Environmental Science

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Selected Topics of Computational and Experimental Fluid Mechanics

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Selected Topics of Computational and Experimental Fluid Mechanics

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Preface

Fluid dynamics is a highly developed branch of science that has been the subject of continuous and expanding research activity both theoretically and experimentally for more than a century and a half. In particular, the relatively recent development of fluid dynamics has been strongly influenced by its numerous applications in a plethora of research fields as well as industrial and technological processes. Current research in physics, biology, engineering, medicine, and environmental sciences rely more and more on the use of the principles of fluid mechanics. While improvements to the nineteenth-century technologies were possible on the basis of common sense, the new technologies require the knowledge of fluid flow behavior under conditions that go beyond our everyday experience.

This book presents recent experimental and theoretical advances in fluid dynamics applied to physics and engineering. It includes invited lectures given during the International Enzo Levi Spring School held at Cinvestav-Abacus, Estado de México, Mexico, May 15–16, 2013, and seminars presented at the XIX National Congress of the Fluid Dynamics Division of the Mexican Physical Society, held at the Mexican Institute of Water Technology, Jiutepec, Morelos, Mexico, November 13–15, 2013.

The Spring School is organized every year in honor of Prof. Enzo Levi, a well-known Mexican scientist, who dedicated his research to the study of fluids. He was one of the founders of the Instituto de Ingeniería (Engineering Institute) of the Universidad Nacional Autónoma de México (UNAM), and of the Instituto Mexicano de Tecnología del Agua (Mexican Institute for Water Technology) of the National Water Commission. He was the mentor of several generations of Mexican Engineers.

The 2013 Enzo Levi School was held at Cinvestav-Abacus, a recently created Centre for Applied Mathematics and High Performance Computing (HPC) that from early 2015 will host one of the largest supercomputers in Latin America, where scientists and engineers in Mexico and other countries will be able to develop projects on Computational Fluid Dynamics requiring very large HPC facilities.

During the Cinvestav-Abacus two-day school, lectures were given by well-known national and international scientists. The meeting was attended by about 50 researchers and about a hundred graduate and undergraduate students.

A wide variety of topics were presented that included asymptotic methods in fluids, convection, computational methods applied to biological systems, interfacial fluid dynamics, colloidal dispersions, and fluid flow in fractured porous media. Among the lectures we want to mention a very interesting description of *Bubble dynamics with biomedical applications* and *Using computers to study fluid dynamics* by Timothy Colonius of the Mechanical and Civil Engineering Department of the California Institute of Technology, two lectures on the *Fluid mechanics of bio-inspired swimming and flying* and *Some problems on the physics of insect-inspired flapping wings* by Ramiro Godoy Diana of the École Supérieure de Physique et de Chimie Industrielles (ESPCI), Paris, France, and Claudio Pastorino of the Departamento de Física, Centro Atómico Constituyentes, CAN-CONICET, Buenos Aires, Argentina, with the two lectures *Polymer brushes exposed to liquid flow: cyclic dynamics, collective behavior and coarse-grained* and *DPD model to simulate soft matter systems in equilibrium and under flow*. Other interesting lectures were *Smoothed Particle Hydrodynamics for free-surface flows: Implementation (CPU and GPU)* and *DualSPHysics code and applications* by Anxo Barreiro, Universidad de Vigo, Spain, *Numerical simulation of multiphase flow* by Leonardo Di G. Sigalotti of the Universidad Autónoma Metropolitana-Azcapotzalco (UAM-A), Mexico and the Instituto Venezolano de Investigaciones Científicas (IVIC), Caracas, Venezuela, *Modeling the dependence of interfacial tension with temperature and ionic strength in mixtures of solvents, organic and water by dissipative particle dynamics* by Estela Mayoral-Villa, ININ, Mexico, and *Surface waves in the vicinity of a singularity* by Gerardo Ruíz Chavarría, FCUNAM, Mexico. Several of these lectures were included in Part I of the book.

The Annual Fluid Dynamics Congress has a different format compared to its previous episodes. In 2013, it lasted three days and was composed of six plenary lectures and many short oral presentations of students and researchers.

In Part I we also included the plenary lectures given during the congress by national and international well-known invited speakers and some of the most interesting short oral contributions. Among the plenary lectures we can mention the following: *Flow coherence: Distinguishing cause from effect* by F.J. Beron Vera of the University of Miami, Florida, USA, *Flows from bins: New Results* by Abraham Medina of ESIME-IPN, Mexico, *Numerical modeling of the extratropical storm Delta over Canary Islands: Importance of high resolution*, by José M. Baldasano of the Barcelona Supercomputing Center, Barcelona, Spain, *Compositional Flow in Fractured Porous Media: Mathematical Background and Basic Physics*, by Leonardo Di G. Sigalotti of the UAM-A, Mexico and IVIC, Venezuela, *Some aspects of the turbulence role in oceanic currents* by Angel Ruiz Ángulo, UNAM, Mexico, and finally *Alya Red CCM: HPC-based cardiac computational modeling* by Mariano Vázquez of the Barcelona Supercomputing Center, Barcelona, Spain.

