



Numerical modeling of multiple length scales in thermal transport processes

Numerical
modeling

Yogesh Jaluria

*Department of Mechanical and Aerospace Engineering, Rutgers University,
Piscataway, New Jersey, USA*

781

Received 5 February 2013

Revised 29 March 2013

Accepted 8 April 2013

Abstract

Purpose – Multiple length and time scales arise in a wide variety of practical and fundamental problems. It is important to obtain accurate and validated numerical simulation results, considering the different scales that exist, in order to predict, design and optimize the behavior of practical thermal processes and systems. The purpose of this paper is to present modeling at the different length scales and then addresses the question of coupling the different models to obtain the overall model for the system or process.

Design/methodology/approach – Both numerical and experimental methods to obtain results at the different length scales, particularly at micro and nanoscales, are considered. Even though the paper focusses on length scales, multiple time scales lead to similar concerns and are also considered. The two circumstances considered in detail are multiple length scales in different domains and those in the same domain. These two cases have to be modeled quite differently in order to obtain a model for the overall process or system. The basic considerations involved in such a modeling are discussed. A wide range of thermal processes are considered and the methods that may be used are presented. The models employed must be validated and the accuracy of the simulation results established if the simulation results are to be used for prediction, control and design.

Findings – Of particular interest are concerns like verification and validation, imposition of appropriate boundary conditions, and modeling of complex, multimode transport phenomena in multiple scales. Additional effects such as viscous dissipation, surface tension, buoyancy and rarefaction that could arise and complicate the modeling are discussed. Uncertainties that arise in material properties and in boundary conditions are also important in design and optimization. Large variations in the geometry and coupled multiple regions are also discussed.

Research limitations/implications – The paper is largely focussed on multiple-scale considerations in thermal processes. Both numerical modeling/simulation and experimentation are considered, with the latter being used for validation and physical insight.

Practical implications – Several examples from materials processing, environmental flows and electronic systems, including data centers, are given to present the different techniques that may be used to achieve the desired level of accuracy and predictability.

Originality/value – Present state of the art and future needs in this interesting and challenging area are discussed, providing the impetus for further work. Different methods for treating multiscale problems are presented.

Keywords Modeling, Numerical simulation, Multiple scales, Multiscale, Thermal processes, Thermal systems

Paper type Research paper



1. Introduction

An important consideration in many thermal processes and systems is that of modeling different length and time scales that arise. In materials processing, for

The author acknowledges the partial support from NSF under grant number 1067141, and from industry for this study and the work done by several graduate students.

International Journal of Numerical
Methods for Heat & Fluid Flow
Vol. 24 No. 4, 2014
pp. 781-796

© Emerald Group Publishing Limited
0961-5539

DOI 10.1108/HFF-02-2013-0044

instance, the basic transformations in the material largely occur at the micro/nanoscale, whereas the devices and products being fabricated and the operating conditions are at the macro or engineering scale (Jaluria, 2003). Similarly, cooling of electronic components, which are generally at engineering length scales, may be efficiently achieved by the flow and heat transfer in microchannels. Numerical simulation of environmental flows, such as the plumes generated by large fires and thermal discharges from power plants and industries into the ambient, involve very different length scales close to the source and those far downstream. In all such cases, depending on the dimensions, different flow regimes arise, which demand different analyses and pose different challenges to experimentation. However, our interest from the overall numerical simulation lies, for instance, in determining the quality of the fabricated product, the effect on the environment, efficiency of heat removal and fire spread. It is thus critical to model the different scales in length and time accurately and then couple these to obtain the overall model for the system or the process.

Several important questions arise in the modeling of multiple length scales. The first one relates to the domains where different scales are applicable. For example, in the chemical vapor deposition process, which is used to fabricate thin films and devices for electronic and optical applications like light-emitting diodes, solar cells and optoelectronic devices, the thin film starts out as a few nanometers in thickness and typically reaches thicknesses of a few microns (Mahajan, 1996; Jaluria, 2009). The basic chemical mechanisms involved in the deposition are quite different from those in the bulk flow. Thus, modeling is carried out at these small length scales with the relevant equations and numerical models. Experimentation may also be used at the small scales to obtain the data that may be provided as inputs to the macroscale model to simulate the overall process. The next aspect relates to how the micro/nanoscale domain is linked with the overall flow and heat transfer in the reactor for process control and optimization. This involves the question of discretization of the different domains and the imposition of appropriate boundary conditions at the boundaries between the different domains. In environmental flows, much finer grids are needed near the source and much coarser grids can be employed far from the source. The underlying mechanisms also change from the region near the source to the flow far downstream, with buoyancy often dominating far from the source and combustion, radiation, and forced convection effects dominating near the source. Similarly, the time scales involved in different components of a furnace, for instance, or in the flow and heat transfer in a natural body of water such as a lake are very different and modeling of the system involves considerations similar to those for multiple length scales. Such multiscale modeling has been of considerable interest in recent years (Joshi, 2012; He and Tao, 2012).

Figure 1 shows a few practical circumstances where multiple length scales are of interest. In chemical vapor deposition, the length scales near the surface, on which the thin film is to be deposited and which is known as the susceptor, are quite different from those in the bulk flow in the reactor. This is also the case in building and forest fires, as well as thermal discharges to the ambient, shown in the figure. In electronic devices, the transport in microchannels needs to be coupled with conduction and convection in the overall system. In data centers, the transport processes at the chip level are at very different length scales as compared to those for the server and the data center. In time-dependent problems, the time scales could similarly be quite different, posing challenges in the modeling of the system.

