5
Modeling of Microfluidic Devices

David F. Fletcher, Brian S. Haynes, Joëlle Aubin, and Catherine Xuereb

5.1
Introduction

This chapter seeks to present the reader with a summary of the modeling challenges that are posed by the miniaturization of chemical and process devices, together with advice on ways to overcome them. The successful use of modeling is demonstrated via a large number of case studies covering both single and multi-phase flows. Here we consider a scale ranging from a few hundred micrometers to a few millimeters. Above this size, the well-known modeling techniques of computational fluid dynamics (CFD), as embodied in a number of commercial packages, are widely used and validated. Below this size, the applications are directed towards nanotechnology and are not considered in detail here, except where novel simulation techniques have been used that have much wider potential application.

At first thought it might be expected that moving to a smaller scale would present few modeling challenges because the well-known difficulties of modeling turbulent flow are usually removed. However, the absence of turbulence in most applications is offset by a number of new physical effects to be included and computational difficulties to be overcome. Before we discuss the modeling challenges faced in a selection of process examples, the physical effects that may come into play in microsystems are discussed.

5.2
Characteristics of Microsystems

In this section, we summarize the features of microsystems that present challenges when modeling them and which are generally absent or straightforward to handle in conventional CFD.

Micro Process Engineering, Vol.1: Fundamentals, Operations and Catalysts
Edited by V. Hessel, A. Renken, J.C. Schouten, and J.-I. Yoshida

ISBN: 978-3-527-31550-5

5.2.1 Non-continuum Effects

In large-scale systems, fluids and gases can almost always be assumed to behave as continua with well-defined pressures, densities, velocity fields, etc. This continuum framework is based on the idea that there are a very large number of collisions between fluid or gas atoms in any small volume, so that it is meaningful to talk about average quantities. This concept is expressed more formally via the Knudsen number, *Kn*, defined via

$$Kn = \frac{\lambda}{L} \tag{5.1}$$

where λ is the molecular mean free path and L is a typical system dimension (e.g. the diameter of a tube). If the Knudsen number is greater than $\sim$0.1, the fluid can no longer be treated as a continuum. This limit does not apply to the systems of interest here, especially to liquids that have very short mean free paths, but must be kept in mind for the flow of gases in very small channels. For channel dimensions greater than 1 μm for liquids and tens of micrometers for gases (the dependence on pressure and temperature is very strong), continuum models can be applied [1, 2]. Outside this regime, the gas flow is characterized first by wall slip effects (for momentum, temperature, concentrations, etc.), which must be modeled, and as the Knudsen number is increased further the behavior of individual molecules must be considered. The need to include this effect arises mostly in gas flows in passages with dimensions of a few micrometers and is therefore much more relevant to lab-on-a-chip applications than for microscale devices applied in chemical process applications. Typical applications include the study of micro-mechanical accelerometers [3], Knudsen pumps [4], thermal management in nanoscale integrated circuits [5] and heterogeneous combustion [6]. There are a wide variety of techniques that are used to solve some form of the Boltzmann equation, using methods as diverse as finite difference techniques [3], orthogonal polynomial expansions [3], the discrete ordinate method [4], the method of moments [7] and Monte-Carlo methods [3, 4, 6].

5.2.2 Laminar Flow

Flow in small-diameter ducts leads frequently to low values of the Reynolds number and hence laminar flow. The Reynolds number, *Re*, defined by

$$Re = \frac{UL}{\nu} \tag{5.2}$$

where U is a typical velocity, L is a typical length-scale and ν is the kinematic viscosity, gives a measure of the relative importance of convective and diffusive momentum transfer. For a duct, flow remains laminar at Reynolds number below around 2300 and becomes "fully" turbulent at a Reynolds number of around 10 000.

Conventional process equipment, such as heat exchangers, mixers, etc., work in the turbulent flow regime, where there is very good mixing by the turbulent eddies present in the flow.

However, in small-diameter devices the flow may be laminar, with consequently very poor mixing. This flow regime is in principle easy to model, as the Navier–Stokes equations can be solved directly with no additional closure assumptions, but there are complexities as the Reynolds number approaches the critical value for transition to turbulence. As the Reynolds number increases there is a transition from steady, laminar flow to unsteady flow which develops more and more turbulent structures before becoming fully turbulent. There is therefore a significant range of Reynolds numbers, even for a straight duct from ~2000 at the lower end to ~10 000 at the upper end, for which there are no developed models. In theory, these flows can be modeled using the Navier–Stokes equations but very fine spatial and temporal resolutions are needed together with very high accuracy numerical schemes, making such calculations very expensive. For duct flows, empirical data are available for frictional loss or the heat transfer rate, but for more complex passages, such as bent ducts, where transition from steady to unsteady flow depends on the geometry, as well as the Reynolds number, there are no easy modeling methodologies. We return to this difficulty later as we describe a number of physical processes that need to be modeled.

It is important to note that early in the study of microscale phenomena many researchers claimed to see transition to turbulence at much lower Reynolds numbers than those observed at the macroscale. However, a very comprehensive review by Hestroni *et al.* [1] has shown that this was due to other causes (surface roughness, experimental errors, etc.) and that for conditions where classical results would be expected to apply, they do. Morini *et al.* [2] have performed a detailed analysis of experimental data for the flow of gases in 100 and 300 μm diameter channels and also concluded that the usual criterion applies for transition to turbulence in this case also. They noted, however, that compressibility effects and inlet and outlet losses can be very significant and that these must be taken into account in many applications if the data are to be interpreted correctly.

5.2.3 Surface Roughness

The treatment of surface roughness in laminar flow is very different from that in turbulent flow. In the latter case, the effect of roughness is treated by modifying the "law of the wall", allowing for the disruption of the laminar sublayer due to the wall roughness. Commercial CFD codes contain models that allow roughness effects to be included at almost no computational overhead by simply modifying the wall treatment. However, in laminar flows the actual rough geometry must be modeled, requiring very large computational meshes, in order to account for any roughness effects. Valdés *et al.* [8] performed a CFD study to explore roughness effects in laminar flow and they highlighted the increased mesh requirements, and consequently simulation times, needed to resolve such flows.

5.2.4
Viscous Energy Dissipation

The effect of viscous energy dissipation is generally negligible and is almost never included in simulations. However, at the microscale this effect can be important because of the large velocity gradients in small-diameter channels. The energy added to the fluid can, for low heat loss at the boundary, cause a sufficient temperature change for the viscosity of the fluid to be reduced, triggering a transition to an oscillatory laminar flow regime. Note that this is not early transition to turbulence, but to a time-dependent laminar flow. A number of workers have investigated this subject, including Koo and Kleinstreuer [9] and Xu *et al.* [10]. The latter group developed a criterion for viscous dissipation effects to be important based on the viscous number (*Vi*):

$$Vi = \frac{\mu U L}{\rho c_p T_{ref} D^2} \tag{5.3}$$

where D is the channel diameter, L is its length, ρ is the fluid density, μ is the dynamic viscosity, c_p is the specific heat capacity and T_{ref} is a reference temperature. For water and adiabatic boundaries, Xu *et al.* [10] showed that viscous dissipation effects are important for $ViPr^{-1} > 0.056$, where Pr is the Prandtl number. The above equation shows that for high flow rates in small-diameter tubes with low heat capacity fluid, the effect is increased. The changes caused by viscous dissipation affect the velocity profile and thus the friction factor. Inclusion of this phenomenon in simulations is generally very easy using commercial CFD software, as this term is available because of its importance in high-speed flow and the user simply has to turn it on.

5.2.5
Gravitational Effects

In most cases the gravitational force plays a very minor role and can be neglected. However, care must be taken in both single-phase flow, where it can be important in natural convection, and multi-phase flows, where phase separation can occur as a result of it. In a detailed literature review, Thome [11] analyzed two-phase flow data and commented that surface tension forces dominate gravitational forces and that stratified flows do not occur in microchannels. Stiles and co-workers [12, 13] investigated a number of flows where two reactants with different densities come into contact and the mixing is enhanced by gravitationally induced flows. They noted this effect to be generally very small except in situations where convective effects are small. They performed an analysis that shows that it is the ratio of the Reynolds number to the Froude number:

$$\frac{Re}{Fr} = \frac{g D^2 \Delta\rho}{\mu U} \tag{5.4}$$

where g is the acceleration due to gravity and $\Delta\rho$ is the difference between the densities of the two fluids, which controls the importance of the gravitational

effects [13]. Examples of flows in a cylinder with a heated wall [12] and coaxial jets of acid and alkali bringing the fluids into contact [13] are presented that illustrate this effect. It is therefore worth keeping in mind that under certain conditions gravity can modify the flow behavior through buoyant convection. For a fixed geometry and pair of fluids, this effect becomes more important as the convective velocities diminish. The above discussion shows that although the effect of gravity is generally insignificant, it is important to make an assessment on a case-by-case basis.

5.2.6 Electric Effects

A variety of electric effects may occur in microchannels and the reader is referred to a recent review by Bayraktar and Pidugu [14] for a detailed discussion. Here we concentrate on the so-called electrokinetic flows that are induced by an applied electric field parallel to the flow direction and electroosmotic flows induced by a surface charge on the channel walls. In both cases it is the electric double layer (EDL) effect that is responsible for the modified flow behavior. The EDL is created if the wall is charged, having say a negative charge: this charge causes a narrow layer of positively charged ions to become immobilized close to the wall (called the Stern layer) and a diffuse (or Gouy–Chapman) layer of mobile positive ions outside of this. An applied electric field causes the ions in this outer layer to move and a plug flow-like velocity profile is induced. A detailed analysis of the effect on the velocity and concentration profiles for an ionic salt dissolved in water was given by Bhattacharyya and co-workers [15].

