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Thermal Processing of Materials: From Basic Research to Engineering

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This paper reviews the active and growing field of thermal processing of materials, with a particular emphasis on the linking of basic research with engineering aspects. In order to meet the challenges posed by new applications arising in electronics, telecommunications, aerospace, transportation, and other areas, extensive work has been done on the development of new materials and processing techniques in recent years. Among the materials that have seen intense interest and research activity over the last two decades are semiconductor and optical materials, composites, ceramics, biomaterials, advanced polymers, and specialized alloys. New processing techniques have been developed to improve product quality, reduce cost, and control material properties. However, it is necessary to couple research efforts directed at the fundamental mechanisms that govern materials processing with engineering issues that arise in the process, such as system design and optimization, process feasibility, and selection of operating conditions to achieve desired product characteristics. Many traditional and emerging materials processing applications involve thermal transport, which plays a critical role in the determination of the quality and characteristics of the final product and in the operation, control, and design of the system. This review is directed at the heat and mass transfer phenomena underlying a wide variety of materials processing operations, such as optical fiber manufacture, casting, thin film manufacture, and polymer processing, and at the engineering aspects that arise in actual practical systems. The review outlines the basic and applied considerations in thermal materials processing, available solution techniques, and the effect of the transport on the process, the product and the system. The complexities that are inherent in materials processing, such as large material property changes, complicated and multiple regions, combined heat and mass transfer mechanisms, and complex boundary conditions, are discussed. The governing equations for typical processes, along with important parameters, common simplifications and specialized methods employed to study these processes are outlined. The field of thermal materials processing is quite extensive and only a few important techniques employed for materials processing are considered in detail. The effect of heat and mass transfer on the final product, the nature of the basic problems involved, solution strategies, and engineering issues involved in the area are brought out. The current status and future trends are discussed, along with critical research needs in the area. The coupling between the research on the basic aspects of materials processing and the engineering concerns in practical processes and systems is discussed in detail. [DOI: 10.1115/1.1621889]

Introduction

Materials processing is one of the most important and active areas of research in heat transfer today. With growing international competition, it is has become crucial to improve the present processing techniques and the quality of the final product. New materials and processing methods are needed to meet the growing demand for special material properties in new and emerging applications related to diverse fields such as environment, energy, bioengineering, transportation, communications, and computers. It is also critical to use the fundamental understanding of materials processing in the design and optimization of the relevant systems.

Heat transfer is extremely important in a wide range of materials processing techniques such as crystal growing, casting, glass fiber drawing, chemical vapor deposition, spray coating, soldering, welding, polymer extrusion, injection molding, and composite materials fabrication. The flows that arise in the molten material in crystal growing due to temperature and concentration differences, for instance, can affect the quality of the crystal and, thus, of the semiconductors fabricated from the crystal. Therefore, it is important to understand these flows and develop methods to minimize or control their effects. Similarly, the profile of the neck-down region in an optical fiber drawing process is largely governed by the viscous flow of molten glass, which is in turn determined by the thermal field in the glass. The buoyancy-driven flows generated in the liquid melt in casting processes strongly influence the microstructure of the casting and the shape, movement and other characteristics of the solid-liquid interface. In chemical vapor deposition, the heat and mass transfer processes determine the deposition rate and uniformity, and thus the quality of the thin film produced. The transport in furnaces and ovens used for heat treatment strongly influence the quality of the product.

As a consequence of the importance of heat and mass transfer in materials processing, extensive work is presently being directed at this area. But what is often lacking is the link between the basic mechanisms that govern diverse processing techniques and the thermal systems needed to achieve the given process. On the one

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Table 1 Different types of thermal materials processing operations, along with examples of common techniques