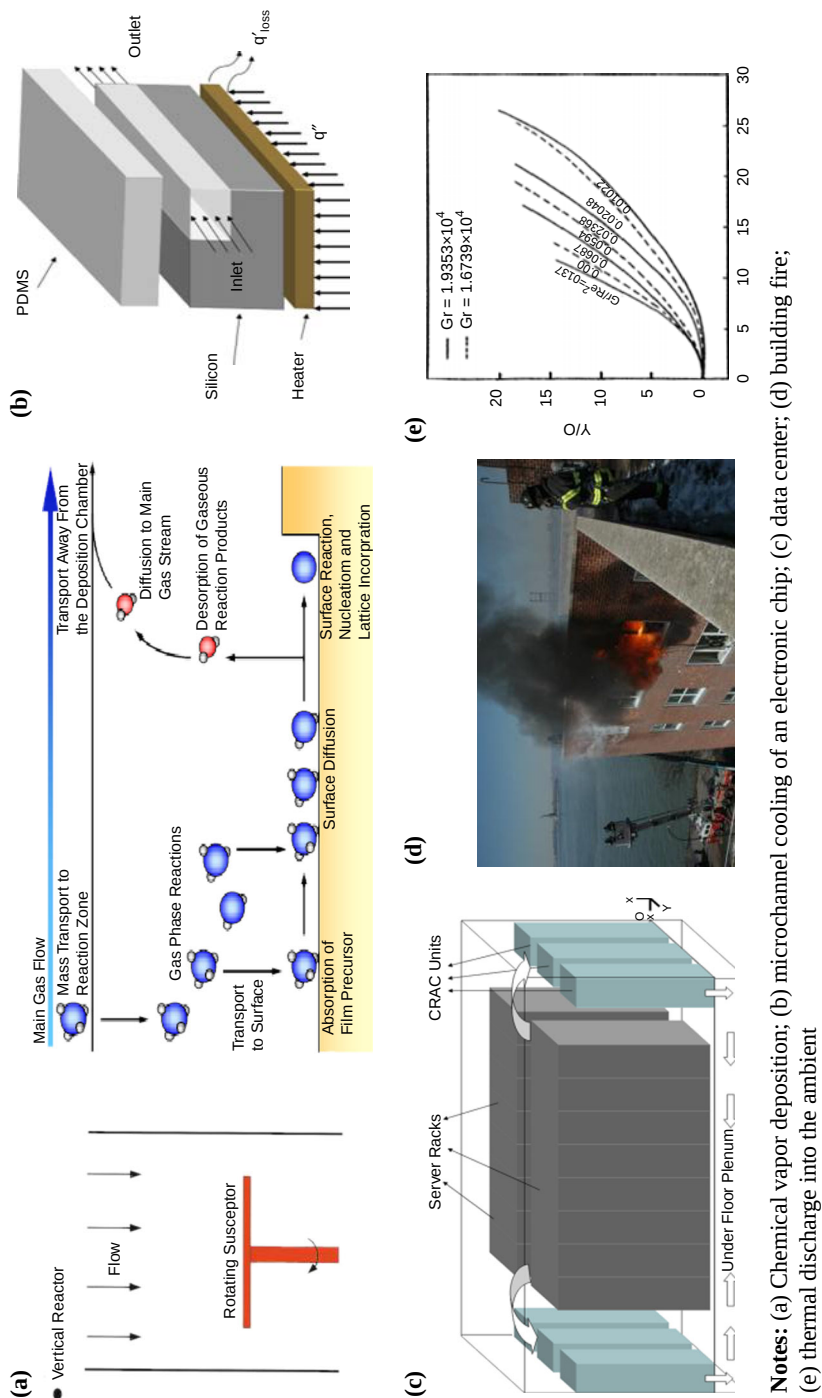


Figure 1.
A few problems where
multiple length scales
are of interest

2. Different circumstances for multiple scales

Multiple length and time scales arise in a wide range of practical processes. There are two main categories that one encounters when dealing with multiple scales. These are:

- (1) multiple scales in different domains; and
- (2) multiple scales within a given domain.

The former circumstance is quite common and is relatively easier to model. Different length or time scales arise in different regions so that each region can be treated separately. In thermal discharges into the environment, for instance, the length scales of interest near in the region close to the discharge point, as shown in Figure 1(e), are often quite different from those far downstream. In typical applications, the former may be of the order of a meter, whereas the length scales are of the order of kilometers far downstream. However, the two regions may be considered separately, with appropriate governing mechanisms and equations, and the solutions in different regions may then be coupled at the boundaries.

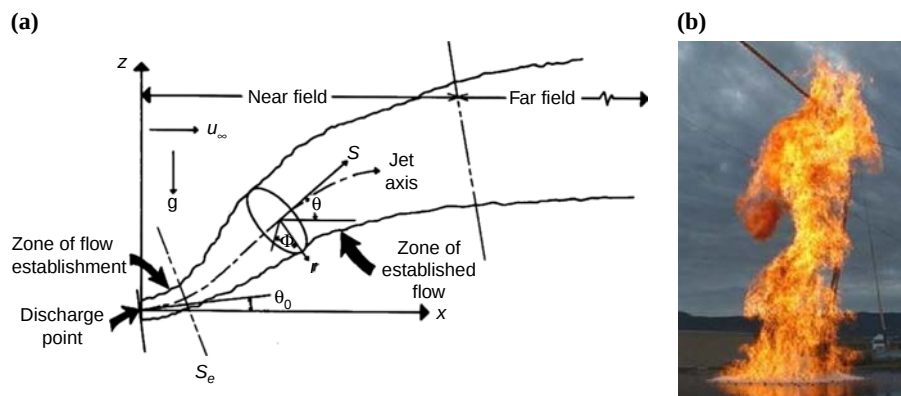
The second circumstance is more involved and is of particular interest in material processing, combustion, chemical conversion, etc. where changes occur at the micro or nanoscale, while the overall system is in the macro or engineering scales, both being in the same domain. An example is provided by chemical vapor deposition, as shown in Figure 1(a), where the thin film and the deposition process occur over much smaller length scales as compared to the bulk flow and transport processes. In such cases, the processes occurring over the small scales have to be experimentally determined or modeled to obtain changes in the material and the results are then coupled with the bulk flow to model, design and optimize the system.

3. Multiple length scales arising in different domains

This is a particularly common circumstance of multiple scales. Different length scales are of interest in different regions of the flow or process. However, the numerical modeling depends on the characteristics of the problem and different techniques are used to simplify the problem. Some of these are outlined here.

3.1 Matching computational results at domain boundaries

Figure 2 shows two important convective flows where multiple scales arise in different regions. Figure 2(a) shows thermal or material discharge into the environment with a cross-flow due to the wind. The flow is of interest in pollution considerations, as well as in the modeling of atmospheric transport processes. As seen in the figure, there is a zone of establishment near the discharge point, where the inflow momentum effects dominate and the flow retains the characteristics of the discharge. Further downstream, the flow establishes itself under the influence of inflow momentum, buoyancy and cross-flow. This is the “near field.” Still further downstream, buoyancy effects dominate, along with the cross-flow, and the effect of the initial momentum input is essentially negligible. This is the “far field.” Clearly, the mechanisms operating in these different regions are different, as are the length scales (Gebhart *et al.*, 1984). Near the discharge, the Reynolds number $Re = UD/\nu$, based on the discharge velocity U and diameter D , where ν is the kinematic viscosity, is the dominant parameter. Similarly, the buoyancy, as given by the Grashof number, Gr , and the Reynolds number based on the cross-flow velocity U_∞ are important far downstream. Clearly, treating the entire flow region as a single computational



Notes: (a) Thermal or material discharge into an ambient medium with cross-flow;
(b) large-scale fire in an open field

Figure 2.
Flows with different
length scales in
different regions

domain is inefficient and time-consuming. It could also lead to inaccurate results in regions where finer scales are of interest.

The basic approach to model this flow is to divide the overall flow into the three regions shown, obtain the relevant equations and boundary conditions, solve these, and match the results obtained at the domain boundaries. The three domains are not known a priori and may be approximated on the basis of the governing parameters such as Reynolds and Grashof numbers, as well as length scales. However, the domains need to be varied in the numerical simulation to ensure that the final results are independent of the chosen regions.