The other short presentations are organized by topics: Multiphase flow and Granular Media (Part II), Convection and Diffusion (Part III), Vortex, Oceanography and Meteorology (Part IV), and General Fluid Dynamics and Applications (Part V).

In Part II, Multiphase Flow and Granular Media, we have focused on petroleum-related applications, where we can find interesting contributions on the tracer transport and natural and forced convection with applications to oil recovery, mixed convection around a heated horizontal cylinder and viscous dissipation, characterization of a bubble curtain for PIV measurements, numerical simulations of gas-stirred ladle with applications to metallurgy, and a study of fluid flow through polymeric complex structures using multiscale simulations.

Convection and Diffusion can be found in Part III, with interesting contributions on conjugate convection in an open cavity, and heat transfer in biological tissues. We can also find two applications on fracture-porous media systems in oxygen transport and combustion, and an interesting study of solidification in the presence of natural convection in a Hele-Shaw cell and of thermal convection in a cylindrical enclosure with a wavy sidewall.

In Part IV, Vortex, Oceanography and Meteorology, we can find three contributions on numerical simulations of the flow past a pair of magnetic obstacles, steady and unsteady vortex flow generated by electromagnetic forcing, as well as numerical simulations of the span-wise vortex in a periodic forced flow, of erosion and deposition of particles in a periodic forced flow and of singularities in surfaces waves.

Finally, in Part V, General Fluid Dynamics and Applications, we find several contributions of fluid dynamics applied to various fields such as biopolymers processes, friction stir welding, dynamical behavior of a drop on a vertically oscillating surface, and critical phenomena of a drop through a stratified fluid.

The book is aimed at fourth year undergraduate and graduate students, and at scientists in the field of physics, engineering, and chemistry who have interest in fluid dynamics from the experimental and theoretical points of view. The material includes recent advances in experimental and theoretical fluid dynamics and is adequate for both teaching and research. The invited lectures are introductory and avoid the use of complicated mathematics. The other selected contributions are also adequate for fourth-year undergraduate and graduate students.

The editors are grateful to the institutions that made possible the realization of the International Enzo Levi Spring School 2013 and the XIX National Congress of the Fluid Dynamics Division of the Mexican Physical Society, especially the Consejo Nacional de Ciencia y Tecnología (CONACYT), the Sociedad Mexicana de Física, the Universidad Autónoma Metropolitana-Azcapotzalco (UAM-A), the Instituto Mexicano de Tecnología del Agua, Jiutepec, Morelos, the Universidad Autónoma de México (UNAM), the ESIME of the Instituto Politécnico Nacional (IPN), Cinvestav-Abacus, and the Instituto Nacional de Investigaciones Nucleares (ININ).

We acknowledge the help of the Editing Committee: Carlos A. Vargas, Salvador Galindo Uribarri, Catalina Stern, Mario Alberto Rodriguez Meza, Estela Mayoral-Villa, Armando Gama, Máximo Pliego Díaz, Leonardo Trujillo, and, in particular, Fernando Aragón and Ruslan Gabbasov for their important and valuable contribution to the final manuscript.

Mexico City, January 2015

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Part I
Invited Lectures

Compositional Flow in Fractured Porous Media: Mathematical Background and Basic Physics

Leonardo Di G. Sigalotti, Eloy Sira, Leonardo Trujillo and Jaime Klapp

Abstract This chapter presents an overview of the equations describing the flow of multiphase and multicomponent fluids through fractured and unfractured porous media using the framework of continuum mixture theory. The model equations and constraint relationships are described by steps of increasing level of complexity. We first describe the governing equations for multiphase flow in both undeformable and deformable porous media. This model is extended to include the transport of chemical species by first describing the flow of a multicomponent, single-phase fluid and then of a compositional (multiphase and multicomponent) fluid in a porous medium. Finally, the equations governing the flow of compositional fluids in fractured porous media are described. The proposed methodology is suitable for modelling any type of fractured media, including dual-, triple-, and multiple-continuum conceptual models.

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1 Introduction

Multiphase and multicomponent fluid flow in fractured rocks occurs in a variety of subsurface flows and transport processes, including contaminant subsurface migration, saltwater intrusion in coastal aquifers, geothermal hydrotransport, subsurface sequestration of CO_2, and oil production and recovery from underground reservoirs, just to mention but a few. In particular, the transport of compositionally complex fluids in fractured porous media has been the subject of extensive research over the past three decades because of its practical interest in petroleum reservoir engineering. Whereas the occurrence of naturally fractured reservoirs over the world is well acknowledged, more than 20 % of the world's oil reserves are estimated to reside in naturally fractured formations (Firoozabadi 2000).

