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CONTENTS

PLENARY LECTURES

KEYNOTE LECTURES

MINI-SYMPOSIA

PARALLEL SESSIONS

NUMERICAL METHODS

POWER PLANTS AND EQUIPMENT SIMULATION

PLENARY LECTURES

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CHALLENGES IN THE ACCURATE NUMERICAL SIMULATION OF PRACTICAL THERMAL PROCESSES AND SYSTEMS

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ABSTRACT

The numerical simulation of practical thermal processes is generally complicated because of multiple transport mechanisms and complex phenomena that commonly arise. In addition, the materials encountered are often not easily characterized and typically involve large property changes over the ranges of interest. The boundary conditions may not be properly defined and or may be unknown. The geometry and interactions between different components are also often quite complicated. However, it is important to obtain accurate and dependable numerical results from the simulation in order to study, design, and optimize most practical thermal processes of current and future interest. The models employed must be validated and the accuracy of the simulation results established if the simulation is to form the basis for improving existing systems and developing new ones in applications areas such as energy, manufacturing, environmental control, electronics cooling, and transportation. This paper focuses on the main challenges that are encountered in obtaining accurate numerical simulation results on practical thermal processes and systems. It considers a wide variety of systems, ranging from materials processing to energy and cooling. Of particular interest are concerns like verification and validation, imposition of appropriate boundary conditions, and modelling 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 modelling 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. The methods that may be used to meet these challenges are discussed, along with typical results for a range of important processes. Future needs in this interesting and challenging area are also outlined.

Key Words: *Thermal processes, thermal systems, numerical simulation, accuracy, challenges*

1. INTRODUCTION

Numerical modelling of thermal processes that are of interest in important applications such as those related to energy, manufacturing, transportation, aerospace, heating, cooling, and to the environment is critical to a detailed study of the resulting phenomena and to the design and optimization of the relevant systems. Most of these practical circumstances are much too complicated to be investigated by analytical methods. Also, relatively limited data are usually available from existing processes and from appropriate experimental studies, which are often expensive and time consuming. In most cases, mathematical models of the processes and systems are developed, followed by numerical modelling and simulation. The models are validated by means of available analytical and experimental results and the numerical simulation is then used to provide the extensive numerical data needed for characterizing the processes and for design, control and optimization [1-3].

Most practical thermal processes and systems involve complex, coupled, transport mechanisms and interacting subsystems that constitute the overall system. As a consequence, several challenges are commonly encountered in obtaining accurate results from the numerical simulation of these systems. Some of the most important challenges are material properties, accurate imposition of boundary

conditions, validation, combined mechanisms, complex phenomena, multiple scales, multi-objective optimization, uncertainties and other additional effects and complexities. This paper considers some of these aspects, presents examples where these considerations are of particular importance and discusses possible approaches to meet these challenges.

As examples of typical practical thermal systems, consider the systems shown in Fig. 1. This figure shows sketches of the fabrication process for a hollow optical fiber, an electronic system cooled by microchannel flow and two configurations of chemical vapour deposition (CVD) reactors for thin film fabrication. These systems involve many of the complexities mentioned above. For instance, material properties of glass in optical fiber drawing are strong functions of temperature, combined modes of radiation, conduction and convection operate at various stages in the process, non-