Electric effects become more important as the channel diameter decreases. For nanometer-scale channels the Stern layer occupies a significant fraction of the cross-section, whereas for microscale channels it is of negligible thickness. Conlisk and co-workers [16, 17] performed a detailed analysis of electrokinetic flow using the Navier–Stokes equations supplemented with equations for ion transport and the electric field density. They showed that such flows can have a plug profile for channel dimensions greater than a critical value, the value of which depends on the electric field strength, mole fraction of salt, etc. They also noted that the volumetric flow rate increases linearly with channel height, in contrast to pressure-driven flows where it varies with the cube of the channel height for a fixed pressure gradient. They cited a case where modest voltages can generate a significant flow in a 10 μm diameter channel that would require a driving pressure of over 8 bar for a conventional Poiseuille flow [16], clearly illustrating the possibilities of this technique.

In such flows, there are significant complications when channels are connected to reservoirs, as expansions or contractions add pressure gradients to the electroosmotic flow induced in the ducts. Yang *et al.* [18] discussed a number of such cases and demonstrated the utility of a detailed CFD model that can be used to investigate such effects. They also presented validation against a number of analytic cases which confirms the accuracy of their model.

Davidson and Sharp [19] performed simulations to study the path of a cylindrical particle in a microchannel where the motion is induced by an applied electric field

acting along the channel. The fluid is an ionic solute and the walls and particles are made of different materials, each having different zeta potentials. The Stokes equations are solved to determine the flow field around the particle and its motion is calculated based on the applied force and torque. The motion of the particle through the mesh is handled using an Arbitrary Lagrangian Eulerian (ALE) method, in which the best features of the two modeling approaches are combined. The computational results show the variety of possible paths that the particle can follow, depending on its initial orientation as it enters the channel.

5.2.7 Surface Tension Effects

In multiphase flows in microchannels, the importance of the surface tension force is much greater than in large-scale systems. This is easily understood, as the internal pressure increase across a bubble is

$$\Delta P = \frac{2\sigma}{R} \tag{5.5}$$

where P is the pressure, σ is the coefficient of surface tension and R is the radius of curvature. From the above equation, it is evident that scale plays an important effect. In microchannels, the important non-dimensional groups are the Bond number, defined as

$$Bo = \frac{\rho g D^2}{\sigma} \tag{5.6}$$

the capillary number, defined as

$$Ca = \frac{\mu U}{\sigma} \tag{5.7}$$

and the Weber number, defined as

$$We = \frac{\rho U^2 D}{\sigma} \tag{5.8}$$

These dimensionless groups give the relative importance of gravitational, viscous and inertial forces to the surface tension force, respectively. Note that the values of all of these numbers decrease significantly as the system size diminishes (small diameters and small velocities), increasing the importance of surface tension effects.

In addition to the effect of the surface tension force at a fluid–fluid interface in droplets or bubbles, surface tension forces play a very important role in fluid behavior at a fluid–solid interface. The wettability of the surface determines the contact angle between the liquid and solid and therefore the magnitude of the resulting surface tension force. This angle has, in general, to be measured experimentally and such experiments have shown that the value is not a constant for a particular fluid–solid pair but shows hysteresis effects, in that the contact angle changes between the cases

of a dry surface being wetted and a wetted surface becoming dry. Baird and Mohseni [20] discussed this effect in terms of its impact on the motion of a droplet in a channel that is propelled along the channel by affects such as electrowetting on a dielectric, dilectrophoresis and thermocapillary pumping. They cited a number of articles addressing calculation of fluid–solid interfacial forces but concluded that at present the required data must be obtained experimentally for each material pair and there are differences between steady-state and dynamic behavior.

5.2.8 Wall Slip Effects

We have already seen that electric effects can produce an effective wall slip at a solid–fluid interface. For a hydrophobic surface, the contact behavior is such that the fluid has a tendency to slip at the interface so that the fluid layer close to the wall moves more freely than if the surface were well wetted. This concept of slip flow has most commonly been seen in rarified gas dynamics, where, as the Knudsen number increases, there is a slip layer close to the wall [21]. However, it can also arise in a number of physical situations [22], including extrusion of pastes where a water film at the wall is generated by squeezing of liquid from the paste or in particle-laden flows where a liquid film separates out at the wall. There is also significant evidence that hydrophobic conditions in microchannel flows can lead to slip flow. Trethway and Meinhart [23] presented experimental data showing that water flow in a $30 \times 300\,\mu m$ channel can yield slip velocities of approximately 10% of the free-stream velocity if the channel surface is coated with a 2.3 nm layer of hydrophobic octadecyltrichlorosilane. A simple model which assumed that a thin layer of fluid containing nanobubbles of gas near the surface could be treated as a gas layer in the slip regime was able to explain the observed behavior [24, 25] and suggests that slip effects can be important for channel flows with dimensions of less than 1 mm.

In addition, gradients of concentration and temperature can also introduce slip effects and, more importantly, a number of effects can be combined [26]. Ajdari and Bocquet [26] analyzed the case of an electroosmotic flow with a clean "solvophobic" surface, so that the two effects could work in tandem to produce significant slip velocities. Hydrophilic effects lead to increased pressure loss and enhanced heat transfer rates and hydrophobic effects lead to reduced pressure loss and heat transfer rates [27, 28].

It is clear from the above discussion that surface properties are extremely important in microscale systems and their importance grows as the characteristic channel dimension decreases. However, there is no straightforward way to take these effects into account, with the models developed to describe this phenomenon being problem specific. Generally they are based on a combination of classical solutions of the Navier–Stokes equations, coupled with *ad hoc* models of molecular slip flow. Therefore, in the simulation of microchannel flows, it is important to keep in mind that the use of the no-slip boundary condition may not be appropriate and that additional physics may need to be included in the modeling to capture the correct behavior.

5.3 The Importance of Appropriate Solution Methods

The last section described a variety of physical effects that may need to be taken into account in the modeling of flow and heat transfer in microdevices. In addition to the importance of including the correct physical models, it is also very import to address numerical solution accuracy, as some of the phenomena require extremely accurate or different numerical methods to capture them correctly. Here we split the discussion into two sections: the first deals with Navier–Stokes solvers and the second introduces novel, physics-specific methods.

5.3.1 Conventional Navier–Stokes Solvers

There is now a wide range of commercial CFD software on the market that provides different levels of sophistication and accuracy to the users, in addition to the specific codes written by individual research groups. Commercial software has many thousands of man-years of effort invested in it, with models that can address almost every conceivable physical phenomenon. They provide a variety of meshing techniques and sophisticated means of post-processing the data to generate both graphical and quantitative data. However, it is important to keep in mind that some of the methods may be inappropriate or the user may need to perform validation checks before applying the software to their problem. We illustrate some of these issues in the following subsections. It should be kept in mind that these issues are on top of the usual requirements for checking grid independence and solution convergence, which may require the use of double precision arithmetic because of the extremely small mass flows.

5.3.1.1 Numerical Diffusion

As already noted, in microsystems the flow is generally laminar so that mass, momentum and energy transport may be controlled by molecular transport properties. In, for example, the mixing of two components dissolved in a liquid, the mass diffusivity is typically of the order of $10^{-9}\,m^2\,s^{-1}$. This means that any numerical diffusion introduced by the numerical scheme must be much smaller than this. Even with high-order methods this level of accuracy is hard to achieve. First-order methods have a false diffusion term that is proportional to the flow velocity multiplied by a typical cell size [29], so to achieve a simulation that is not dominated by numerical diffusion would require a mesh size of less than 0.1 μm for a $1\,mm\,s^{-1}$ flow. Even with second-order methods, numerical dispersion can still be important and lead to significant smearing. For this reason, it is often better to use a Lagrangian method to track the location of a particular component, as such methods can be much more accurate [30–32]. Despite the ample evidence that Eulerian methods can be very diffusive, their use continues and the presented results obtained using them clearly show numerical diffusion [33, 34]. In recent work, MacInnes *et al.* [35] compared an Eulerian solution for species transport with a Monte Carlo based calculation of the

concentration field and showed that at low Péclet numbers these are equivalent but at high Péclet numbers the Eulerian result is much too diffusive.

5.3.1.2 Interfacial Surface Location and Parasitic Currents

In the calculation of flows involving free surfaces and surface tension forces, there are significant numerical issues regarding how the surface location is determined and how the surface tension force is included. In a typical calculation, the location of the gas–liquid interface needs to be determined, then the local curvature must be calculated and, finally, a surface force must be implemented on a three-dimensional, finite-volume grid. The manner in which these tasks are undertaken has a huge impact on the accuracy of the solution.

The task of determination of the location of the interface is often performed using a volume of fluid (VOF) method [36] in which the two fluids are represented via a volume fraction and the location of the interface is determined by solving an advection equation for the volume fraction of fluid, α:

$$\frac{D\alpha}{Dt} = 0 \tag{5.9}$$

and then determining the free surface by either using a threshold value of the volume fraction (i.e. $\alpha = 0.5$) or using surface reconstruction [37, 38]. In the former case, compressive differencing of the advection terms is used to avoid numerical diffusion as much as possible. In the latter case, the advection step is followed by a geometric reconstruction step, in which assumptions regarding the shape of the interface are used to reconstruct the interface profile. These methods can be time consuming but have the potential to reduce greatly the smearing of the interface.