1.	PROCESSES WITH PHASE CHANGE	casting, continuous casting, crystal growing, drying
2.	HEAT TREATMENT	annealing, hardening, tempering, surface treatment, curing, baking
3.	FORMING OPERATIONS	hot rolling, wire drawing, metal forming, extrusion, forging
4.	CUTTING	laser and gas cutting, fluid jet cutting, grinding, machining
5.	BONDING PROCESSES	soldering, welding, explosive bonding, chemical bonding
6.	POLYMER PROCESSING	extrusion, injection molding, thermoforming
7.	REACTIVE PROCESSING	chemical vapor deposition, food processing
8.	POWDER PROCESSING	powder metallurgy, sintering, sputtering, processing of nano-powders and ceramics
9.	GLASS PROCESSING	optical fiber drawing, glass blowing, annealing
10.	COATING	thermal spray coating, polymer coating
11.	OTHER PROCESSES	composite materials processing, microgravity materials processing, rapid prototyping

hand, considerable effort has been directed at specific manufacturing systems, problems and circumstances in order to develop new products, reduce costs and optimize the process. Much of this effort has been based on expensive and time-consuming experimentation on practical systems. On the other hand, detailed research has been carried out to extract the main underlying features of the processes, develop new solution methods to simulate complex transport circumstances that arise, and to obtain a much better understanding of the governing mechanisms. However, quantitative information on the dependence of product quality, process control and optimization on the thermal transport is often unavailable The coupling between practical engineering systems and the basic transport mechanisms is a very important aspect that should be considered, so that the current and future research on thermal materials processing has a strong impact on the design, control and optimization of the relevant thermal systems. For instance, an understanding of the microscale mechanisms that determine material characteristics is important, but these must be linked with the boundary conditions that are usually imposed at the macroscale level in the system.

This review paper is directed at these important issues, focusing on the heat and mass transfer involved with materials processing and linking these with the characteristics of the product and with the system. However, it must be noted that the concerns, questions and considerations presented in this paper are not unique to the field of materials processing. Other traditional and emerging areas like those concerned with safety, cooling of electronic systems, automobile and aircraft systems, space, and energy also involve research on the basic transport processes and these need to be linked with engineering issues.

Thermal Processing of Materials

Thermal processing of materials refers to manufacturing and material fabrication techniques that are strongly dependent on the thermal transport mechanisms. With the substantial growth in new and advanced materials like composites, ceramics, different types of polymers and glass, coatings, specialized alloys and semiconductor materials, thermal processing has become particularly important since the properties and characteristics of the product, as well as the operation of the system, are largely determined by heat transfer mechanisms. A few important materials processing techniques in which heat transfer plays a very important role are listed in Table 1.

This list contains both traditional processes and new or emerging methods. In the former category, we can include welding, metal forming, polymer extrusion, casting, heat treatment and drying. Similarly, in the latter category, we can include crystal growing, chemical vapor deposition and other thin film manufacturing techniques, thermal sprays, fabrication of composite materials, processing of nano-powders to fabricate system components, optical fiber drawing and coating, microgravity materials processing, laser machining and reactive extrusion. The choice of an appropriate material for a given application is an important consideration in the design and optimization of processes and systems [1].

A few thermal materials processing systems are also sketched in Fig. 1. These include the optical glass fiber drawing process in which a specially fabricated glass preform is heated and drawn into a fiber, thin film fabrication by chemical vapor deposition (CVD), Czochralski crystal growing in which molten material such as silicon is allowed to solidify across an interface as a seed crystal is withdrawn, and screw extrusion in which materials such as plastics are melted and forced through a die to obtain specific dimensions and shape. In all these processes, the quality and characteristics of the final product and the rate of fabrication are strong functions of the underlying thermal transport processes. Many books and review articles have discussed important practical considerations and the fundamental transport mechanisms in the area of manufacturing and materials processing [2–8].

Basic Research Versus Engineering

Research in thermal materials processing is largely directed at the basic processes and underlying mechanisms, physical understanding, effects of different transport mechanisms and physical parameters, general behavior and characteristics, and the thermal process undergone by the material. It is usually a long-term effort, which leads to a better quantitative understanding of the process under consideration. However, it can also provide inputs, which can be used for design and development.

Engineering studies in materials processing, on the other hand, are concerned with the design of the process and the relevant thermal system, optimization, product development, system control, choice of operating conditions, improving product quality, reduction in costs, process feasibility, enhanced productivity, repeatability, and dependability.