An important aspect in the numerical modeling is obviously the grid used for the solution of the equations. Different length scales demand different grid dimensions and this must be addressed before proceeding to the solution. Generally, fine grids are needed near the discharge point, with much larger and coarser grids far downstream. Different strategies of generating such non-uniform grids are available in the literature (Minkowycz and Sparrow, 1997; Minkowycz *et al.*, 2006) and commercial codes, like Fluent, have the flexibility and ease to use a wide variety of appropriate grids. Similar considerations apply for the large-scale fire shown in Figure 2(b). The fire is modeled as a combustion phenomenon using the chemical kinetics and radiative transport, along with the flow. The region beyond the flames is dominated by buoyancy and is solved as a buoyancy-driven flow, with inputs obtained at the boundaries from the fire model.

3.2 Imposition as boundary condition

In many circumstances, different length scales can be treated in a simpler, though more approximate, manner. The region of smaller length scales is solved accurately and the inputs in terms of heat or mass transfer rate, flow rate, etc. are obtained. These are then given as boundary conditions for the solution of the transport processes in the region with larger length scales.

Figure 3 shows the flows driven by a localized fire, such as a pool fire, in an enclosure such as a room with a door. Again, the fire region and the buoyancy-driven flow away from the fire may be treated in terms of two different domains, as outlined earlier. However, in many cases, the heat release rate by the fire can be obtained by

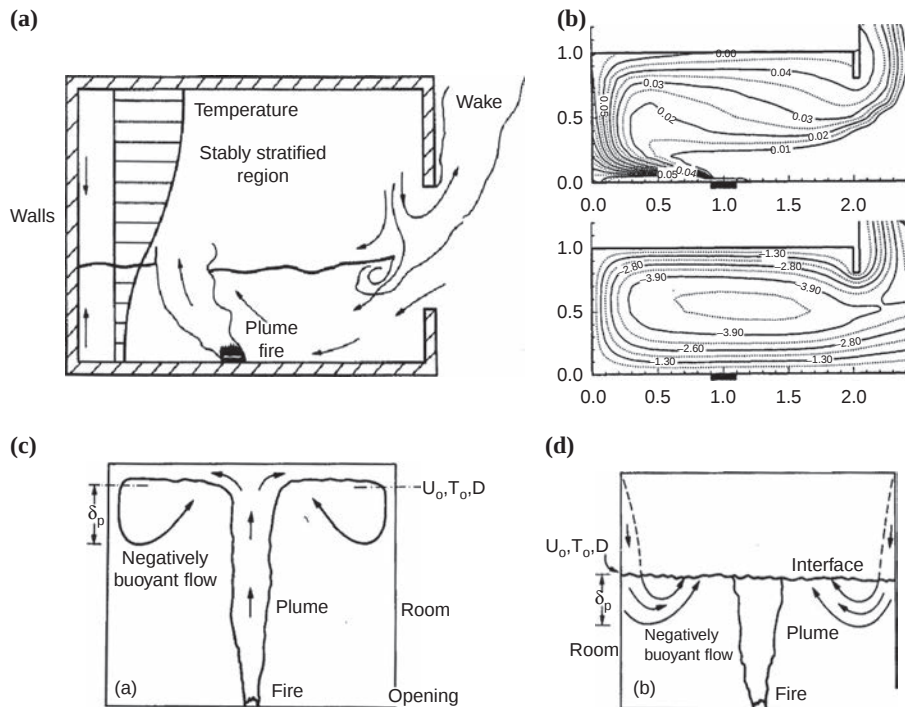


Figure 3.
Buoyancy-driven flows
due to fire in a room
with an opening

Notes: (a) Basic flow; (b) streamlines and isotherms in turbulent flow; (c) starting fire; (d) wall flows in a steady state situation

analysis, experiment or numerical modeling at the relevant length scales. The heat release rate is then provided as input of heat flux over a specified region, as shown. The focus is on the flow driven by this heat input at various stages of fire growth or under steady state conditions that arise in some cases. Figure 3(a) shows the physical nature of the problem associated with a fire in a room with an opening. Figure 3(b) shows the computed streamlines and isotherms for a typical turbulent flow circumstance. Figure 3(c) shows the starting plume, ceiling jet and the flow turning downward at the corner, at the early stages of the fire. Finally, Figure 3(d) shows wall flows generated in a stratified environment for the steady state situation. Various such flows have been investigated to evaluate the changing environment in a room due to a fire (Abib and Jaluria, 1995; Jaluria and Cooper, 1989). It is interesting to note that this approach has been used extensively to model fire growth and spread in buildings using the heat release rate from a fire as obtained experimentally or numerically.

Numerical simulation can be used quite conveniently to solve for the velocity, temperature and pressure. The boundary conditions are the usual no-slip, adiabatic, conditions at the walls, except for the source and the inflow-outflow conditions at the opening. Except for relatively small fires and rooms, the flow is turbulent, which requires an appropriate closure model. Simulation has been carried out by several investigators using eddy viscosity models, as well as the κ - ϵ mode (Jaluria and Torrance, 2003).

Mixed convection flows arise if a cross-flow exists, as in Figure 2(a), or in the simulation of a buoyant jet such as the ceiling jet or wall flows shown in Figure 3. The governing non-dimensional differential equations for laminar mixed convection flow, with constant thermophysical properties, can be written for three-dimensional flow in the following form for continuity, momentum and energy:

$$\nabla \cdot \bar{V} = 0 \quad (1)$$

$$\frac{\partial \bar{V}}{\partial t} + \bar{V} \cdot \nabla \bar{V} = -\nabla P + \frac{1}{\text{Re}} \nabla^2 \bar{V} - \frac{Gr}{\text{Re}^2} \theta \bar{g} \quad (2)$$

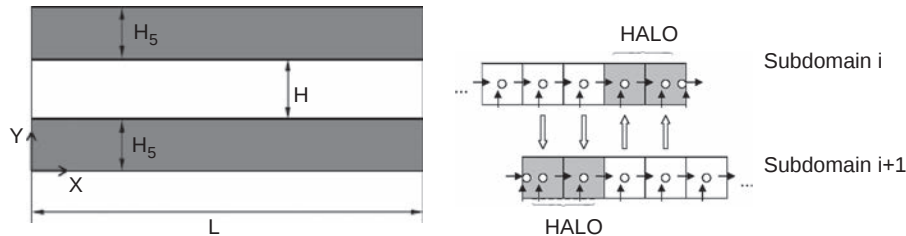
$$\frac{\partial \theta}{\partial t} + \bar{V} \cdot \nabla \theta = \frac{1}{\text{RePr}} \nabla^2 \theta \quad (3)$$

where $\bar{V}$ is the velocity, P the pressure, θ the temperature, $\bar{g}$ the gravitational acceleration, Pr the Prandtl number and t the time. Again, the numerical modeling is well established and can be used to study the flow driven by a heat or momentum source for laminar or turbulent flow.