A more sophisticated approach to the basic VOF method is the Level Set method [39], which is similar to a VOF method in that a variable, ϕ, is advected in the same manner as conventional VOF but the variable ϕ is an indicator function and is used to define the interface which is located at $\phi = 0$. A redistancing step is performed at each time step to ensure that $|\nabla\phi| = 1$ at the interface and therefore that ϕ remains a distance function and the interface is spread across only a couple of computational cells.

Once the surface between the fluids has been determined, there remain two important additional steps before surface forces can be included. First, the curvature of the surface must be calculated from the discrete location values available on the computational grid. Then the surface tension force is applied by replacing a surface force by an equivalent volume force in a zone adjacent to the interface, with most commercial software using a version of the Continuum Surface Force (CSF) method derived by Brackbill *et al.* [40]. The manner in which this force is implemented can lead to the appearance of spurious velocities, known as parasitic currents. A recent study by Harvie *et al.* [41] has shown that these parasitic currents cannot be removed by mesh refinement alone and they can have a significant effect in certain conditions.

It is clear from the discussion in this section that great care needs to be taken in the computation of two-phase flows that involve surface tension forces. At present, most commercial software has algorithms that lend themselves to generality of application, speed of solution and robustness rather than accuracy for the particular flows of

interest here. It is therefore essential that their accuracy be quantified by users before reliance is placed on the results.

5.3.1.3 Heat Transfer Simulations

The simulation of heat transfer in microsystems poses no particular problem unless there are complexities such as wall slip present. However, it is worth pointing out that the boundaries of the system to be considered may need to be enlarged in the microsystem case. Typically heat transfer simulations are performed with either a constant wall temperature or some form of constant heat flux boundary condition. Tiselj *et al.* [42] studied heat transfer to water in a triangular microchannel with a hydraulic diameter of 160 μm inside a silicon substrate. Their experimental results showed a non-monotonic temperature change along the channel which at first sight seems unphysical. However, simulations in which they increased the domain considered to include the solid material, via a conjugate heat transfer (CHT) simulation, explained the results. For their conditions, axial conduction was very important and inclusion of this mechanism in the simulations was essential to obtain the correct results. A similar observation has been made by Li *et al.* [43], who also made detailed comparisons between experimental and simulation results for tube diameters ranging from 10 to 1570 μm. In both cases the important issue is being aware of the need to treat the problem using a CHT simulation, as all the major commercial codes are able to treat this accurately. The simulations are much larger in size and require more geometry to be meshed, but these are simply resource requirements that are straightforward to overcome.

5.3.2 Advanced Solution Methods

Almost all commercially available software falls into the category already discussed, in that it is based on either a finite-volume or finite-element approach to solve the Navier–Stokes equations. However, as noted earlier in this chapter, there are certain situations in which these equations do not apply.

The calculation of wall slip at high Knudsen numbers from a fundamental point of view has been performed using molecular dynamics simulations. Arya *et al.* [44] simulated rarefied gases flowing in a microchannel by simulating non-interacting gas molecules interacting with rigid atoms forming a wall. Nagayama and Cheng [21] used similar techniques to study the effect of surface wettability in microchannel flows. The choice of models to represent wall roughness and the attraction between the gas molecules and the wall material is crucial to achieving meaningful results. This method is described here for completeness as it provides very useful results in understanding slip phenomena, but its use is reserved for specialists. Ideally, the outcome of such simulations would be an effective boundary condition that could be implemented in standard CFD codes to include the effect of wall slip, as has been done in the past for wall slip arising in the extrusion of polymers [45].

Lattice Boltzmann methods are proving to be very popular in the simulation of flows in microdevices. These methods can be used to solve flow problems that could

also be solved using the Navier–Stokes equations or they can be extended to include other effects, such as wall slip effects due to a hydrophobic surface [46, 47] or electrokinetically-driven flows that promote mixing [48]. Essentially, in this approach the solution variables are not pressure and velocity; rather, the single-particle velocity distribution function is determined on a grid of points via a simplified Boltzmann equation. Again, these methods require much more specialist knowledge than conventional CFD but their ability to include wall material effects and their extension to multi-component flows allows them to be used to understand, for example, the effects of wall slip, making them extremely powerful tools to understand complex physics that cannot be addressed by traditional Navier–Stokes solvers.

5.4 Single-phase Simulations

In this section, we present some examples of modeling being performed in single-phase flows to design a variety of equipment ranging from heat exchangers to mixers. The aim is to present the reader with a variety of different studies that show the potential of such modeling, rather than to provide an exhaustive review of the area.

5.4.1 Heat Transfer Enhancement

As noted earlier, the absence of turbulence in microchannel flows means that the traditional means of enhancing heat transfer via the use of baffles or periodic roughness must be modified or avoided due to the very different construction methods in microscale systems. The flow channels must be designed in such a way that good mixing is caused by the geometry of the channels or some other means that disrupts the thermal boundary layer.

Chung and Tucker [49] performed a very comprehensive study of the heat transfer enhancement of a ribbed channel caused by a 180° bend with application to microchip cooling. They performed very careful CFD studies of transient, laminar flow and studied the development of Tollmein–Schlichting waves induced by a single fin upstream of the bend. They investigated a number of differencing schemes for the convective terms and a number of different algorithms for determination of the pressure. They concluded that central differencing and the Crank–Nicholson schemes performed the best and that the results were relatively insensitive to the chosen pressure determination algorithm. Their results showed that in the periodic grooved channel the flow had to pass around five ribs before it became periodic, setting some important constraints for cooling of chips. In the case of the fin upstream of the 180° bend, they were able to obtain very significant increases in the heat transfer rate, by a factor of five, by choosing a fin height and location that shortened the downstream recirculation length and generated oscillatory flow. They also looked at active control methods, such as flow modulation and identified strategies that could enhance heat transfer with only a modest increase in pressure loss.

There are a large number of computational studies of the effect of flow and heat transfer development in microchannels. Typically these use commercial software and can include effects such as viscous dissipation and variable properties. In some circumstances, allowing for variable fluid properties can be important, especially in small-diameter ducts. Liu *et al.* [50] made a detailed study of the effect of having a variable fluid thermal conductivity and viscosity for water in a two-dimensional channel that was 100 μm wide. They sandwiched a heated section of wall (where a constant wall heat flux was applied) between two adiabatic sections and examined the influence of the variable properties on the flow field and the Nusselt number. Variable properties were shown to induce a non-negligible cross-flow at low Reynolds numbers, which led to a non-negligible heat transfer enhancement.

Enhancement of the heat transfer rate can be obtained by the generation of Dean vortices at bends in ducts. These can be bends in two-dimensional ducts [30] or in three-dimensional structures [32]. The generation of Dean vortices was originally investigated as a means of enhancing mixing of two fluid streams but applies equally well to the mixing of hot and cold fluids. The authors cited above studied the effect of the Dean number, defined by

$$Dn = Re\sqrt{\frac{d}{R}} \tag{5.10}$$

where Re is the Reynolds number, d is the hydraulic diameter of the channel and R is radius of the curvature of the channel. In both cases, commercial software was used to solve for the flow field and then particle tracking was used to examine the properties of the flow field with regard to interface stretching, residence time distribution and chaotic convection. As the Dean number increases, so does the strength of the Dean vortices generated at bends, although beyond a certain point the number of vortices can change and more or less stable flow patterns can develop.

Wang and Liu [51] made a very careful study of the flow bifurcation behavior in a slightly curved microscale duct ($d/R = 5 \times 10^{-6}$) where they examined the effect of increasing Dean number on the flow structure for a square section channel. A high-accuracy finite volume method was used to determine the bifurcation structure of the system. Their results showed that this simple system exhibits very complex behavior with a two-cell state at low Dean numbers changing to a temporally periodic oscillation, another steady two-cell state, a temporally intermittent oscillation and finally a chaotic temporal oscillation as the Dean number is increased. This work highlights the complexity of this very simple system and the need for high-fidelity simulations.

Fletcher, Haynes and co-workers have investigated the effect of channel-section shape and path on the enhancement of the heat transfer rate and the concomitant pressure drop increase in periodic channels that are made by sweeping a given cross-section along a path lying in a plane. This geometry represents flow paths of various constructions, ranging from etching or milling to pipe networks. They investigated the behavior of channel section (circular [52], square [53] and semicircular [54]) for serpentine paths, circular and semicircular sections following a sinusoidal path [55] and semicircular section ducts following a trapezoidal path (a path that can be varied from a zig-zag to a serpentine) [56]. A common feature in all of the results is the

substantial heat transfer improvement, by factors of around two to three for Reynolds number of around 200, for only a modest increase in pressure drop. They provide detailed results for the effect of Reynolds number, Prandtl number and path geometry for these cases. In all of the geometries Dean vortices are formed at bends which lead to local enhancement of the heat transfer rate with a relatively small increase in pressure drop because flow separation either does not occur (at low Reynolds number) or occupies only a small volume of the duct at higher Reynolds numbers. Their results also showed the transition from two to four vortices in some geometries and more complex structures in, for example, semicircular section ducts. They characterized this behavior using the volume integrated helicity, which is a measure of how well the vortices are aligned with the flow.