Figure 2 shows a schematic of the different steps that are typically involved in the design and optimization of a system. The iterative process to obtain an acceptable design by varying the design variables is indicated by the feedback loop connecting simulation, design evaluation and acceptable design. There is a feedback between simulation and modeling as well, in order to improve the model representation of the physical system on the basis of observed behavior and characteristics of the system, as obtained from simulation. Optimization of the system is undertaken after acceptable designs have been obtained.

Some of the important considerations that arise when dealing with the thermal transport in the processing of materials are given in Table 2. All these considerations make the mathematical and numerical modeling of the process and the associated system for materials processing very involved and challenging. Special procedures and techniques are generally needed to satisfactorily simulate the relevant boundary conditions and material property variations. The results from the simulation provide inputs for the design and optimization of the relevant system, as well as for the choice of the appropriate operating conditions. Experimental techniques and results are also closely linked with the mathematical modeling in order to simplify the experiments and obtain useful results in terms of important dimensionless parameters.

It is necessary for heat transfer researchers to thoroughly understand the concerns, intricacies and basic considerations that

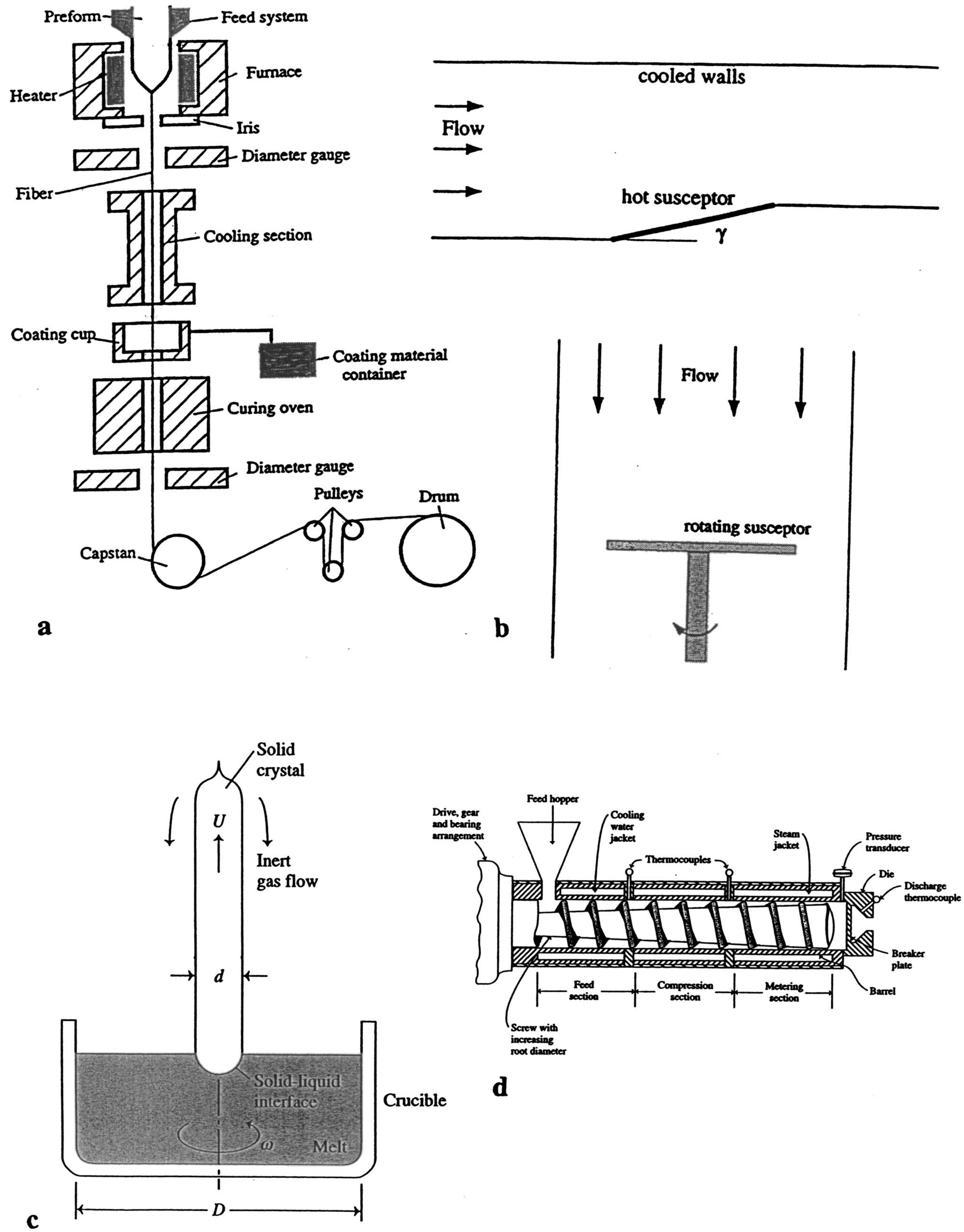

Fig. 1 Sketches of a few common manufacturing processes that involve thermal transport in the material being processed: (a) optical fiber drawing; (b) chemical vapor deposition; (c) Czochralski crystal growing; and (d) plastic screw extrusion.

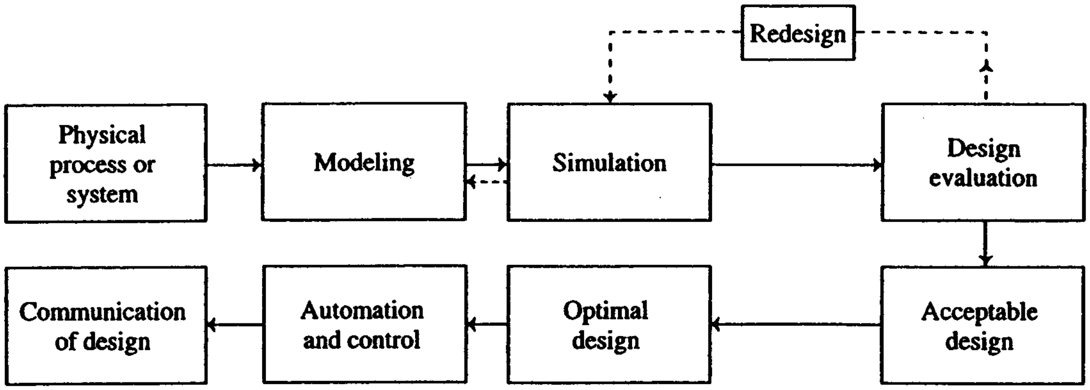

Fig. 2 Various steps involved in the design and optimization of a thermal system and in the implementation of the design