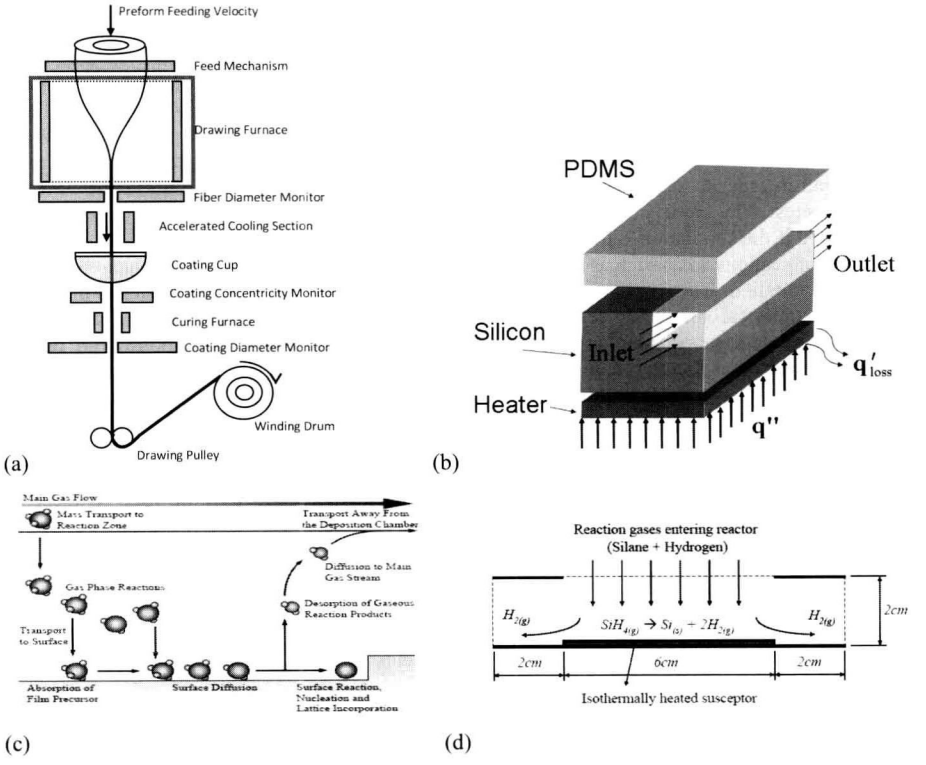

FIGURE 1. Common thermal processes and systems: (a) Hollow fiber drawing; (b) Microchannel flow for electronic cooling and (c) and (d) Chemical vapor deposition (CVD) systems for thin film fabrication.

Newtonian fluids are generally used for the fiber coating process and large changes in glass diameter occur in the draw furnace [4]. Similarly, the microchannel flow in electronic cooling is coupled with the system simulation at a much larger length scale. CVD involves chemical kinetics, which vary strongly with temperature and concentration [5]. The boundary conditions are fairly complicated in all cases and combined transport mechanisms are of interest. Similar considerations arise in other practical processes, as outlined later in this extended abstract and in the presentation.

A brief discussion of the challenges posed by the complexities in practical systems is given in this paper, considering a few selected examples such as the ones shown in Fig. 1.

2. NUMERICAL MODELING OF PRACTICAL PROCESSES

Let us consider the basic characteristics of mathematical and numerical modelling of typical thermal processes and systems. Considering the optical fiber drawing process, the flow of the glass and of the aiding purge gas in a cylindrical furnace is assumed to be axisymmentric. The governing equations for the glass and the gas are then given as,

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

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

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial r}+v\frac{\partial u}{\partial z}=-\frac{1}{\rho}\frac{\partial p}{\partial r}+\frac{2}{r}\frac{\partial}{\partial r}\left(r\upsilon\frac{\partial u}{\partial r}\right)+\frac{\partial}{\partial z}\left[\upsilon\left(\frac{\partial v}{\partial r}+\frac{\partial u}{\partial z}\right)\right]-\frac{2\upsilon u}{r^2} \tag{3}$$

$$\rho C_p\left(\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial r}+v\frac{\partial T}{\partial z}\right)=\frac{1}{r}\frac{\partial}{\partial r}\left(rK\frac{\partial T}{\partial r}\right)+\frac{\partial}{\partial z}\left(K\frac{\partial T}{\partial z}\right)+\Phi+S_r \tag{4}$$

Where u, v are the velocity components in the axial and radial directions, z and, r, respectively, p is the local pressure, T the temperature, t the time, υ the kinematic viscosity, ρ the density, K the thermal conductivity, C_p the specific heat at constant pressure, Φ is the viscous dissipation term and S_r is the radiation source term. For glass, the material properties are strong functions of the temperature T. They also vary with composition and changes in the microstructure, the main effect being on the radiation properties. The variation in the viscosity is the most critical one for the flow, since it varies quite dramatically with temperature. An equation based on the curve fit of available data for kinematic viscosity υ is written for silica, in S.I. units, as

$$\upsilon = 4545.45 \exp\left[32\left(\frac{T_{melt}}{T}-1\right)\right] \tag{5}$$

indicating the strong, exponential, variation of υ with temperature. Here, T_{melt} is the glass softening temperature, being around 1900 K for silica glass. The radiative source term S_r in Eq. (4) is non-zero for the glass preform/fiber because glass emits and absorbs energy. The variation of the absorption coefficient with wavelength λ can often be approximated in terms of bands with constant absorption over each band. Because of the small fiber diameter, being around 125 μm, there is a temptation to assume uniform temperature across the fiber. However, because of the high temperature dependence of the viscosity, this assumption does not yield accurate results and a large number of grid points, typically around 50, are needed across the fiber radius of around 62.5 μm to capture changes in temperature and the consequent effects on properties, viscous dissipation, thermally induced defects, and dopant movement.