Their work also investigated a number of different boundary conditions, including constant wall temperature (T), constant axial flux with uniform peripherally-averaged temperature (H1) and constant wall heat flux (H2). Whereas the T and H2 boundary conditions are available in all commercial software, the H1 boundary condition is not. However, it represents an important case as it corresponds most closely to the real situation in which there is conduction in the channel walls that tends to even out hot spots that can occur in the corners of ducts. They presented a novel algorithm that can be used to solve for this case based around Newton iteration to determine the wall temperature field [57]. Lee and Garimella [58] also looked at the H1 boundary condition but for developing flow in a rectangular channel. They implemented the condition by solving a conjugate heat transfer problem in which a conducting boundary wall, with a high circumferential conductivity but negligible axial conduction, was added around the channel. This is a very efficient way to solve the problem for straight channels but can only be used for simple geometries where an anisotropic thermal conductivity can be defined to ensure negligible axial heat transfer.

The utility of the simulation results to designers of heat transfer equipment was addressed by consideration of not only heat transfer enhancement but also of the fact that the choice of channel path has design implications. In microdevices, it is important to be able to stack the channels efficiently on, for example, a plate and to do this in a manner that is consistent with manufacturing and structural limitations [56]. The concept of heat transfer intensification, which gives a measure of the improvement of the heat transfer rate compared with using straight channels occupying the same plate area, was introduced. Based on these ideas, it was shown that designs consisting of swept zig-zag paths give the greatest heat transfer enhancement when all factors are taken into account.

5.4.2 Mixing

Due to the predominantly laminar flow present in microchannels, mixing in these devices is largely controlled by molecular diffusion. In the scale of dimensions considered here, i.e. channel widths/depths ranging from a few hundred micrometers to a few millimeters, the mixing process by molecular diffusion is extremely slow, since the mixing time is proportional to d_1^2/D_m, where d_1 is the characteristic

diffusional path (typically the channel width) and D_m is the molecular diffusivity. This is especially true for liquids, which have small diffusivities. Thus, in order to mix effectively at this scale in a reasonable time, fluids must be manipulated so that the interfacial surface area between the fluids is increased massively and the diffusional path is decreased, thereby enhancing molecular diffusion to complete the mixing process. Various mechanisms for contacting and mixing fluids exist and have been dealt with elsewhere in this handbook. Of course in order to design microchannels for mixing operations effectively, a methodology that enables the mixing performance to be evaluated is required. Modeling the mixing phenomena by CFD and other methods is an attractive option, since it provides local three-dimensional flow information, which is difficult or even impossible to access with most experimental techniques. As a result, there are a large number of computational studies of mixing in microchannels. The majority of these employ commercial CFD software packages to provide qualitative and/or quantitative characterization of the mixing quality.

One method to evaluate mixing quality in microchannel devices relies on the resolution of the Navier–Stokes equation and the convection-diffusion equation of a concentration field. This technique has been used widely as it is analogous to the mixing of two miscible components that can be observed experimentally [33, 59–67]. The results give access to concentration maps throughout the volume of the microdevice, which can be used to quantify mixing quality. The most common approach for evaluating mixing quality is based on Danckwerts' intensity of segregation [68], which is defined by

$$I_s = \frac{\sigma^2}{\sigma^2_{max}} \tag{5.11}$$

where σ^2_{max} is the maximum variance of the mixture and σ^2 is the variance of the mixture around the mean concentration:

$$\sigma^2 = \frac{1}{n-1}\sum_{i=1}^{n}(c_i - \bar{c})^2 \tag{5.12}$$

where n is the number of sampling points, c_i is the concentration at sample point i and $\bar{c}$ is the mean value of the concentration field. I_s is equal to 1 at the state of maximum unmixedness and decays to zero for perfect mixing.

Despite the fact that this Eulerian method is often used for evaluating mixing in microchannel devices, it has an important drawback that jeopardizes the accuracy of the results. As discussed previously in this chapter and pointed out clearly by Hardt and Schönfeld [69], the discretization of the convective term in the transport equation gives rise to numerical errors introducing an unphysical diffusion mechanism, which can be greater than the diffusive mass transfer of the studied species. This results in a smearing of the mixed components and a prediction of mixing times that are too short. Examples of this are given in [33, 59]. Even with a highly refined grid of approximately 9×10^6 computational cells and a grid resolution of 1 μm in the mixing region, Bothe *et al.* [66] showed that some extremely fine flow structures are still smeared due to numerical diffusion. In order to avoid numerical diffusion in high

Péclet number mixing, Hardt, Schönfeld and co-workers [69, 70] have developed some theoretical models that are based on the solution of the diffusion equation with simplifying assumptions. Although these models are rather simple, they enable quantitative information on mixing to be obtained that is both free of numerical diffusion and in good agreement with experimental data.

Another approach for evaluating mixing in microdevices is to use a Lagrangian method to compute the trajectories of mass-less tracer particles in the flow. Although the solutions of the velocity field and the integration algorithm for the computation of trajectories are still subject to some discretization errors, this method eliminates the problem of numerical diffusion. Typically, the results allow the spatial location of a particular component to be tracked, which enables the mixing mechanism to be visualized [31, 32, 69, 71–74]. Various methods can then be applied to quantify the mixing quality. One method is to carry out a dynamic systems analysis to construct Poincaré sections allowing the chaotic nature of the flow to be characterized or to deduce Lyaponov exponents, which characterize the exponential growth of the interface between two components and can be used to evaluate mixing efficiency [30, 32, 74, 75]. Alternatively, a number-based variance that is analogous to Equation (5.12) can be determined to obtain information on the intensity of segregation [71]:

$$\sigma^2 = \frac{1}{M-1}\sum_{i=1}^{M}(N_i - \bar{N})^2 \tag{5.13}$$

where M is the number of equal-sized bins or quadrats placed in the domain, N_i is the number of particles in bin i and $\bar{N}$ is the mean number of particles per bin. Although this methodology is useful for quantifying the rate at which the tracer particles are spatially spread throughout the micromixer or device, its value is highly dependent on the size and number of bins used and it filters out all segregation patterns that are smaller than the scale of the bin employed in the analysis. In addition, a decrease in quadrat size requires a massive increase in the number of particles in order to represent correctly the statistics of the flow, hence this technique can rapidly become very computationally demanding.

To avoid the dependency of mixing quality on quadrat size and the number of particles, Aubin *et al.* [31] proposed an alternative method based on the analysis of spatial point patterns. This method differs from quadrat analysis mentioned above in that it is based on the distance x_i from each point to the nearest event (tracer particle) for a chosen lattice of m sample points in the domain and therefore it does not require the studied region to be divided into quadrats. The variance of the point-event distances around distance x_R [Equation (5.14)] provides a means to evaluate the mixedness of a system with respect to a 'well-mixed' criterion. This predefined criterion is set by the distance x_R, which corresponds to the scale of segregation whereby two events are considered spatially close enough to be mixed. In this case the variance is defined via

$$\sigma^2 = \frac{1}{m-1}\sum_{i=1}^{m}(x_i - x_R)^2 \tag{5.14}$$

If $x_R \neq 0$, any value of $x_i < x_R$ is considered "better mixed" than the desired scale of segregation. However, according to Equation (5.14) this will give rise to unphysical increases in the variance. To avoid this, Aubin *et al.* [31] suggested the use of a threshold such that in the case where $x_i < x_R$, x_i is assigned a value equal to x_R. This means that the variance will tend towards a value of zero as the spatial distribution of the tracer particles approaches uniformity in the limit of the defined scale of segregation.

Another means of characterizing mixing in microchannels from Lagrangian particle tracking data is to use a measure based on Shannon entropy or information entropy [72–74]. A system with maximum entropy implies an absence of any information and is therefore completely disordered. This corresponds to perfect distributive mixing. In the case of mixing of incompressible fluids, the density at any point in the system remains constant over time and therefore the entropy of the spatial distribution of the mixture also remains constant. This means that the conditional Shannon entropy, S_c, can be used alone to evaluate the local mixing quality averaged over space [73]:

$$S_c = -\sum_{i=1}^{M}\left[P_i \sum_{j=1}^{N_s}\left(P_{j/i}\ln P_{j/i}\right)\right] \tag{5.15}$$

where M is the number of bins, i is the bin number, N_s is the number of species, j is the species number, P_i is the probability of having any species in bin i and $P_{j/i}$ is the probability of having species j in bin i. A mixing index, $\propto_m$, is then deduced by normalizing the conditional Shannon entropy by its maximum value:

$$\propto_m = \frac{S_c}{\ln N_s} \tag{5.16}$$

A mixing index equal to one represents perfect mixing, whereas a value of zero indicates total segregation. As for quadrat analysis, the mixing quality determined by Shannon entropy is dependent on the number and therefore the size of bins. For a large number of bins, i.e. small bin size, perfect mixing is harder (or takes longer) to attain because the required scale of segregation for "complete" mixing is more stringent.

The lattice Boltzmann method has also been used as an alternative to the traditional finite-volume or finite element approaches to assess mixing in microchannels [76, 77]. Lattice Boltzmann methods can simulate hydrodynamics and mass transport phenomena by tracking particle probability distribution functions at lattice positions over time. As a result, the particle concentration is known at the lattice points in the domain. As for Eulerian and Lagrangian methods, the degree of mixing can be assessed by computing the variance of the particle concentration at the lattice points around the mean concentration of the field [76]. Although the lattice Boltzmann method is a means to avoid numerical diffusion, the accuracy of the results depends, of course, on the refinement of the lattice grid. Li and Chen [76] admitted that the lattice used in their simulations was not fine enough, resulting in a poor resolution of concentration fields that filtered out the small scales of mixing.