characterize materials processing in order to make a significant impact on the field and to play a leadership role. The dependence of the characteristics of the final product on the heat transfer must be properly understood and characterized so that analysis or experimentation can be used to design processes to achieve desired product characteristics and production rates.

Mathematical Modeling

Modeling is one of the most crucial elements in the design and optimization of thermal materials processing systems. Practical processes and systems are generally very complicated and must be simplified through idealizations and approximations to make the problem solvable. This process of simplifying a given problem so that it may be represented in terms of a system of equations, for analysis, or a physical arrangement, for experimentation, is termed modeling. Once a model is obtained, it is subjected to a variety of operating conditions and design variations. If the model is a good representation of the actual system under consideration, the outputs obtained from the model characterize the behavior of the given system. This information is used in the design process as well as in obtaining and comparing alternative designs by predicting the performance of each design, ultimately leading to an optimal design.

A mathematical model is one that represents the performance and behavior of a given system in terms of mathematical equations. These models are the most important ones in the design of thermal systems, since they provide considerable flexibility and versatility in obtaining quantitative results that are needed as inputs for design. Mathematical models form the basis for simulation, so that the behavior and characteristics of the system may be investigated without actually fabricating a prototype. In addition, the simplifications and approximations that lead to a mathematical model also indicate the dominant variables in a problem. This helps in developing efficient physical or experimental models. Numerical models are based on the mathematical model and allow one to obtain, using a computer, quantitative results on the system behavior for different operating conditions and design parameters.