In contrast to crystalline rocks in which any void space is due to fractures, void space in fractured porous media is predominantly formed by pores, which manifest themselves as microscopic perforations of the fracture matrix interface that alter in-plane flow when fracture aperture is less than or equal to the grain size (Mätthai and Belayneh 2004). Although above a certain aperture and length, fractures may become preferential flow pathways that dominate fluid transport throughout the reservoir (Phillips 1991), their actual impact on the transport is in general difficult to predict because multiple fractures may exhibit self-similar and fractal properties in a wide range of scales, with different orientations and intersecting each other. The problem of compositional (i.e., multiphase and multicomponent) flow in fractured porous rocks becomes even more complex owing to the strong nonlinear couplings among viscous, gravitational, and capillary forces in the reservoir which manifest themselves differently in the fracture and rock matrix domains.

The physics of multiphase flows in porous media seems to be reasonably well established and it has been mostly developed in the framework of continuum mixture theory (Allen 1985; Bear 1988; Adler and Brenner 1988; Miller et al. 1998; Chen et al. 2006), where a multiphase mixture is treated as a set of overlapping continua called constituents. In porous media a multiphase fluid mixture consists of several phases if on the scale of typical pore apertures they are separated by sharp interfaces. If, on the other hand, the fluid mixture consists of several chemical species, or components, in which their spatial segregation is only observable at intermolecular length scales, we call it a multicomponent mixture. In underground petroleum reservoirs, we deal in general with multiphase flows in which each phase comprises several chemical species and so we refer to them as multiphase and multicomponent flows, or simply, as compositional flows. In recent years, research efforts have gone mostly into modelling compositional flow in fractured porous media in order to optimize the recovery of hydrocarbons. The partial differential equations governing this type of flows were presented already in 1960 by Barenblatt et al. (1960), and since then they have undergone little modifications. However, their solution still remains a challenge owing to the nonlinear couplings among the variables, the scale-varying heterogeneity of the fractured porous medium, and the large variations in key material properties. At present, there is no a general satisfactory methodology for quantitatively describing flow and reactive transport in multiscale media.

The key issue for simulating flow in fracture rocks, however, is how to handle fracture-matrix interaction under different conditions. For instance, under multiphase and nonisothermal conditions, a critical aspect involves the interaction of mass and thermal energy at fracture-matrix interfaces. In general, most mathematical models rely on continuum approaches and involve developing conceptual models. They incorporate the geometrical information of the fracture-matrix system, define mass and energy conservation equations for the fracture-matrix domains, and solve a number of discrete nonlinear algebraic and constitutive equations, which express relations and constraints of physical processes, variables, and parameters as functions of primary unknowns. Conceptual models employed to represent fractured porous media include: the discrete fracture and matrix models (DFM) (Lichtner 1988; Steefel and Lichtner 1998a, b; Stothoff and Or 2000), the effective-continuum method (ECM) (Wu 2000), the dual-continuum methods, including double- and multi-porosity, dual-permeability models, and the more general Multiple Interacting Continuum (MINC) approach (Barenblatt et al. 1960; Barenblatt and Zheltov 1960; Warren and Root 1963; Pruess and Narasimhan 1985; Wu and Pruess 1988; Bai et al. 1993). A dual porosity model of multidimensional, compositional flow in naturally fractured reservoirs as derived by the mathematical theory of homogenization was presented by Chen (2007). The dual-continuum model, such as the double-porosity and the dual-permeability concept, has been the most widely used approach for modelling fluid flow, heat transfer, and chemical transport through fractured reservoirs because of its computational efficiency and its ability to match many types of field-observed data. A unified scheme based on the dual-continuum method has been recently reported by Wu and Qin (2009), which can be used with different fracture-matrix conceptual models. The mathematical formulation of dual-continuum models as used in industrial simulators and the-state-of-the-art modelling of the physical mechanisms driving flows and interactions/exchanges within and between fractures and matrix media have been described in two separate papers by Lemonnier and Bourbiaux (2010a, b).