5.4.3
Modeling of Mass Transfer and Chemical Reaction

Many of the mixing simulations described in the previous section deal with the modeling of mass transfer between miscible fluids [33, 70–77]. These are the simulations which require a solution of the convection–diffusion equation for the concentration fields. For the most part, the transport of a dilute species with a typical diffusion coefficient $\sim 10^{-9}\,m^2\,s^{-1}$ between two miscible fluids with equal physical properties is simulated. It has already been mentioned that due to the discretization of the convection–diffusion equation and the typically small diffusion coefficients for liquids, these simulations are prone to numerical diffusion, which may result in an over-prediction of mass transfer efficiency. Using a lattice Boltzmann method, however, Sullivan *et al.* [77] successfully simulated not only the diffusion of a passive tracer but also that of an active tracer, whereby two miscible fluids of different viscosities are mixed. In particular, they used a coupled hydrodynamic/mass transfer model, which enabled the effects of the tracer concentration on the local viscosity to be taken into account.

Other mass transfer studies in the literature concern mass transport between a single-phase fluid and the microchannel wall, which is a first step towards the simulation of catalytic reactions in which the catalyst is a coating on the channel wall. Van Male *et al.* [78] employed a more global approach to study mass transfer between a gas and the walls of a square microchannel. They used a commercial CFD package to simulate initially heat transport in the microchannel. Using these results, they calculated the Nusselt number at the channel wall, which was then converted to a mass transfer correlation (involving the Sherwood number) via the Chilton–Colburn analogy. The derived Sherwood number correlation permits the calculation of the mass transport coefficient along the length of the microchannel, which can subsequently be used to determine the reaction rate.

Kirtland *et al.* [79] performed simulations of a mass transfer process between reactive solute molecules in a Stokes flow with a reactive channel wall. They simulated a convection–diffusion reaction by tracking the advection of passive Lagrangian tracers in a 3D flow field given by an approximate model. In addition to particle convection, that was calculated at each time step via integration of the velocity field, a diffusive step was implemented, which enabled the three-dimensional, isotropic, diffusive displacement of the particle to be determined. When a particle comes into contact with a reactive microchannel wall it is considered to react, thus allowing calculation of the reactive flux. Using this methodology, a local mass transfer coefficient (averaged over the channel width) and consequently a local Sherwood number were determined.

The modeling of chemical reactions between miscible fluids has been considered in relatively few studies. This may be due to a number of reasons, including the complexity of chemical reaction systems, the lack of intrinsic kinetic data and the inherent numerical problems associated with the resolution of the convection–diffusion reaction equation using typical CFD methods. Within these limits and certain simplifications, the simulation of gas-phase reactions is feasible, as demonstrated

in [80, 81]. Rebrov *et al.* [80] simulated ammonia oxidation on a platinum catalyst in a microstructured reactor/heat exchanger. The detailed kinetic data for ammonia oxidation on Pt catalyst previously obtained by the authors were used to create a simplified rate expression with a power law form, which included two kinetic parameters with Arrhenius temperature dependence. The oxidation reaction on the surface of the channel walls was a boundary condition for the chemical species. This allowed the simulation of the reactions within a given temperature range which were in good agreement with experimental data. Similarly, Deshmukh *et al.* [81] modeled the production of hydrogen from ammonia decomposition on ruthenium. Again, the authors developed a detailed kinetic model for the reaction which they simplified to a reduced rate expression for use in the CFD simulations. The ammonia decomposition was assumed to be a surface reaction and a reduced rate expression was used for the determination of the surface reaction rates. Additionally, isothermal conditions are assumed by setting the heat of reaction to zero. Despite the use of a reduced chemistry model, good agreement between the simulations and the experimental data was observed.

Although the accurate computation of liquid-phase reactions remains difficult due to numerical issues, Aoki *et al.* [82] performed simulations of various model reaction systems, allowing relative comparisons. In particular, they studied the effects of the width of the fluid lamellae and the rate constants on reactant conversion and product selectivity. Qualitatively, the results reveal a strong dependence of the product selectivity on the lamellar width. From these CFD simulations, a model was developed that relates lamellar width, rate constants and product selectivity for various multiple reactions and reaction conditions.

5.5 Multi-phase Simulations

In this section, we look at some examples of multi-phase flows from the simulation perspective. These have very important applications in wide range of microtechnologies.

5.5.1 Taylor Bubble Simulations

Taylor bubbles have been the focus of many simulation exercises because of their occurrence in a variety of flow situations of importance in chemical reaction engineering. They present an example of a flow where the location of a fluid–gas interface must be determined as part of the simulation. A variety of approaches have been used, as discussed below.

Kreutzer *et al.* [83] performed Taylor bubble simulations in which the fluid region around the bubble is meshed and the grid is morphed to determine the location of the gas-liquid interface. The flow inside the bubble is not considered, so it is assumed that its density and viscosity are negligible compared with those of the liquid. The

effect of gravity was ignored, which is equivalent to having a very small Bond number. A two-dimensional, axisymmetric simulation was performed in a frame of reference moving with the bubble. This means that the bubble remains stationary but the wall moves past at the speed of bubble, which has to be determined as part of the simulation. The laminar regime was considered and therefore a parabolic flow was introduced at the inlet and was assumed to leave at the outlet of the tube. The pressure was set to a reference value of zero inside the bubble and the angle of the interface with the axis was set to 90°. The known surface tension coefficient was then used to set the pressure on the fluid side of the interface and the shear at the interface was determined from the gradient of the surface tension, allowing Marangoni effects to be included.

The mesh was fixed far from the bubble but near the interface the nodes were allowed to move along spline curves. The flow was determined without mesh motion and then the nodes were moved according to the boundary conditions. A transient simulation was run until a steady state was achieved. They used around 4000 nodes in their simulations, which was sufficient to give grid-independent results. Their results were found to agree well with theoretical results and experimental data. The use of a discontinuous interface is clever in that it avoids any numerical smearing and ensures that there is a high quality mesh in the very thin liquid fluid layer separating the bubble from the wall.

The same group further developed the model to include mass transfer effects, where mass is transferred from the gas phase to a reacting wall [84]. Given a solution for the bubble shape, it is a simple matter to include mass transfer, as this involves only the addition of a scalar equation with the flow-field kept "frozen". The entire approach represents a clever use of CFD both to determine the bubble hydrodynamics and then to explore the influence of the flow on mass transfer, enabling them to generate useful data for the design of multi-phase monolith reactors.

van Baten and Krishna [85] performed a similar analysis for Taylor bubbles in a vertical tube but they set the bubble shape and velocity as constants and solved for the resulting flow-field. Parametric simulations were performed to investigate the effect of film thickness and bubble velocity. They then used these results to perform transient mass transfer simulations, using extremely fine meshes to resolve the concentration boundary layer. They used these simulations to validate a much simpler model that could be used in monolith reactor design.

Fukagata *et al.* [86] used the Level Set method described earlier to simulate the flow of air bubbles in water in a 20 μm diameter tube with heat transfer. They specified the pressure drop, wall heat flux, bubble period and void fraction. The model then calculated the bubble shape and the flow-field around the bubble assuming a periodic flow boundary condition. From this they then determined the superficial velocities of the gas and liquid and the two-phase multiplier for frictional loss. They noted that the period of the bubbles has a significant effect on the flow field. Their simulation results compared well with experimental data.

Qian and Lawal [87] used the VOF model in Fluent 6.1 (a basic VOF model with the CSF method for the surface tension force; see Section 5.3.1.2) to study Taylor bubble formation via a T-junction made from circular ducts with diameters in the

range 0.25–3 mm, in which gas and liquid are injected from separate legs and a stream of bubbles is produced in the tube. They point out that their results are somewhat approximate as their mesh, comprising 6600 cells, is not fine enough to resolve the bubble shape or the liquid film separating the bubble from the wall. In addition, most simulations are performed for a 2D planar geometry. However, their results are shown to reproduce a number of quantities measured experimentally, including pressure drop and the dependence of slug length on liquid holdup. It is surprising that a modeling approach that clearly does not resolve the flow correctly is capable of producing useful insights into the behavior of this system.

Mukherjee and Kandlikar [88] simulated the growth of a small vapor bubble, in a superheated liquid, located at the center of a 200 μm square section channel. The interface was tracked using the Level Set method coupled with a fifth-order weighted discretization of the Level Set function. Their results predicted a bubble that initially grew in a spherical shape and then developed an elongated form. This shape was seen to occur because as the bubble grew the thin liquid films near the wall resulted in very rapid evaporation and local dryout. Typical starting conditions were water superheated by 2 °C and a wall superheat of 7 °C for a Reynolds number of 100. They found that the bubble growth rate increased with wall superheat, decreased with increased Reynolds number and was insensitive to the presence of gravity.

5.5.2 Droplet Simulations

Many of the issues discussed above apply also in the case of droplet simulations, where again there is a need to model free surfaces accurately and to account for interfacial surface forces. There is a wide range of microscale applications that use droplets, so this area has been well studied. Typical applications include the formation of emulsions via primary breakup of a fluid stream, the further fragmentation of a droplet stream and the encapsulation of a second fluid and/or particles within a droplet.

Schönfeld and Rensink [89] used the VOF model in the commercial code CFX4 to study the formation of a pendant droplet exiting through a 1 mm diameter nozzle. Having validated the single droplet case they then simulated a dual nozzle in which two nozzles located adjacent to each other were used to inject two different fluids that mixed within the droplet. Finally, they used various designs of three nozzles to inject two solutions that were separated by a lamella of water. The computed flow field predicted a vortex formed within the droplet that was similar to those observed experimentally. However, the numerical diffusion was so large that the modeling could not be used to study inter-mixing of the solutions or subsequent reaction.

