**Operating pressure: 4.5 MPa**
Region	**Type**	**Specification**
Inlet	Velocity inlet	Liquid velocity = 1 m/s; liquid temperature = 471.8 K
Outlet	Pressure outlet	Backflow void: 0; vapor temperature = 530.55 K
Wall-heated	Wall	Heat flux: 570 kW/m^2 (uniform)

Source: Bartolomei and Chanturiya [31].

2.8.4.1 Nodalization for the One-Dimensional Models

Figure 2.7 shows the nodalization considered for the Bartolomei and Chanturiya, case [31]. The tube is divided into eight equal volumes with length 0.25 m. Time-dependent volumes are connected to maintain the pressure at the outlet, and time-dependent junction is connected to the pipe for maintaining the flow at the inlet (liquid velocity 1 m/s). Heat structure is provided for heating the tube at outer periphery. Three cases of one-D models viz three-equation, five-equation, and six-equation models have been selected to analyze the experimental data. Besides, the same case has also been analyzed with CFD.

2.8.4.2 Model Details

Table 2.5 shows the details of various models selected for simulation of the Bartolomei and Chanturiya, experiment of subcooled boiling [31]. Three-equation

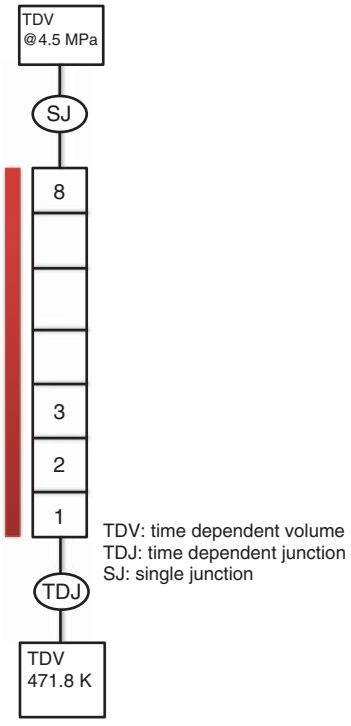

Figure 2.7 One-D nodalization for Bartolomei and Chanturiya, case. Source: Bartolomei and Chanturiya [31].

Table 2.5 Models details used for simulation.

Equation solved ↓	Three equation model	Five equation model	Six equation model
Mass conservation	1	2	2
Momentum conservation	1	1	2
Energy conservation	1	2	2