Fluid motion in a petroleum reservoir is governed by the laws of conservation of mass, momentum, and energy. These physical laws are often represented mathematically on the macroscopic level by a set of partial differential or integral equations, referred to as the governing equations. As long as compressible or multiphase flow or heat transfer is involved, these equations are inherently nonlinear. A mathematical model for describing the flow and transport processes in fractured porous media consists of these equations, together with appropriate constitutive relations and a set of boundary and/or initial conditions. In this paper we intend to develop such a model by steps of increasing level of complexity. We first describe in Sect. 2 the equations governing the simultaneous flow of two or more fluid phases within a porous medium. In Sect. 3 we write down the equations used to model the transport of multicomponents in a fluid phase in a porous medium. This model is extended in Sect. 4 to describe compositional flow in a general fashion, where each phase may involve many components and mass transfer between the phases is an important effect. Chemical flooding, i.e., the injection of chemical components in production wells is an important technique employed in enhanced oil recovery to reduce the fluid mobility and increase

the sweep efficiency of a reservoir. In view of its practical importance in petroleum engineering, Sect. 5 extends the equations of Sect. 4 to describe chemical flooding compositional flows in a porous medium. The equations for modelling compositional flow in a fractured porous medium are introduced in Sect. 6. The proposed methodology is suitable for modelling any type of fractured reservoirs, including double-, triple-, and other multiple-continuum conceptual models.

2 Multiphase Flow in Porous Media

In fluid mechanics, multiphase flow is treated as a generalization of the modelling of a two-phase immiscible flow, where the two fluids are not chemically related and coexist in contact separated by well-defined interfaces at the microscopic scale. In reservoir simulations, we are typically interested in the simultaneous flow of two or more fluid phases coexisting within the porous solid matrix. In principle, the physics of such flows can be described using the framework of continuum mixture theory for the development of the governing equations, in which the various phases are considered as distinct fluids with individual thermodynamic and transport properties and with different flow velocities. The transport phenomena are mathematically described by the basic principles of conservation for each phase separately and by appropriate kinematic and dynamic conditions at the interfaces. Whereas the detailed structure of these interfaces and the fluid volumes bounded by them are in general inaccessible to macroscopic observation, their geometry influences the dynamics of the multiphase mixture. To cover this difficulty, mixture theory makes use of the *volume fraction* ϕ_α of phase α, which is defined as a scalar function of position $\mathbf{x}$ and time t such that $0 \leq \phi_\alpha \leq 1$. Therefore, for any volume $\mathscr{V}$ in the mixture, the integral

$$\int_{\mathscr{V}} \phi_\alpha(\mathbf{x}, t) d\mathbf{x}, \tag{1}$$

gives the instantaneous fraction of volume $\mathscr{V}$ that is occupied by the fluid phase α. Another quantity which is important in the description of multiphase flow is the phase *saturation* S_α, defined as the fraction of void space of a porous medium that is filled by phase α,

$$S_\alpha = \frac{\phi_\alpha}{\phi}, \tag{2}$$

where ϕ denotes the skeletal *porosity* of the solid matrix, which is the sum of the fluid volume fractions in a saturated porous medium. In other words, it is the total fraction of void space in the material that can be occupied by the fluid phases.

2.1 Undeformable Porous Media

Consider first a porous medium that is statistically homogeneous and undeformable, and assume that the system has four phases: a solid phase (R) and three fluid phases, namely water (W), gas (G), and oil (O). The water phase wets the porous medium more than the oil phase, and so it is called the *wetting phase*. In general, water is the wetting fluid relative to oil and gas, while oil is the wetting fluid relative to gas. Each phase has its own intrinsic mass density ρ_α, velocity $\mathbf{v}_\alpha$, and volume fraction ϕ_α, with the latter obeying the constraint

$$\sum_\alpha \phi_\alpha = 1. \tag{3}$$

The mass conservation equation for phase α can be written as

$$\frac{\partial\left(\phi_\alpha \rho_\alpha\right)}{\partial t} + \nabla \cdot \left(\rho_\alpha \mathbf{v}_\alpha\right) = I_\alpha, \tag{4}$$

where I_α is an interfacial mass transfer rate from all other phases to phase α. In the absence of any external mass source or sink, the reaction rates must satisfy the constraint

$$\sum_\alpha I_\alpha = 0 \tag{5}$$

in order to ensure mass conservation in the overall mixture. In addition, the fact that all fluid phases jointly fill the void space in the solid matrix implies the further relation

$$\sum_\alpha S_\alpha = 1, \qquad \text{or} \qquad S_W + S_O + S_G = 1. \tag{6}$$

Using relations (2) and (3) and noting that $\phi + \phi_R = 1$, Eq. (4) can be expressed in terms of the saturation and porosity as

$$\frac{\partial\left(\phi S_\alpha \rho_\alpha\right)}{\partial t} + \nabla \cdot \left(\rho_\alpha \mathbf{v}_\alpha\right) = I_\alpha, \tag{7}$$

for the fluid phases, and

$$\frac{\partial\left[\left(1-\phi\right)\rho_R\right]}{\partial t} + \nabla \cdot \left(\rho_R \mathbf{v}_R\right) = I_R, \tag{8}$$

for the solid (rock) phase. If the rock phase is chemically inert, $I_R = 0$. In addition, if the solid medium is immobile then $\mathbf{v}_R = 0$ and Eq. (8) reduces to $\rho_R = const$.