Table 2 Important considerations in thermal materials processing

1.	COUPLING OF TRANSPORT WITH MATERIAL CHARACTERISTICS different materials, properties, behavior, material structure
2.	VARIABLE MATERIAL PROPERTIES strong variation with temperature, pressure and concentration
3.	COMPLEX GEOMETRIES complicated domains, multiple regions
4.	COMPLICATED BOUNDARY CONDITIONS conjugate conditions, combined modes
5.	INTERACTION BETWEEN DIFFERENT MECHANISMS surface tension, heat and mass transfer, chemical reactions, phase change
6.	MICRO-MACRO COUPLING micro-structure changes, mechanisms operating at different length and time scales
7.	COMPLEX FLOWS non-Newtonian flows, free surface flows, powder and particle transport
8.	INVERSE PROBLEMS non-unique multiple solutions, iterative solution
9.	DIFFERENT ENERGY SOURCES laser, chemical, electrical, gas, fluid jet, heat
10.	SYSTEM OPTIMIZATION AND CONTROL link between heat transfer and manufacturing system

Governing Equations

General Equations. The governing equations for convective heat transfer in materials processing are derived from the basic conservation principles for mass, momentum and energy. For a pure viscous fluid, these equations may be written as

$$\frac{D\rho}{Dt}+\rho\nabla\cdot\bar{V}=0 \tag{1}$$

$$\rho\frac{D\bar{V}}{Dt}=\bar{F}+\nabla\cdot\underline{\underline{\tau}} \tag{2}$$

$$\rho C_p\frac{DT}{Dt}=\nabla\cdot(k\nabla T)+\dot{Q}+\beta T\frac{Dp}{Dt}+\mu\Phi \tag{3}$$

Here, D/Dt is the substantial or particle derivative, given in terms of the local derivatives in the flow field by $D/Dt=\partial/\partial t+\bar{V}\cdot\nabla$. The other variables are defined in the Nomenclature.

For a solid, the energy equation is written as

$$\rho C_p\frac{DT}{Dt}=\frac{\partial T}{\partial t}+\bar{V}\cdot\nabla T=\nabla\cdot(k\nabla T)+\dot{Q} \tag{4}$$

where the specific heats at constant pressure and at constant volume are essentially the same for an incompressible fluid. If the solid is stationary, the convection term drops out and the particle derivative is replaced by the transient term $\partial/\partial t$, resulting in the conduction equation. In a deforming solid, as in wire drawing, extrusion or fiber drawing, the material is treated as a fluid, with an appropriate constitutive equation, and the additional terms due to pressure work and viscous heating are generally included. In the preceding equations, the material is taken as isotropic, with the properties, which are taken as variable, assumed to be the same in all directions. For certain materials, such as composites, the nonisotropic behavior must be taken into account.

The stress tensor in Eq. (2) can be written in terms of the velocity $\overline{V}$ if the material characteristics are known. For instance, if μ is taken as constant for a Newtonian fluid, the relationships between the shear stresses and the shear rates, given by Stokes, are employed to yield

$$\rho \frac{D\overline{V}}{Dt} = \overline{F} - \nabla p + \mu \nabla^2 \overline{V} + \frac{\mu}{3} \nabla(\nabla \cdot \overline{V}) \tag{5}$$

Here, the bulk viscosity $K = \lambda + (2/3)\mu$ is taken as zero. For an incompressible fluid, ρ is constant, which gives $\nabla \cdot \overline{V} = 0$ from Eq. (1). Then, the last term in Eq. (5) drops out.

Buoyancy Effects. The body force $\overline{F}$ is important in many manufacturing processes, such as crystal growing and casting where it gives rise to the thermal or solutal buoyancy term. The governing momentum equation is obtained from Eq. (5), when thermal buoyancy is included, as

$$\rho \frac{D\overline{V}}{Dt} = -\overline{e}g\rho\beta(T - T_a) - \nabla p_d + \mu \nabla^2 \overline{V} \tag{6}$$

where p_d is the dynamic pressure, obtained after subtracting out the hydrostatic pressure p_a. Therefore, p_d is the component due to fluid motion, as discussed by Jaluria [9] and Gebhart et al. [10]. Boussinesq approximations, that neglect the effect of the density variation in the continuity equation and assume a linear variation of density with temperature, are employed here. However, in many practical cases, these approximations can not be used. The governing equations are coupled because of the buoyancy term in Eq. (6) and must be solved simultaneously [11].