The similar problem of encapsulating sub-micrometer particles within a carrier fluid has been investigated computationally using a lattice Boltzmann model for binary fluids, together with a Brownian motion model for the particles [90]. The modeling approach allows the inclusion of different fluid–fluid, fluid–solid and fluid–surface interactions into the free energy of the system and hence into their simulations as the dynamics equations depend on the free energy. This novel

approach allowed them to determine the flow patterns and morphology of the fluid system. They illustrate the power of the modeling approach via the simulation of the microencapsulation of solid particles inside a fluid droplet that is immersed in a carrier fluid. This represents a very powerful modeling approach because of the models ability to account for the various phase-interaction physics.

Hardt *et al.* [91] performed both a stability analysis and VOF simulations to study the behavior of a liquid stream passing through a focusing micromixer in order to understand the jet breakup behavior. By understanding the manner in which the jets break up it is possible to operate in a range where a well-controlled droplet size is generated leading to highly controllable emulsion properties. The breakup mechanism was via a "bead-on-string" instability which then generated both larger droplets (the "beads") and smaller droplets from the "string". Their CFD analysis showed that linear stability theory over-predicted the breakup rate as it did not take into account factors such as the rapid acceleration of the fluid at the outlet of the focusing device or the role of wall shear on the subsequent breakup within the capillary tube.

The formation of a microemulsion from an array of microtubes has been studied experimentally and computationally by Kobayashi and co-workers [92, 93]. They used the commercial code CFD-ACE, which uses a piecewise linear interface construction (PLIC) method to determine the interface. They used quarter symmetry, as the channels were elliptical in shape, but the simulations still required 7–14 days on a 2.5 GHz Pentium IV processor. The simulations captured the main features observed experimentally, including the change of regime from continuous outflow of oil if the channel was below a critical aspect ratio, to a stream of droplets above this threshold. The model was also used to predict the droplet size as a function of oil properties and generally agreed well with the experimental data.

Van de Graff *et al.* [94] used a lattice Boltzmann code to predict the effect of velocity and interfacial tension on the formation of droplets in a T-shaped microchannel. Very good agreement between the simulations and experimental data was obtained and the model was used to show that a combination of the capillary number and the flow rate of the fluid to be dispersed control the droplet size.

A novel approach that uses the moving particle semi-implicit (MPS) method to solve the Navier–Stokes equation via a particle interaction model has been used to study droplet formation at a junction between two microchannels [95]. This modeling approach tracks particles with collision rules that allow them to mimic the Navier–Stokes equations. There is no numerical diffusion in this method and a sub-time-stepping treatment of the surface tension force makes the code very stable and accurate in its handling of surface tension forces. The model generally reproduced the experimental data very well, except for some minor differences attributed to the application of a 2D model to a 3D experimental setup.

The modeling of electrohydrodynamic droplet generation from a microchannel within a microchip via an applied electric field has been studied by Kim *et al.* [96]. They modeled the droplet formation using a Level Set method coupled with a Poisson solver for the electric field. The model was used to determine the role of the surface properties of the microtube. They demonstrated that the system could generate mono-sized droplets at a regular frequency with no satellite droplets. The

simple model did not include all of the electric effects but forms a good starting point for a more comprehensive model.

The behavior of elongated droplets of water contained in silicone oil within a 60 μm square-section channel was studied experimentally and numerically by Sarrazzin *et al.* [97]. Their simulations used a research code that solves the Navier–Stokes equations together with a VOF method on a structured mesh. Very fine meshes were needed, with a mesh size of 1/200 of the tube dimension resulting in 10 cells across the liquid film between the droplet and the wall. Simulations required 49 days on a 3 GHz Pentium IV processor. The model results agreed well with microPIV data. In addition to calculating the flow field and droplet shape, they injected a tracer into the droplet at various locations to determine the mixing time. They observed that the counter-rotating vortices within the droplet prevented the mixing of the tracer throughout the droplet.

Harvie and co-workers [98, 99] simulated the behavior of droplets as they pass through an axisymmetric, microcontraction with an aspect ratio of 4:1. Their study was aimed at understanding how such a device could be used to break up further an already formed droplet to a controlled final size for applications such a formation of a microemulsion. Their numerical model used a modified form of the advection scheme of Rudman [38]. They studied a wide range of conditions, including Newtonian droplets suspended in a fluid with a viscosity 1000 times larger and shear thinning fluids for either the droplet or the carrier fluid. A variety of different behaviors were observed, ranging from droplets that elongate and pass through the constriction without fragmenting to cases where a stream of small droplets is formed. They were also able to characterize the behavior of the shear thinning results in terms of results for an equivalent constant viscosity, but the value of this viscosity is only known once a simulation is made and compared with Newtonian simulations.

The effect of the wetting angle at the wall on the droplet breakup behavior for the system described above has been studied using the commercial code CFD-ACE [100]. It was shown that, keeping all other variables constant, lower contact angles induce droplet breakup through the contraction, whereas for higher contact angles the droplet deforms to form a slug, the shape of which depends on the contact angle.

5.6 Summary and Perspective

It is clear from the examples presented above that there is now an enormous amount of work being performed on simulations of flows of relevance to microsystems. This is a very new field, as evidenced by the fact that most of the references cited have been published within the last 3 years. There are some common conclusions that can be drawn from the above work that are summarized below:

1. For flow of a single fluid there exist a number of commercial codes that can be used to investigate flow and heat transfer behavior.
2. Great care must be taken to avoid the effect of numerical diffusion, as this swamps the effect of the real diffusion in many applications.

3. There are a number of additional physical phenomena, such as wall slip, electric effects and viscous energy dissipation, which may need to be taken into account. Generally applicable models are not available for some of these effects, particularly wall slip.
4. In heat transfer applications, the conjugate heat transfer in the substrate may play an important role in determining the thermal behavior of the system.
5. In multi-phase systems, there is the additional complexity of tracking a moving interface. There are a number of different approaches that can be used either to determine the location of the interface from a two-phase flow model or to fit an interface and use interface conditions to determine its shape.
6. Commercial software does not generally have algorithms of sufficient accuracy to determine interface locations and to represent surface tension forces. The Level Set algorithm appears to be the most widely used technique in research codes.
7. Accurate surface tension modeling is also a key component of many simulations but is difficult as a surface force must be represented on a volumetric grid. In addition, the wall contact angle plays a very important role in many cases and this is often a highly uncertain parameter.
8. There is growing use of lattice Boltzmann and other particle-based codes that can circumvent many of the problems of traditional Navier–Stokes-based solvers. However, their use requires specialist knowledge and they are not available commercially.
9. Based on the observation that most of the work cited here was performed in the last 3 years, this area will see considerable growth and numerical methods and models will be developed to resolve many of the outstanding issues discussed in this chapter.

Acknowledgment

Funding of this research via an Australian Research Council Discovery grant is gratefully acknowledged.

References

1 G. Hestroni, A. Mosyak, E. Pogrebnyak, L.P. Yarin, Fluid flow in microchannels, *Int. J. Heat Mass Transfer*, **2005**, *48*, 1982–1998.

2 G.L. Morini, M. Lorenzini, S. Colin, A. Geoffroy, Experimental analysis of pressure drop and laminar to turbulent transition for gas flows in smooth microtubes, *Heat Transfer Eng.*, **2007**, *28*, 670–679.

3 S. Lorenzani, L. Gibelli, A. Frezzotti, A. Frangi, C. Cercignani, Kinetic approach to gas flows in microchannels, *Nanoscale Microscale Thermophys. Eng.*, D **2007**, *11*, 211–226.

4 Y.-L. Han, E.P. Muntz, A. Alexeenko, M. Young, Experimental and computational studies of temperature gradient-driven molecular transport in gas flows through nano/microscale channels, *Nanoscale Microscale Thermophys. Eng.*, **2007**, *11*, 151–175.

5 U. Kursun, J.S. Kapat, Modelling of microscale gas flows in transition regime. Part I. Flow over backward facing steps, *Nanoscale Microscale Thermophys. Eng.*, **2007**, *11*, 15–30.

6 B. Xu, Y. Ju, Concentration slip and its impact on heterogeneous combustion in a micro scale chemical reactor, *Chem. Eng. Sci.*, **2005**, *60*, 3561–3572.

7 X.J. Gu, R.W. Barber, D.R. Emerson, How far can 13 moments go in modeling microscale gas phenomena?, *Nanoscale Microscale Thermophys. Eng.*, **2007**, *11*, 85–97.

8 J.R. Valdés, M.J. Mianna, J.L. Pelegay, J.N. Núñez, T. Pütz, Numerical investigation of the influence or roughness on the laminar incompressible fluid flow through annular microchannels, *Int. J. Heat Mass Transfer*, **2007**, *50*, 1865–1878.

9 J. Koo, C. Kleinstreuer, Viscous dissipation effects in microtubes and microchannels, *Int. J. Heat Mass Transfer*, **2004**, *47*, 3159–3169.

10 B. Xu, K.T. Ooi, C. Mavriplis, M.E. Zaghloul, Evaluation of viscous dissipation in liquid flow in microchannels, *J. Micromech. Microeng.*, **2003**, *13*, 53–57.

11 J.R. Thome, State-of-the-art overview of boiling and two-phase flows in microchannels, *Heat Transfer Eng.*, **2006**, *27*, 4–19.

12 P.J. Stiles, D.F. Fletcher, I. Morris, The effect of gravity on the rate of a simple liquid-state reaction in a small unstirred cylindrical vessel (II), *Phys. Chem. Chem. Phys.*, **2001**, *3*, 3651–3655.