3.3 Multiple length scales in different components

In many practical systems, transport processes in various components or subsystems are at different length or time scales. The governing equations for different components are different and thus the numerical approaches used may be quite different. As an example, consider the numerical simulation of pressure-driven nitrogen slip flow in long microchannels, with conjugate heat transfer at the walls of the heat removal system under a uniform heat flux wall boundary condition, as sketched in Figure 1(b).

Figure 4(a) shows a sketch of this problem. For the gas phase, the two-dimensional momentum and energy equations are solved, considering variable properties, rarefaction, which involves velocity slip, thermal creep and temperature jump, compressibility, and viscous dissipation. Even with liquids, though slip conditions may not arise, the basic concerns with pressure, viscous dissipation, variable properties and fine grids have to be considered at these scales. For conduction in the solid region, on the other hand, the energy equation is solved with variable properties. Figure 4(b) shows a domain decomposition that may be used for parallelization of the computation process, as well as for different components or subsystems.



Notes: (a) Sketch of the microchannel; (b) domain decomposition for parallel computation of the microchannel flow, as well as of the various components

Figure 4.
Nitrogen flow in
a microchannel, with
conjugate transport
at the walls

Due to rarefaction, discontinuous boundary conditions are applied at the wall, particularly for gases, depending on the Knudsen number, $Kn = \lambda/H$, where λ is the mean free path of the gas molecules and H is the channel height for two-dimensional rectangular channels. Continuum flow is assumed for $Kn \leq 10^{-3}$; slip flow occurs when $10^{-3} \leq Kn \leq 10^{-1}$; transition flow arises $10^{-1} \leq Kn \leq 10$; and free-molecular flow refers to the case of $Kn > 10$. For isothermal walls, the wall boundary conditions are (Sun and Jaluria, 2011):

$$\begin{aligned} \text{At } y=0 \text{ and } y=H, u &= \frac{2-\sigma_v}{\sigma_v} \lambda \left(\frac{\partial u}{\partial n} \right)_w + \frac{3}{4} \frac{\mu}{\rho T} \left(\frac{\partial T}{\partial x} \right)_w, v = 0, \\ T_g - T_w &= \frac{2-\sigma_T}{\sigma_T} \left[\frac{2\gamma}{\gamma+1} \right] \frac{\lambda}{Pr} \left(\frac{\partial T}{\partial n} \right)_w \end{aligned} \quad (4)$$

The coefficients σ_v and σ_T depend on gas properties and surface qualities. They represent the fraction of the molecule's tangential momentum and energy loss through the interactions with the solid wall, respectively. The substrates are governed by the energy equation:

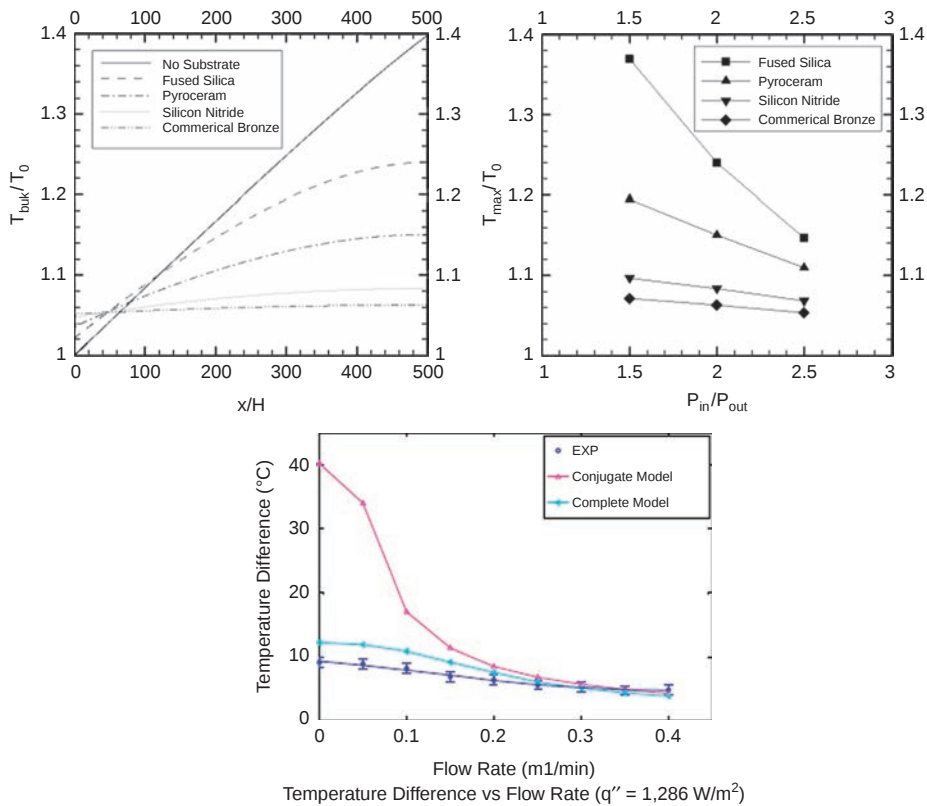
$$c_p \left[\frac{\partial \rho T}{\partial t} + \frac{\partial \rho u T}{\partial x} + \frac{\partial \rho v T}{\partial y} \right] = \left[\frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) \right] \quad (5)$$

Here, u and v are velocity components in x and y coordinate directions, respectively, n is the normal to the wall, λ is the specific heat ratio, c_p the specific heat at constant pressure, ρ the density and k the thermal conductivity. The boundary conditions in the y -direction, i.e., at $y=0$ and $y=2H_s+H$ are given by $q=q_w$, q being the heat flux and subscript w referring to the wall. The temperature at the fluid-solid interface is obtained by solving the two equations:

$$\begin{aligned} T_g - T_w &= \frac{2-\sigma_T}{\sigma_T} \left[\frac{2\gamma}{\gamma+1} \right] \frac{\lambda}{Pr} \left(\frac{\partial T}{\partial n} \right)_w \\ q_g &= q_s \end{aligned} \quad (6)$$

where the first equation is due to the temperature jump at the gas-solid interface, and the second one arises from the fact that no energy can be stored in the interface.

Typical results for different substrate materials, including commercial bronze, silicon nitride, pyroceram and fused silica are shown in Figure 5(a) and (b). The effects of substrate axial conduction, material thermal conductivity and substrate thickness are clearly seen. It was found that substrate axial conduction leads to a flatter bulk temperature profile along the channel, lower maximum temperature and lower Nusselt number. The effect of substrate thickness on the conjugate heat transfer is very similar to that of the substrate thermal conductivity. That is, in terms of axial thermal resistance, the increase in substrate thickness has the same effect as that caused by an increase in its thermal conductivity. Figure 5(c) shows the comparison between the numerical results and experimental data when only the walls are considered and also when the entire system is considered for simulation. This simple example illustrates the simulation of different components with different length scales, followed by coupling of the results to obtain the model for the entire system. This is particularly valuable in electronic thermal management systems (Incropera, 1999; Wei and Joshi, 2004).