Viscous Dissipation. The viscous dissipation term $\mu\Phi$ in Eq. (3) represents the irreversible part of the energy transfer due to the shear stress. Therefore, viscous dissipation gives rise to a thermal source in the flow and is always positive. For a Cartesian coordinate system, Φ is given by the expression

$$\Phi = 2\left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial z}\right)^2\right] + \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z}\right)^2 + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)^2 - \frac{2}{3}(\nabla \cdot \overline{V})^2 \tag{7}$$

Similarly, expressions for other coordinate systems may be obtained. This term becomes important for very viscous fluids, such as glass, plastics and food, and at high speeds.

Processes With Phase Change. Many material processing techniques, such as crystal growing, casting, and welding, involve a phase change. Two main approaches have been used for the numerical simulation of these problems. The first one treats the two phases as separate, with their own properties and characteristics. The interface between the two phases must be determined so that conservation principles may be applied there [7,12]. This becomes fairly involved since the interface location and shape must be determined for each time step or iteration.

In the second approach, the conservation of energy is considered in terms of the enthalpy H, yielding the governing energy equation as

$$\rho \frac{DH}{Dt} = \rho \frac{\partial H}{\partial t} + \rho \overline{V} \cdot \nabla H = \nabla \cdot (k \nabla T) \tag{8}$$

where each of the phase enthalpies H_i is defined as

$$H_i = \int_0^T C_i dT + H_i^o \tag{9}$$

C_i being the corresponding specific heat and H_i^0 the enthalpy at $0K$. Then, the solid and liquid enthalpies are given by, respectively,

$$H_s = C_s T \quad H_l = C_l T + [(C_s - C_l)T_m + L_h] \tag{10}$$

where L_h is the latent heat of fusion, and T_m the melting point. The continuum enthalpy and thermal conductivity are given, respectively, as

$$H = H_s + f_l(H_l - H_s) \quad k = k_s + f_l(k_l - k_s) \tag{11}$$

where f_l is the liquid mass fraction, obtained from equilibrium thermodynamic considerations. The dynamic viscosity μ is expressed as the harmonic mean of the phase viscosities, employing the limit $\mu_s \to \infty$, i.e., $\mu = \mu_l / f_l$. This model smears out the discrete phase transition in a pure material. But the numerical modeling is much simpler since the same equations are employed over the entire computational domain and there is no need to keep track of the interface between the two phases [13–15]. In addition, impure materials, mixtures and alloys can be treated very easily by this approach.

Chemically Reactive Flows. Combined thermal and mass transport mechanisms are important in many materials processing circumstances, such as chemical vapor deposition and processing of food, reactive polymers, and several other materials with multiple species. Chemical reactions occurring in chemically reactive materials substantially alter the structure and characteristics of the product [16,17].

A simple approach to model the chemical conversion process in reactive materials, such as food, is based on the governing equation for chemical conversion, given as [18]

$$\frac{d}{dt}[(1 - \tilde{X})] = -K(1 - \tilde{X})^m \tag{12}$$

where $\tilde{X}$ is the degree of conversion, defined as,

$$\tilde{X} = \frac{M_i - M_t}{M_i - M_f} \tag{13}$$

here M is the amount of unconverted material, with subscripts i, f, and t referring to the amounts at the initial condition, final condition and at time t. The order of the reaction is m and K is the reaction rate, these generally being determined experimentally. Similarly, chemical kinetics play a critical role in the deposition of material from the gas phase in chemical vapor deposition systems [19,20].

Idealizations and Simplifications

In order to develop an appropriate mathematical model for a given materials processing system, several idealizations and simplifications are made to make the problem amenable to an analytical or numerical solution. A general procedure, which includes considerations of transient versus steady-state transport, number of spatial dimensions needed, neglecting of relatively small effects, idealizations such as isothermal or uniform heat flux conditions, and characterization of material properties, may be adopted to obtain the usual simplifications in analysis [1].

Boundary Conditions. Many of the boundary and initial conditions used in materials processing are the usual no-slip conditions for velocity and the appropriate thermal or mass transfer conditions at the boundaries. Similarly, the normal gradients are taken as zero at an axis or plane of symmetry, temperature and heat flux continuity is maintained in going from one homogeneous region to another, and initial conditions are often taken as zero flow at the ambient temperature, representing the situation before the onset of the process. For periodic processes, the initial conditions are arbitrary.