13 P.J. Stiles, D.F. Fletcher, Effects of gravity on the steady state of a reaction in a liquid-state microreactor – deviations from Poiseuille flow, *Phys. Chem. Chem. Phys.*, **2003**, *5*, 1219–1224.

14 T. Bayraktar, S.B. Pidugu, Characterization of liquid flow in microfluidic systems, *Int. J. Heat Mass Transfer*, **2006**, *49*, 815–824.

15 S. Bhattacharyya, Z. Zheng, A.T. Conlisk, Electro-osmotic flow in two-dimensional charged micro and nanochannels, *J. Fluid Mech.*, **2005**, *540*, 247–267.

16 A.T. Conlisk, J. McFerran, Z. Zheng, D. Handsford, Mass transfer and flow in electrically charged micro and nanochannels, *Anal. Chem.*, **2002**, *74*, 2139–2150.

17 A.T. Conlisk, A. Kumar and A. Rampersaud, Ionic and biomolecular transport in nanochannels, *Nanoscale Microscale Thermophys. Eng.*, **2007**, *11*, 177–199.

18 R.-J. Yang, T.-L. Tseng, C.-C. Chang, End effects on electro-osmotic flows in channels, *J. Micromech. Microeng.*, **2005**, *15*, 254–262.

19 S.M. Davidson, K.V. Sharp, Transient electrophoretic motion of cylindrical particles in capillaries, *Nanoscale Microscale Thermophys. Eng.*, **2007**, *11*, 71–83.

20 E.S. Baird, K. Mohseni, A unified velocity model for digital micriofluidics, *Nanoscale Microscale Thermophys. Eng.*, **2007**, *11*, 109–120.

21 G. Nagayama, P. Cheng, Effects of interface wettability on microscale flow by molecular dynamics simulation, *Int. J. Heat Mass Transfer*, **2004**, *47*, 501–513.

22 A.V. Ramamuthy, Wall slip in viscous fluids and influence of material of construction, *J. Rheol.*, **1986**, *30*, 337–357.

23 D.C. Trethway, C.D. Meinhart, Apparent fluid slip at hydrophobic microchannel walls, *Phys. Fluids*, **2002**, *14*, L9.

24 D.C. Trethway, C.D. Meinhart, A generating mechanism for apparent fluid slip in hydrophobic microchannels, *Phys. Fluids*, **2004**, *16*, 1509–1515.

25 D.C. Trethway, C.D. Meinhart, Erratum: A generating mechanism for apparent fluid

slip in hydrophobic microchannels [Phys. Fluids 16, 1509 (2004)], *Phys Fluids*, **2006**, *18*, 109901.

26 A. Ajdari, L. Bocquet, Giant amplification of interfacially driven transport by hydrodynamic slip: diffusio-osmosis and beyond, *Phys. Rev. Lett.*, **2006**, *96*, 186102, 1–4.

27 H.Y. Wu, P. Cheng, An experimental study of convective heat transfer in silicon microchannels with different surface conditions, *Int. J. Heat Mass Transfer*, **2003**, *46*, 2547–2556.

28 G. Rosengarten, J. Cooper-White, G. Metcalfe, Experimental and analytical study of the effect of contact angle on liquid convective heat transfer in microchannels, *Int. J. Heat Mass Transfer*, **2006**, *19*, 4161–4170.

29 S.V. Patankar, *Numerical Heat Transfer and Fluid Flow*, Taylor and Francis, London, **1980**, p. 105.

30 F. Jiang, K.S. Drese, S. Hardt, M. Küpper, F. Schönefeld, Helical flow and chaotic mixing in curved microchannels, *AIChE J.*, **2004**, *50*, 2297–2305.

31 J. Aubin, D.F. Fletcher, C. Xuereb, Design of micromixers using CFD modeling, *Chem. Eng. Sci.*, **2005**, *60*, 2503–2516.

32 M. Yi, H.H. Bau The kinematics of bend-induced mixing in microconduits, *Int. J. Heat Fluid Flow*, **2003**, *24*, 645–656.

33 Y.Z. Liu, B.J. Kim, H.J. Sung, Two-fluid mixing in a microchannel, *Int. J. Heat Fluid Flow*, **2004**, *25*, 986–995.

34 S.H. Wong, P. Bryant, M. Ward, C. Wharton, Investigation of mixing in a cross-shaped micromixer with static mixing elements for reaction kinetics studies, *Sens. Actuators B*, **2003**, *95*, 414–424.

35 J.M. MacInnes, A. Vikhansky, R.W.K. Allen, Numerical characterization of folding flow in microchannel mixers, *Chem. Eng. Sci.*, **2007**, *62*, 2718–2727.

36 C.W. Hirt, B.D. Nichols Volume of fluid method for the dynamics of free surface boundaries, *J. Comput. Phys.*, **1981**, *39*, 323–345.

37 W.J. Rider, D.B. Kothe, Reconstructing volume tracking, *J. Comput. Phys.*, **1998**, *141*, 112–152.

38 M. Rudman, Volume-tracking methods for interfacial flow calculations, *Int. J. Num. Methods Fluids*, **1997**, *24*, 671–691.

39 M. Sussman, E. Fatemi, P. Smereka, S. Osher, An improved Level Set method for incompressible two-phase flows, *Comput. Fluids*, **1998**, *27*, 663–680.

40 J.U. Brackbill, D.B. Kothe, C. Zemach, A continuum method for modeling surface tension, *J. Comput. Phys.*, **1992**, *100*, 335–354.

41 D.J.E. Harvie, M.R. Davidson, M. Rudman, An analysis of parasitic current generation in volume of fluid simulations, *Appl. Math. Model.*, **2006**, *30*, 1056–1066.

42 I. Tiselj, G. Hestroni, B. Mavko, A. Mosyak, E. Pogrebnyak, Z. Segal, Effect of axial conduction on the heat transfer in microchannels, *Int. J. Heat Mass Transfer*, **2004**, *47*, 2551–2565.

43 Z. Li, Y.-L. He, G.-H. Tang, W.-Q. Tao, Experimental and numerical studies of liquid flow and heat transfer in microtubes, *Int. J. Heat Mass Transfer*, **2007**, *50*, 3447–3460.

44 G. Arya, H.C. Chang, E.J. Maginn, Molecular simulations of Knudsen wall-slip: effect of wall morphology, *Mol. Simul.*, **2003**, *29*, 697–709.

45 E.E. Rosenbaum, S.G. Hatzikiriakos, Wall slip in the capillary flow of molten polymers subject to viscous heating, *AIChE J.*, **1997**, *43*, 598–608.

46 C.Y. Lim, C. Shu, X.D. Niu, Y.T. Chew, Application of lattice Boltzmann method to simulate microchannel flows, *Phys. Fluids*, **2002**, *14*, 2299–2308.

47 L. Zhu, D. Tretheway, L. Petzold, C. Meinhart, Simulation of fluid slip at 3D hydrophobic walls by the lattice Boltzmann method, *J. Comput. Phys.*, **2005**, *202*, 181–195.

48 D. Wang, J. Summers, P.H. Gaskell, Modelling of electrokinetically driven flow mixing enhancement in

microchannels with patterned heterogeneous surface and blocks, *Nanoscale Microscale Thermophys. Eng.*, **2007**, *11*, 1–13.

49 Y.M. Chung, P.G. Tucker, Numerical studies of heat transfer enhancements in laminar separated flows, *Int. J. Heat Fluid Flow*, **2004**, *25*, 22–31.

50 J.-T. Liu, X.-F. Peng, W.-M. Yan, Numerical study of fluid flow and heat transfer in microchannel cooling passages, *Int. J. Heat Mass Transfer*, **2007**, *50*, 1855–1864.

51 L. Wang, F. Liu, Forced convection in slightly curved microchannels, *Int. J. Heat Mass Transfer*, **2007**, *50*, 881–896.

52 N.R. Rosaguti, D.F. Fletcher, B.S. Haynes, Laminar flow and heat transfer in a periodic serpentine channel, *Chem. Eng. Technol.*, **2005**, *28*, 353–361.

53 P.E. Geyer, N.R. Rosaguti, D.F. Fletcher, B.S. Haynes, Thermohydraulics of square-section microchannels following a serpentine path, *Microfluidics Nanofluidics*, **2006**, *2*, 195–204.

54 N.R. Rosaguti, D.F. Fletcher, B.S. Haynes, Laminar flow and heat transfer in a periodic serpentine channel with semi-circular cross-section, *Int. J. Heat Mass Transfer*, **2006**, *49*, 2912–2923.

55 N.R. Rosaguti, D.F. Fletcher, B.S. Haynes, Low Reynolds number heat transfer enhancement in sinusoidal channels, *Chem. Eng. Sci.*, **2007**, *62*, 694–702.

56 P.E. Geyer, D.F. Fletcher, B.S. Haynes, Laminar flow and heat transfer in a periodic trapezoidal channel with semi-circular cross-section, *Int. J. Heat Mass Transfer*, **2007**, *50*, 3571–3480.

57 N.R. Rosaguti, D.F. Fletcher, B.S. Haynes, A general implementation of the H1 boundary condition in CFD simulations of heat transfer in swept passages, *Int. J. Heat Mass Transfer*, **2007**, *50*, 1833–1842.

58 P.-S. Lee, S.V. Garimella, Thermally developing flow and heat transfer in rectangular microchannels of different aspect ratios, *Int. J. Heat Mass Transfer*, **2006**, *49*, 3060–3067.