Notes: (a) Bulk temperature distribution for different wall materials; (b) maximum temperature as a function of the imposed pressure difference for different wall materials; (c) comparison between numerical results and experimental data for the system shown in Figure 1(b)

Figure 5.
Conjugate transport
in microchannels

3.4 Reduced complexity or order in components

In many cases, the large difference in length or time scales between different components can be treated by simplifying the model for some of the components by reducing the order. Lumping in certain directions or over time is used to simplify the model for components where small length scales are of interest, while full-field models may be employed for other components (Joshi, 2012). If temperature variations are relatively small in certain regions, these could easily be lumped. An example that may be mentioned is that of a plastic insulated cable, where the metal core, whose scales are relatively small, may be taken as lumped while the temperature distribution in the plastic is calculated by solving the full-field equations. Such models are well known and have been used in the literature for different thermal systems, using length or time scales to decide the simplification to be employed (Jaluria, 2008).

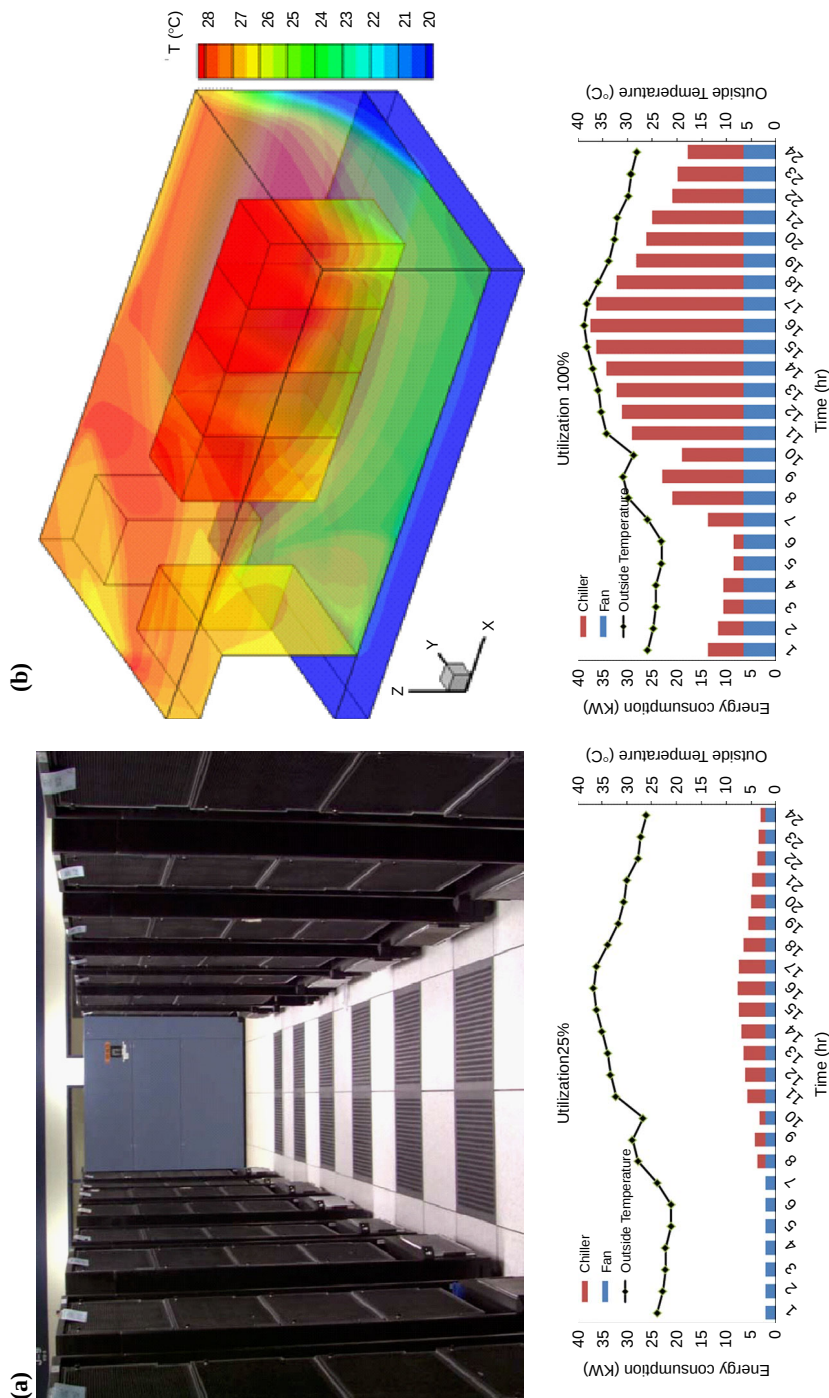
A particularly important and relevant example is that of data centers, which are used for data storage and retrieval by financial companies, internet servers, defence and security agencies, etc. The length scales go from submicron at the chip level to

several meters at the room or enclosure level, with servers at intermediate length scales. Field equations can be solved for the flow and heat transfer in the room and also in the racks. But this cannot be easily extended to the device level without incurring prohibitive time and cost. Some of the preceding approaches discussed for multiscale modeling may be employed to simulate the entire data center. However, the use of reduced order modeling for components at smaller scales is particularly useful in such cases. The reduced order may be obtained by lumping over certain dimensions in steady state or over certain time periods in transient behavior. The devices then become heat sources and the racks may be modeled as porous media with localized or uniformly distributed sources. Several such racks can then be considered and the convective flow in the room modeled, with different inflow and outflow configurations and conditions, in order to minimize the energy needed for thermal management (Patankar, 2010; Joshi and Kumar, 2012).

Figure 6(a) shows a typical data center and Figure 6(b) the calculated thermal field with a relatively small number of racks in the room, using a model based on the preceding approach. It is quite easy to vary the positioning of the racks, as well as of the inflow/outflow ports. The use of chillers to reduce the inflow temperature to levels below the ambient can be included. Then, the energy consumption to achieve desired temperature levels in the electronic systems can be determined for a variety of locations, ambient conditions, load on the data center and so on. Figure 6(c) and (d) show the energy consumption for two different loads at a data center located in Princeton, NJ, USA, considering the chiller and the fan, separately. It is possible to use such simulations to optimize the use of data centers. For instance, we can distribute the load among various data centers on the basis of the ambient conditions to minimize the energy consumption (Le *et al.*, 2011). A full-field model for the entire system is much too costly and may also yield details that are not needed for the desired optimization. Then, reduced order models can be used advantageously to treat this multiscale problem. Similar considerations apply for a wide range of thermal systems, such as those related to energy and transportation.