Similarly, the fiber coating process may be modeled. Typical coating thicknesses are of the order of 40-50 μm and are applied to the uncoated fiber or as secondary coating to a coated fiber. The basic coating process involves drawing the fiber of diameter around 125 μm through a reservoir of coating fluid, with inlet and outlet dies. This is immediately followed by a curing process of the polymer coating material around the fiber. A balance between surface tension, viscous, gravitational, and pressure forces results in an upstream meniscus at the cup entrance, as well as a downstream meniscus at the die exit. At high speeds, the upper meniscus breaks down and air is entrained into the coating. The use of high draw

rates requires consideration of alternate pressurized applicator designs, where pressure induced motion of the coating material is used to reduce the shear at the fiber surface and helps in the establishment of a stable free surface flow. The control of the coating characteristics is of major concern in industry. These considerations have become particularly important as the coating speeds have been increased to values beyond 20 m/s to enhance productivity and as the interest in specialty fibers and fibers of different materials, including polymer fibers, has grown. The physical properties of the polymer coating materials, particularly the viscosity, and their dependence on temperature are of primary importance in the coating process. Surface tension has a significant effect on the flow near the free surface, which represents the interface between a liquid and a gas in many cases, and on the shape, stability and other characteristics of the interface.

Similarly, consider an electronic component cooled by the microchannel single-phase flow of a coolant, as shown in Fig. 1(b). Depending on the fluid, dimensions and operating conditions, the Knudsen number for the flow may be determined, leading to continuum flow, slip flow or molecular flow [6]. The overall system, on the other hand, is at engineering, or macro-scale, and can be modeled using the usual conservation equations. The typical equations are of the form:

Mass:

$$\nabla\cdot(\rho\tilde{V})=0 \tag{6}$$

Momentum:

$$\tilde{V}\cdot\nabla(\rho\tilde{V})=-\nabla p+\nabla\cdot(\mu\nabla\tilde{V}) \tag{7}$$

Energy:

$$\tilde{V}\cdot\nabla(\rho C_p T)=\nabla\cdot(k\nabla T) \tag{8}$$

where μ is the dynamic viscosity, k is the fluid thermal conductivity and $\tilde{V}$ is the velocity vector. For the solid region, the conduction equation is used, with thermal conductivity of the solid k, as

$$\frac{\partial}{\partial x_i}(k\frac{\partial T}{\partial x_i})=0 \tag{9}$$

For conjugate problem, the heat conduction in the solid region and the flow in the fluid region are solved separately and then coupled at the solid–fluid interface.

The chemical kinetics plays a critical role in the deposition of material from the gas phase in chemical vapor deposition systems [5]. The concentrations of the chemical species in the reactor affect the chemical kinetics, which in turn affect the 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. For instance, 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 [7]

$$\hat{K}=\frac{K_o p_{SiH4}}{1+K_1 p_{H2}+K_2 p_{SiH4}} \tag{10}$$

where the surface reaction rate $\hat{K}$ is in mole of Si/m^2s, K_O = 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. However, the chemical processes are typically much more complicated, with several intermediate reactions in the gaseous phase and several at the surface. This is particularly true for the deposition of SiC and GaN.

3. RESULTS AND DISCUSSIONS

A few practical processes and systems have been mentioned in the preceding, along with some of the challenges faced in an accurate simulation. Several of these are considered in greater detail here, along with relevant examples. However, only a brief outline and a few selected examples are considered. Further details and examples will be given in the presentation.

3.1. Material properties, variations and characteristics

The accuracy of any numerical simulation is dependent on the material properties used. This is particularly critical in practical processes where the properties vary with the local conditions like temperature and pressure and where changes in the material during the process can affect the properties. However, property data are often not available to the needed accuracy and often at conditions that are different from those of the process. This is particularly problematic for the manufacture of optical fibers which strongly depends on the physical properties of silica glass and their variation with the temperature T. The exponential dependence of viscosity on temperature was given earlier. The radiation properties, such as the variation of the absorption coefficient with wavelength λ have been measured for certain compositions and glasses. But these data are often available only at room temperature, whereas the process is at much higher temperatures. Also, data may not be available for the particular glass or composition that is being simulated.

Dopants such as rare earth materials are often used to modify the transmission characteristics of optical fibers and for specialized applications. Even though accurate models may be developed for the process [8], the data on the effect of the dopants on radiation properties and on viscosity are very limited [9], as shown here.