59 S.H. Wong, P. Bryant, M. Ward, C. Wharton, Investigation of mixing in a cross-shaped micromixer with static mixing elements for reaction kinetics studies, *Sens. Actuators B*, **2003**, *95*, 414–424.

60 H. Wang, P. Iovenitti, E. Harvey, S. Masood, Numerical investigation of mixing microchannels with patterned grooves, *J. Micromech. Microeng.*, **2003**, *13*, 801–808.

61 M. Engler, N. Kockmann, T. Kiefer, P. Woias, Numerical and experimental investigations on liquid mixing in static micromixers, *Chem. Eng. J.*, **2004**, *101*, 315–322.

62 S.W. Lee, D.S. Kim, S.S. Lee, T.H. Kwon, A split and recombination micromixer fabricated in a PDMS three-dimensional structure, *J. Micromech. Microeng.*, **2006**, *16*, 1067–1072.

63 J. Cha, J. Kim, S.-K. Ryu, J. Park, Y. Jeong, Se. Park, Su. Park, J.C. Kim, K. Chun, A highly efficient 3D micromixer using soft PDMS bonding, *J. Micromech. Microeng.*, **2006**, *16*, 1778–1782.

64 N. Kockmann, T. Kiefer, M. Engler, P. Woias, Convective mixing and chemical reactions in microchannels with high flow rates, *Sens. Actuators B*, **2006**, *117*, 495–508.

65 X. Fu, S. Liu, X. Ruan, H. Yang, Research on staggered oriented ridges static micromixers, *Sens. Actuators B*, **2006**, *114*, 618–624.

66 D. Bothe, C. Stemich, H.-J. Warnecke, Fluid mixing in a T-shaped micromixer, *Chem. Eng. Sci.*, **2006**, *61*, 2950–2958.

67 L. Wang, J.-T. Yang, P.-C. Lyu, An overlapping crisscross micromixer, *Chem. Eng. Sci.*, **2007**, *62*, 711–730.

68 P.V. Danckwerts, The definition and measurement of some characteristics of mixtures, *Appl. Sci. Res.*, **1952**, *A3*, 279–296.

69 S. Hardt, F. Schönfeld, Laminar mixing in different interdigital micromixers: II. Numerical simulations, *AIChE J.*, **2003**, *49*, 578–584.

70 S. Hardt, H. Pennemann, F. Schönfeld, Theoretical and experimental characterization of a low-Reynolds number split-and-recombine mixer, *Microfluidics Nanofluidics*, **2006**, *2*, 237–248.

71 J. Aubin, D.F. Fletcher, J. Bertrand, C. Xuereb, Characterization of mixing quality in micromixers, *Chem. Eng. Technol.*, **2003**, *26*, 1262–1270.

72 T.G. Kang, T.H. Kwon, Colored particle tracking method for mixing analysis of chaotic micromixers, *J. Micromech. Microeng.*, **2004**, *14*, 891–899.

73 M. Camesasca, I. Manas-Zloczower, M. Kaufman, Entropic characterization of mixing in microchannels, *J. Micromech. Microeng.*, **2005**, *15*, 2038–2044.

74 C.-C. Chang, R.-J. Yang, A particle tracking method for analyzing chaotic electroosmotic flow mixing in 3D microchannels with patterned charged surfaces, *J. Micromech. Microeng.*, **2006**, *16*, 1453–1462.

75 X. Niu, Y.-K. Lee, Efficient spatial–temporal chaotic mixing in microchannels, *J. Micromech. Microeng.*, **2003**, *13*, 454–462.

76 C. Li, T. Chen, Simulation and optimization of chaotic micromixer using lattice Boltzmann method, *Sens. Actuators B*, **2005**, *106*, 871–877.

77 S.P. Sullivan, B.S. Akpa, S.M. Matthews, A.C. Fisher, L.F. Gladden, M.L. Johns, Simulation of miscible diffusive mixing in microchannels, *Sens. Actuators B*, **2007**, *123*, 1142–1152.

78 P. van Male, M.H.J.M. de Croon, R.M. Tiggelaar, A. van den Berg, J.C. Schouten, Heat and mass transfer in a square microchannel with asymmetric heating, *Int. J. Heat Mass Transfer*, **2004**, *47*, 87–99.

79 J.D. Kirtland, G.J. McGraw, A.D. Stroock, Mass transfer to reactive boundaries from steady three-dimensional flows in microchannels, *Phys. Fluids*, **2006**, *18*, 073602.

80 E.V. Rebrov, S.A. Duinkerke, M.H.J.M. de Croon, J.C. Schouten, Optimization of heat transfer characteristics, flow distribution and reaction processing for a microstructured reactor/heat-exchanger for optimal performance in platinum catalyzed ammonia oxidation, *Chem. Eng. J.*, **2003**, *93*, 201–216.

81 S.R. Deshmukh, A.B. Mhadeshwar, D.G. Vlachos, Microreactor modeling for hydrogen production from ammonia decomposition on ruthenium, *Ind. Eng. Chem. Res.*, **2004**, *43*, 2986–2999.

82 N. Aoki, S. Hasebe, K. Mae, Mixing microreactors: effectiveness of lamination segments as a form of feed on product distribution for multiple reactions, *Chem. Eng. J.*, **2004**, *101*, 323–331.

83 M.T. Kreutzer, F. Kapteijn, J.A. Moulijn, C.R. Kleijn, J.J. Heiszwolf, Inertial and interfacial effects on pressure drop of Taylor flow in capillaries, *AIChE J.*, **2005**, *51*, 2428–2440.

84 M.T. Kreutzer, F. Kapteijn, J.A. Moulijn, J.J. Heiszwolf, Multi-phase monolith reactors: chemical reaction engineering of segmented flow in microchannels, *Chem. Eng. Sci.*, **2005**, *60*, 5895–5916.

85 van Baten J.M., Krishna R., CFD simulations of mass transfer from Taylor bubbles rising in circular capillaries, *Chem. Eng. Sci.*, **2004**, *59*, 2535–2545.

86 K. Fukagata, N. Kagagi, P. Ua-arayaporn, T. Himeno, Numerical simulation of gas–liquid two-phase flow and convective heat transfer in a micro tube, *Int. J. Heat Fluid Flow*, **2007**, *28*, 72–82.

87 D. Qian, A. Lawal, Numerical study on gas and liquid slugs for Taylor flow in a T-junction microchannel, *Chem. Eng. Sci.*, **2006**, *61*, 7609–7625.

88 A. Mukherjee, S.G. Kandlikar, Numerical simulation of growth of a vapor bubble during flow boiling of water in a microchannel, *Microfluidics Nanofluidics*, **2005**, *1*, 137–145.

89 F. Schönfeld, D. Rensink, Simulation of droplet generation by mixing nozzles, *Chem. Eng. Technol.*, **2003**, *26*, 585–591.

90 R. Verberg, J.M. Yeomans, A.C. Balazs, Modeling the flow of fluid/particle mixtures in microchannels: encapsulating nanoparticles within monodisperse droplets, *J. Chem. Phys.*, **2005,** *123*, 224706.

91 S. Hardt, F. Jiang, F. Schönfeld, A computational analysis of the hydrodynamic instability of a liquid jet focused into a converging microchannel, *Int. J. Multi-phase Flow,* **2005,** *31*, 739–756.

92 I. Kobayashi, S. Mukataka, M. Nakajima, CFD simulations and analysis of emulsion droplet formation from straight-through microchannels, *Langmuir,* **2004,** *20*, 9868–9877.

93 I. Kobayashi, S. Mukataka, M. Nakajima, Effects of type and physical properties of oil phase on oil-in-water emulsion droplet formation in straight-through microchannel emulsification, experimental and CFD studies, *Langmuir,* **2005,** *21*, 5722–5730.

94 S. van de Graff, T. Nisisako, C.G.P.H. Schroën, R.G.M. van de Samn, R.M. Broom, Lattice Boltzmann simulations of droplet formation in a T-shaped microchannel, *Langmuir,* **2006,** *22*, 4144–4152.

95 T. Harada, Y. Suzuki, S. Koshizuka, T. Arakawa, S. Shoji, Simulation of droplet generation in micro flow using MPS method, *JSME Int. J., Ser. B*, **2006,** *49*, 731–736.

96 S.J. Kim, Y.-A. Song, P.L. Skipper, J. Han, Elecrohydrodynamic generation and delivery of monodisperse picoliter droplets using a poly(dimethylsiloxane) microchip, *Anal. Chem.*, **2006,** *78*, 8011–8019.

97 F. Sarrazin, K. Loubière, L. Prat, C. Goudron, T. Bonometti, J. Magnaudet, Experimental and numerical study of droplet hydrodynamics in microchannels, *AIChE J.*, **2006,** *52*, 4061–4070.

98 D.J.E. Harvie, M.R. Davidson, J.J. Cooper-White, M. Rudman, A parametric study of droplet deformation through a microfluidic contraction: Low viscosity Newtonian droplets, *Chem. Eng. Sci.*, **2006,** *61*, 5149–5158.

99 D.J.E. Harvie, M.R. Davidson, J.J. Cooper-White, M. Rudman, A parametric study of droplet deformation through a microfluidic contraction: Shear thinning liquids, *Int. J. Multi-phase Flow,* **2007,** *33*, 545–556.

100 G. Rosengarten, D.J.E. Harvie, J. Cooper-White, Contact angle effects on microdroplet deformation using CFD, *Appl. Math. Model.*, **2006,** *30*, 1033–1042.