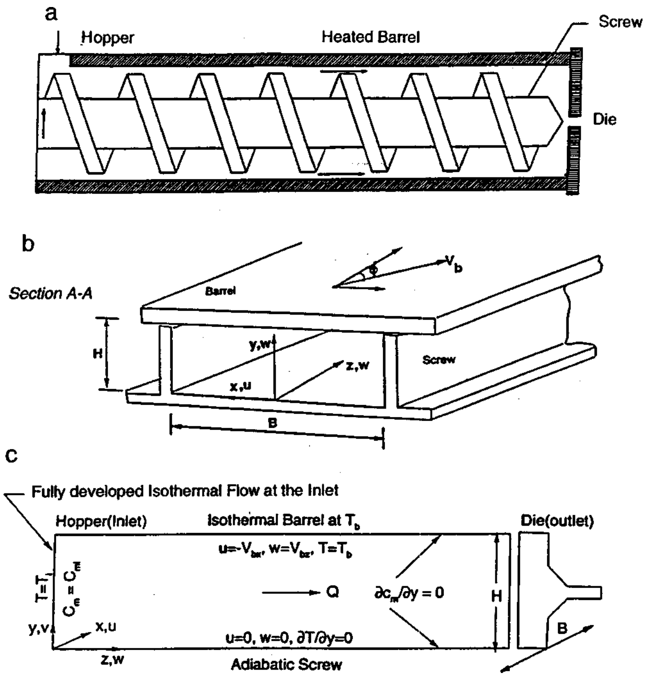

Fig. 3 Screw channel and simplified computational domain for a single-screw extruder

At a free surface, the shear stress is often specified as zero, yielding a Neumann condition of the form $\partial V/\partial n = 0$, if negligible shear is applied on the surface. In general, a balance of all the forces acting at the surface is used to obtain the interface. As considered in detail by Roy Choudhury et al. [21] and as presented later, the free surface may be determined numerically by iterating from an initial profile and using the imbalance of the forces for correcting the profile at intermediate steps, finally yielding a converged profile. In a stationary ambient medium, far from the solid boundaries, the velocity and temperature may be given as $\underline{V} \rightarrow 0$, $T \rightarrow T_a$ as $n \rightarrow \infty$. However, frequently the condition $\partial \underline{V}/\partial n \rightarrow 0$ is used, instead, in order to allow for entrainment into the flow. The use of this gradient, or Neumann, condition generally allows the use of a much smaller computational domain, than that needed for a given value, or Dirichlet condition, imposed on the velocity $\underline{V}$ [22].

If a change of phase occurs at the boundary, the energy absorbed or released due to the change of phase must be taken into account. Thus, the boundary conditions at the moving interface between the two phases must be given if a two-zone model is being used. This is not needed in the enthalpy model mentioned earlier. For one-dimensional solidification, this boundary condition is given by the equation

$$k_s \frac{\partial T_s}{\partial y} - k_l \frac{\partial T_l}{\partial y} = \rho L_h \frac{d\delta}{dt} \tag{14}$$

where $y = \delta$ is the location of the interface. This implies that the energy released due to solidification is conveyed by conduction in the two regions. Similarly, the boundary condition may be written for two or three-dimensional solidification [12]. For a stationary interface, as in crystal growing shown in Fig. 1(c) and for continuous casting, the appropriate boundary condition has been given by Siegel [23].

Other Simplifications. In the case of material flow in a moving cylindrical rod or a plate for extrusion or hot rolling, the temperature T is a function of time and location if a Lagrangian approach is used to follow a material element. However, by placing the coordinate system outside the moving material, a steady problem is obtained if the edge of the rod is far from the inlet and if the boundary conditions are steady. Transient problems arise for small lengths of the rod at short times following the onset of the process, and for boundary conditions varying with time [24]. Similarly, coordinate transformations are employed to convert transient problems to steady state ones in other circumstances.