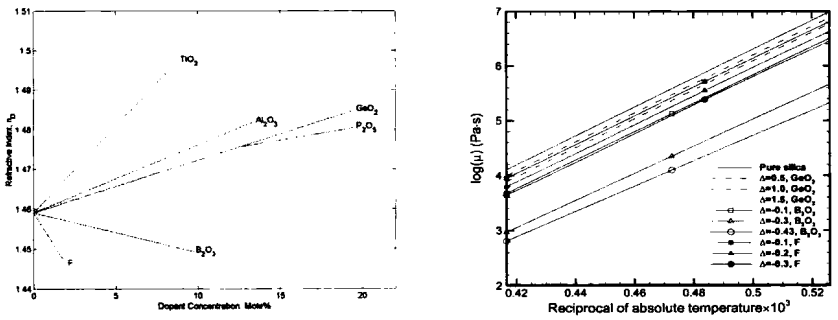

FIGURE 2. Effect of various dopants on the refractive index and viscosity of silica glass in the optical fiber drawing process.

Similarly, the coating process involves non-Newtonian materials and large material property changes. The fluid viscosity is often taken as

$$\mu = \mu_0 (\dot{\gamma} / \dot{\gamma}_0)^{n-1} \exp (b/T) \tag{11}$$

where $\dot{\gamma}$ is the total strain rate, b the temperature coefficient of viscosity, subscript o indicates reference conditions and n is the power-law index of the fluid. The jacketing material is thus treated as a Generalized Newtonian fluid [10]. Other rheological models may also be used, depending on the fluid. Similarly, chemical kinetics play a critical role in chemical vapor deposition. Simple equations like the given earlier for Silicon are generally not available or applicable for the wide

variety of materials of practical interest. A large number of chemical reactions have to be solved in most cases and, again, the results are strongly affected by the material property and chemical kinetics employed. Lack of accurate property data is clearly a major hurdle in obtaining accurate simulation results in this case.

Besides temperature and concentration, the material properties are also often sensitive to the conditions under which the material is stored as well as the fabrication process, age and raw materials used. The properties may also change with time, resulting in different values for experiments done at different times. This is particularly of concern with biological materials, polymers and chemicals. It is therefore important to know what material and under what conditions it is being employed so that the appropriate properties can be used in simulation. Also, in some cases, properties may be measured for more accurate inputs. Interpolation may be used with available data to obtain the best estimate of the properties under the operating conditions.

3.2. Verification and validation of the mathematical and numerical models

Generally, simplifications and idealizations are employed in the modeling of practical thermal processes and systems because of the complexities that arise. Therefore, it is critical to verify and validate the mathematical and numerical models to ensure that the results obtained are applicable, realistic and accurate [11]. Unless the models are satisfactorily validated, the simulation results cannot be used as the basis for design and optimization. Among the approaches used are a consideration of the physical behavior of the results obtained, comparisons with available analytical and numerical results, particularly benchmark solutions, and comparisons with available experimental data. It is also important to ensure that the results are essentially independent of the grid and other arbitrarily chosen numerical parameters.

Because of the critical importance of validation, extensive efforts have to be made to obtain experimental data, whenever possible, for comparison with numerical predictions. In several cases, a separate, well-designed, experimental set-up may need to be fabricated to achieve this. In the modeling and simulation of single and twin-screw polymer extruders, a specially designed cam-driven thermocouple system was employed to obtain the temperature profile in the rotating screw and two rotating cylinders were used to study the mixing phenomena and thus validate the model for twin-screw extrusion [12].

In the manufacture of optical fibers, a polymer coating is applied, as shown in Fig. 1(a), for protection against abrasion and to increase strength. Typical coating thicknesses are of the order of 40-50 μm and are applied to the uncoated fiber or as secondary coating to a coated fiber. The basic coating process involves drawing the fiber of diameter around 125 μm through a reservoir of coating fluid, with inlet and outlet dies. This is immediately followed by a curing process of the polymer coating material around the fiber. At the die exit, the coating material is drawn out with the fiber, forming a downstream meniscus, which influences the coating characteristics.

Thus, an important consideration in the coating process is the exit meniscus, which represents the profile of the free surface as the fluid exits from the die due to the viscous drag from the moving wire or fiber. The governing equations are solved to obtain the temperature and flow distributions, from which the shear at the free surface is determined. The additional forces due to gravity, surface tension and external shear due to air are included to determine the overall force balance. The force imbalance is used to generate an iteration scheme, starting with a guessed profile, till the force balance is satisfied and a converged meniscus is obtained [13]. Figure 3 shows the numerical results and compares these with experimental data on the exit meniscus profile. A good agreement is observed, indicating the validity and accuracy of this approach. Overall, it is necessary to make all possible efforts to validate the mathematical/numerical models, even if it means spending considerable time and effort in developing an experimental arrangement to obtain the data needed for comparisons.