4. Multiple scales within the flow

In a wide range of thermal processes, different length or time scales arise within the same domain such as the flow in an enclosure or in a moving fluid. There are two main approaches to the numerical solution of such multiscale problems, which are usually more complicated than the problems with different length scales in different regions considered earlier. The first and the most commonly used approach is to solve the micro or nanoscale problem separately and feed the results as inputs to the macroscale modeling of the process. The smaller scale problem may often be treated experimentally to obtain, for instance, the relevant chemical kinetics. A wide range of experimental techniques are available for this purpose, such as the Differential Scanning Calorimeter (DSC) for studying chemical conversion of food materials or reactive polymers. Once the chemical kinetics has been determined as function of temperature, shear and concentration, one could incorporate the results in the numerical simulation of the flow and the heat and mass transfer in the overall system. Similarly, numerical methods such as molecular dynamics may be employed to study the transformations of interest and obtain the relevant material properties, conversion or transformation rates, and changes in material characteristics. Again, these results are then incorporated in the simulation of the system and the final results employed for prediction, design and optimization of the process. In the second approach, the simulation at the smaller length scales is carried out



Notes: (a) A typical data center; (b) calculated thermal field in a room containing a simple data center; (c) and (d) energy consumption for the cooling of a data center in Princeton, NJ, USA, at 25 and 100 percent utilization of the center, respectively

Figure 6.
Thermal management
of data centers

concurrently, rather than separately, with the system simulation. Though more involved than the earlier approach, this allows greater flexibility and accuracy in the simulation. A few examples are given here using the former approach, first with modeling and then with experimental results on the smaller length scales.

Changes at the molecular level are considered in the generation of thermally induced E' defects in optical fiber drawing. The E' defect is a point defect, which is generated at high temperature during the drawing process. Its presence causes transmission loss and mechanical strength degradation in the fiber. The differential equation for the time dependence of the E' defect concentration was formulated on the basis of the thermodynamics of lattice vacancies in crystals. The E' defects are generated through the breaking of the $Si-O$ band, and, at the same time, a portion of the defects recombine to form $Si-O$ again. Depending on the cooling, or annealing process, the final concentration of defects can be varied. The net concentration of the E' defects is the difference between the generation and the recombination. The equation for E' defect concentration is given as (Hanafusa *et al.*, 1985):

$$v \frac{dn_d}{dz} = n_p(0)v \exp\left(-\frac{E_p}{KT}\right) - n_d v \left[\exp\left(-\frac{E_p}{KT}\right) + \exp\left(-\frac{E_d}{KT}\right) \right] \quad (7)$$

where, n_d and E_d represent the concentration and activation energy of the E' defect; while n_p and E_p represent those of the precursors, v is a frequency factor and K the Boltzmann constant. The initial values and constants are defined by Hanafusa *et al.* (1985). Figure 7(a) shows the neck-down region in a fiber drawing process, as the silica glass goes from a

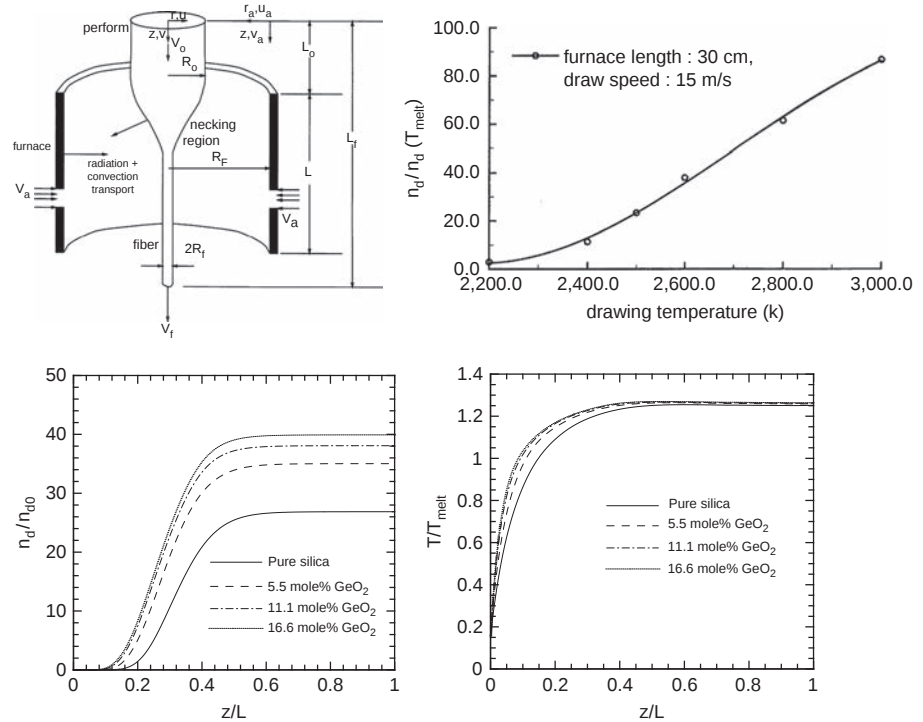


Figure 7.
(a) Neck-down region in optical fiber drawing;
(b) dependence of average concentration of E' defects on furnace wall temperature; (c) concentration of E' defects along the centerline for various GeO_2 concentrations in a doped fiber; (d) temperature distribution in a doped fiber

perform of diameter around 10 cm to a fiber of diameter of around 125 μm (Paek, 1999). The governing equations involve strong property changes and high-viscous dissipation Φ due to the large viscosity ν of glass. For an axisymmetric flow, the equations are given in terms of radial r and axial coordinate z as (Chen and Jaluria, 2009):

$$\frac{\partial v}{\partial z} + \frac{1}{r} \frac{\partial(ru)}{\partial r} = 0 \quad (8)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial r} + v \frac{\partial v}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r} \left[rv \left(\frac{\partial v}{\partial r} + \frac{\partial u}{\partial z} \right) \right] + 2 \frac{\partial}{\partial z} \left(v \frac{\partial v}{\partial z} \right) \quad (9)$$

$$\begin{aligned} \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial r} + v \frac{\partial u}{\partial z} &= -\frac{1}{\rho} \frac{\partial p}{\partial r} + \frac{2}{r} \frac{\partial}{\partial r} \left(rv \frac{\partial u}{\partial r} \right) + \frac{\partial}{\partial z} \left[v \left(\frac{\partial v}{\partial r} + \frac{\partial u}{\partial z} \right) \right] - \frac{2vu}{r^2} \\ \rho C_p \left(\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial r} + v \frac{\partial T}{\partial z} \right) &= \frac{1}{r} \frac{\partial}{\partial r} \left(rk \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) + \Phi + S_r \end{aligned} \quad (10)$$

The dependence of the average concentration of E' defects in the fiber on the drawing temperature is shown in Figure 7(b), which clearly indicates an increase with temperature as expected from the higher breakage of the Si-O bond. Similarly, dopants, such as rare-earth elements, are added to the preform to fine tune the transmission characteristics of the optical fiber. Using similar strategies for modeling, the drawing of doped fibers may be simulated (Chen and Jaluria, 2009). Figure 7(c) shows the defects in a doped fiber and Figure 7(d) shows the temperature distribution. Clearly, the effect can be controlled by doping and by varying the operating conditions, particularly the furnace temperature.

Similarly, in thermal processing of materials such as food and reactive polymers, the microscopic changes in the material are linked with the operating conditions that are imposed at the engineering scale on the system. The chemical conversion process is represented by the chemical kinetics, which is dependent on the temperature and the concentration (Wang *et al.*, 1989). These micro and nanoscale conversion mechanisms may be coupled with the flow and heat transfer in a die or a screw extruder to obtain the degree of conversion, pressure, bulk temperature and other important quantities. Figure 8(a) gives a sketch of some of the relevant conversion mechanisms for food. The dependence of the chemical kinetics on the temperature and the shear can then be determined experimentally and fed into the model of the system. Figure 8(b) shows the sketch of an extrusion die and the corresponding simulation and experimental results. The strong agreement between the two lends support to the experimentally determined chemical kinetics and the model.

Similarly, chemical kinetics plays a critical role in the deposition of material from the gas phase in chemical vapor deposition systems (Jensen *et al.*, 1991; Wu *et al.*, 2003; Wang *et al.*, 2006). The concentrations of the chemical species in the reactor affect the chemical kinetics, which in turn affect the film deposition. In many cases, the process is chemical kinetics limited, implying that the transport processes are quite vigorous and the deposition is restricted largely by the kinetics. The chemical kinetics for several materials is available in the literature and is often complicated by the large number of reactions and species involved. In addition, there are reactions at the surface as well as within the gas. Considering a fairly simple case, the chemical kinetics for the

deposition of Silicon from Silane (SiH_4) with Hydrogen as the carrier gas in a CVD reactor is given by the expression (Eversteyn *et al.*, 1970)

$$K = \frac{K_0 P_{\text{SiH}_4}}{1 + K_1 P_{\text{H}_2} + K_2 P_{\text{SiH}_4}} \tag{11}$$

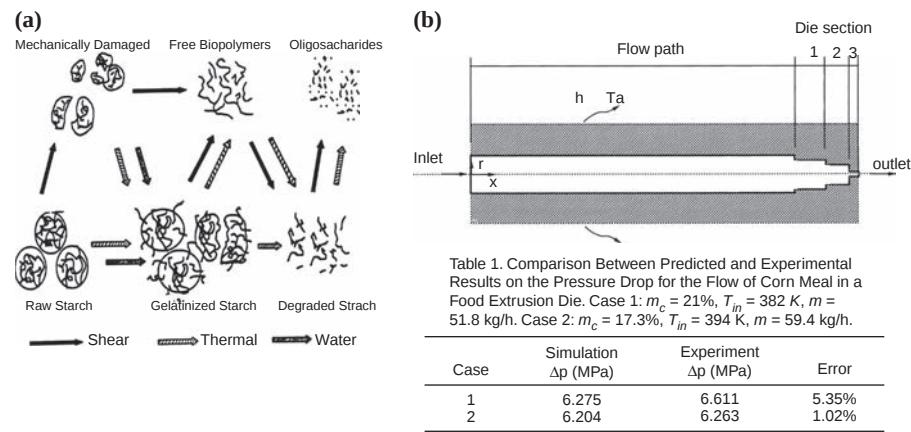
where the surface reaction rate K is in mole of $\text{Si}/\text{m}^2\text{s}$, $K_0 = A \exp(-E/RT)$, E being the activation energy, and A , K_1 and K_2 are constants which are obtained experimentally. The p 's are the partial pressures of the two species in the reactor.

Some typical results are shown in Figure 9 for an impingement type CVD reactor for Silicon. A major concern is the non-uniformity of the deposited film and efforts are made to achieve better uniformity by controlling the operating conditions like susceptor temperature and inflow velocity and concentration. Substantial work has been done in this area, considering the deposition of materials like TiN , SiC , GaN and GaAs for a wide variety of applications. This brief outline indicates the approach for modeling this multiscale problem, which involves microscale mechanisms at the surface and transport at engineering scales in the reactor.

5. Conclusions

This paper considers the numerical simulation of multiscale problems in the area of thermal science and engineering. Many basic and applied thermal processes and systems involve significantly different length and time scales over different components or regions. It is important to obtain accurate numerical models to predict the behavior and performance and to design and optimize the systems. Several different circumstances are considered here. The first and most common situation is when the different scales occur in different regions. In this case, the different regions are often characterized by different equations and the solution methodology may also be quite different. The results obtained in different regions are matched at the boundaries, or one region, particularly the one with much smaller scales, provides the boundary conditions for the larger scale domain. In many cases, reduced order models may be used for certain components to simplify the simulation. Large differences in time scales are handled in a fairly similar manner. Examples are taken from a range of practical systems to illustrate these approaches and to present characteristic results from simulation.

Figure 8.
(a) Basic chemical conversion processes in starch, driven by shear and temperature;
(b) sketch of an extrusion die and the comparison between the calculated and experimentally obtained pressure drop in the die. Here m_c is the moisture content and $\dot{m}$ the mass flow rate



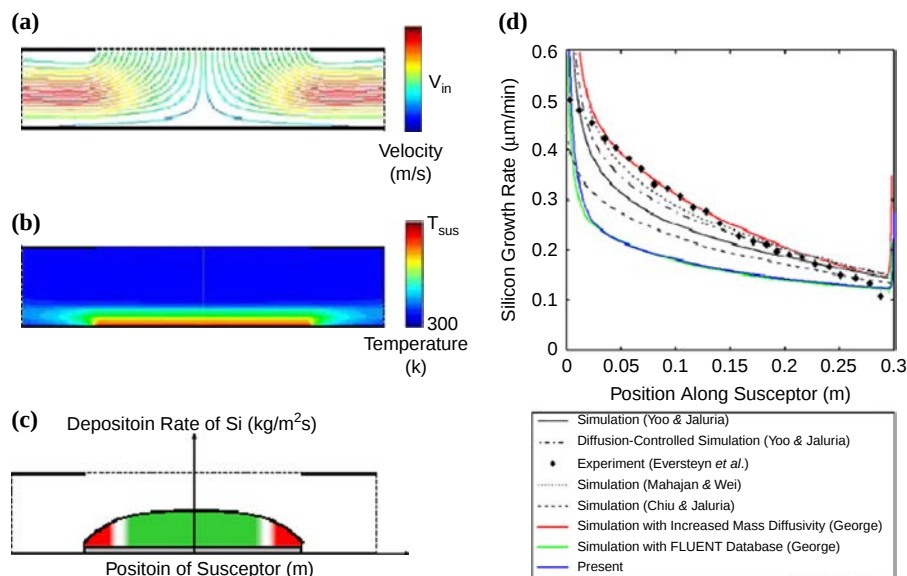


Figure 9.
(a) Calculated streamlines
in an impingement CVD
reactor for Silicon;
(b) isotherms in the
reactor; (c) typical thin
film deposited, showing
the non-uniformity;
(d) comparison between
numerical and
experimental results
on Si deposition

The second multiscale circumstance of interest is the one in which multiple scales arise in the same domain. This is the situation, for instance, in combustion, materials processing and chemical energy storage. Taking examples from materials processing, the basic approach of solving the micro or nanoscale problem separately by analysis or experimentation and then feeding the results as inputs to the numerical model of the system is discussed in detail. Considering generation of defects in optical fiber drawing, thin film fabrication in chemical vapor deposition and chemical conversion in the extrusion of reactive polymers, the use of both numerical modeling and experimentation to provide the inputs is presented. Typical results from the simulation of the overall system are presented and discussed.

Multiscale problems are quite common in thermal processes and systems. It is important to link the simulation at different scales to obtain results that can form the basis for system control and optimization to obtain high-quality products and high productivity. Some of the basic considerations in this important area are outlined in this paper and appropriate strategies for accurate and efficient numerical simulation are discussed.

References

- Abib, A. and Jaluria, Y. (1995), "Turbulent penetrative and recirculating flow in a compartment fire", *ASME J. Heat Transfer*, Vol. 117 No. 13, pp. 927-935.
- Chen, C. and Jaluria, Y. (2009), "Effects of doping on the optical fiber drawing process", *Int. J. Heat Mass Transfer*, Vol. 52 No. 21, pp. 4812-4822.
- Eversteyn, F.C., Severin, P.J.W., Brekel, C.H.J. and Peek, H.L. (1970), "A stagnant layer model for the epitaxial growth of silicon from silane in a horizontal reactor", *J. Electrochem. Soc.*, Vol. 117 No. 7, pp. 925-931.
- Gebhart, B., Hilder, D.S. and Kelleher, M. (1984), "The diffusion of turbulent jets", *Advances in Heat Transfer*, Vol. 16, pp. 1-57.
- Hanafusa, H., Hibino, Y. and Yamamoto, F. (1985), "Formation mechanism of drawing-induced E' centers in silica optical fibers", *J. Appl. Phys.*, Vol. 58 No. 3, pp. 1356-1361.

- He, Y.L. and Tao, W.Q. (2012), "Multiscale simulations of heat transfer and fluid flow problems", *ASME J. Heat Transfer*, Vol. 134 No. 3, pp. 031018-1-031018-13.
- Incropera, F.P. (1999), *Liquid Cooling of Electronic Devices by Single-Phase Convection*, John Wiley & Sons, New York, NY.
- Jaluria, Y. (2003), "Thermal processing of materials: from basic research to engineering", *ASME J. Heat Transfer*, Vol. 125 No. 6, pp. 957-979.
- Jaluria, Y. (2008), *Design and Optimization of Thermal Systems*, 2nd ed., CRC Press (Taylor & Francis), Boca Raton, FL.
- Jaluria, Y. (2009), "Microscale transport phenomena in materials processing", *ASME J. Heat Transfer*, Vol. 131 No. 3, pp. 033111-1-033111-17.
- Jaluria, Y. and Cooper, L.Y. (1989), "Negatively buoyant wall flows generated in enclosure fires", *Prog. Energy Combust. Sci.*, Vol. 15 No. 2, pp. 159-182.
- Jaluria, Y. and Torrance, K.E. (2003), *Computational Heat Transfer*, 2nd ed., Taylor and Francis, New York, NY.
- Jensen, K.F., Einset, E.O. and Fotiadis, D.I. (1991), "Flow phenomena in chemical vapor deposition of thin films", *Ann. Rev. Fluid Mechanics*, Vol. 23, pp. 197-232.
- Joshi, Y. (2012), "Reduced order thermal models of multiscale microsystems", *ASME J. Heat Transfer*, Vol. 134 No. 3, pp. 031008-1-031008-11.
- Joshi, Y. and Kumar, P. (Eds), (2012), *Energy Efficient Thermal Management of Data Centers*, Springer, New York, NY.
- Le, K., Zhang, J., Meng, J., Bianchini, R., Jaluria, Y. and Nguyen, T.D. (2011), "Reducing electricity cost through virtual machine placement in high performance computing clouds", *SC 11 Int. Conf. High Perf. Comput., Networking, Storage & Anal.*, Seattle, WA, November.
- Mahajan, R.L. (1996), "Transport phenomena in chemical vapor-deposition systems", *Advances in Heat Transfer*, Vol. 28, pp. 339-425.
- Minkowycz, W.J. and Sparrow, E.M. (Eds), (1997), *Advances in Numerical Heat Transfer*, Vol. 1, Taylor & Francis, Philadelphia, PA.
- Minkowycz, W.J., Sparrow, E.M. and Murthy, J. (Eds), (2006), *Handbook of Numerical Heat Transfer*, Wiley, New York, NY.
- Paek, U.C. (1999), "Free drawing and polymer coating of silica glass optical fibers", *ASME J. Heat Transfer*, Vol. 121 No. 4, pp. 774-788.
- Patankar, S.V. (2010), "Airflow and cooling in a data center", *ASME J. Heat Transfer*, Vol. 132 No. 7, pp. 073001-1-073001-17.
- Sun, Z. and Jaluria, Y. (2011), "Conjugate thermal transport in gas flow in long rectangular microchannel", *ASME J. Elect. Pkg.*, Vol. 133 No. 2, pp. 021008-1-021008-11.
- Wang, S.S., Chiang, C.C., Yeh, A.I., Zhao, B. and Kim, I.H. (1989), "Kinetics of phase transition of waxy corn starch at extrusion temperatures and moisture contents", *J. Food Sci.*, Vol. 54 No. 5, pp. 1298-1301.
- Wang, R., Ma, R. and Zupan, M. (2006), "Modeling of chemical vapor deposition of large-area silicon carbide thin film", *Journal of Crystal Growth & Design*, Vol. 6 No. 11, pp. 2592-2597.
- Wei, J. and Joshi, Y. (2004), "Stacked microchannel heat sinks for liquid cooling of microelectronic components", *Journal of Electronic Packaging*, Vol. 126 No. 1, pp. 60-66.
- Wu, B., Ma, R. and Zhang, H. (2003), "Epitaxy growth kinetics of GaN films", *Journal of Crystal Growth*, Vol. 250 Nos 1-2, pp. 14-21.

Corresponding author

Professor Yogesh Jaluria can be contacted at: JALURIA@JOVE.RUTGERS.EDU