In the case of a single-screw extruder, shown in Fig. 3, the coordinate system is generally fixed to the rotating screw and the channel straightened out mathematically, ignoring the effects of curvature. Then the complicated flow in the extruder is replaced by a simpler pressure and shear driven channel flow, with shear arising due to the barrel moving at the pitch angle over a stationary screw.

The basic nature of the underlying physical processes and the simplifications that may be obtained under various circumstances can be best understood in terms of dimensionless variables that arise when the governing equations and the boundary conditions are nondimensionalized. The commonly encountered governing dimensionless parameters are the Strouhal number Sr, the Reynolds number Re, the Grashof number Gr, the Prandtl number Pr and the Eckert number Ec. These are defined as

$$\mathrm{Sr} = \frac{L}{V_c t_c}, \quad \mathrm{Re} = \frac{V_c L}{\nu}, \quad \mathrm{Gr} = \frac{g\beta(T_s - T_a)L^3}{\nu^2}, \quad \mathrm{Pr} = \frac{\nu}{\alpha},$$

$$\mathrm{Ec} = \frac{V_c^2}{C_p(T_s - T_a)} \tag{15}$$

where V_c is a characteristic speed, L a characteristic dimension, and t_c a characteristic time. The dimensionless equations may be used to determine the various regimes over which certain simplifications can be made, such as creeping flow at small Re and boundary layer at large Re.

Material Considerations

Variable Properties. The properties of the material undergoing thermal processing are very important in the modeling of the process, in the interpretation of experimental results and in the determination of the characteristics of the final product. The ranges of pressure, concentration and temperature are usually large enough to make it necessary to consider material property variations. Usually, the dependence of the properties on temperature T is the most important effect. This leads to nonlinearity in the governing equations and couples the flow with the energy transport. Thus the solution of the equations and the interpretation of experimental results become more involved than for constant property circumstances. Average constant property values at different reference conditions are frequently employed to simplify the solution [25,26]. However, most manufacturing processes require the solution of the full variable-property problem for accurate predictions of the resulting transport.

The variation of dynamic viscosity μ requires special consideration for materials such as plastics, polymers, food materials, several oils and rubber, that are of interest in a variety of manufacturing processes. Most of these materials are non-Newtonian in behavior, implying that the shear stress is not proportional to the shear rate. Thus, the viscosity μ is a function of the shear rate and, therefore, of the velocity field. The viscosity is independent of the shear rate for Newtonian fluids like air and water, but increases or decreases with the shear rate for shear thickening or thinning fluids, respectively. These are viscoinelastic (purely viscous) fluids, which may be time-independent or time-dependent, the shear rate being a function of both the magnitude and the duration of shear in the latter case.

Various models are employed to represent the viscous or rheological behavior of fluids of practical interest. Frequently, the fluid is treated as a Generalized Newtonian Fluid (GNF) with the non-Newtonian viscosity function given in terms of the shear rate which is related to the second invariant of the rate of strain tensor.

For instance, time-independent viscoinelastic fluids without a yield stress are often represented by the power-law model, given by [27]

$$\tau_{yx}=K_c\left|\frac{du}{dy}\right|^{n-1}\frac{du}{dy} \tag{16}$$

where K_c is the consistency index, and n the power law fluid index. Note that $n=1$ represents a Newtonian fluid. For $n<1$, the behavior is pseudoplastic (shear thinning) and for $n>1$, it is dilatant (shear thickening). Then the viscosity variation may be written as [27]

$$\mu=\mu_o\left(\frac{\dot{\gamma}}{\dot{\gamma}_o}\right)^{n-1}e^{-b(T-To)} \tag{17}$$

where

$$\dot{\gamma}=\left[\left(\frac{\partial u}{\partial y}\right)^2+\left(\frac{\partial w}{\partial y}\right)^2\right]^{1/2}, \quad \text{with} \quad \tau_{yx}=\mu\frac{\partial u}{\partial y}, \quad \tau_{yz}=\mu\frac{\partial w}{\partial y} \tag{18}$$

for a two-dimensional flow, with u and w varying only with y. Similarly, expressions for other two- and three-dimensional flows may be written. Here $\dot{\gamma}$ is the shear strain rate, the subscript o denotes reference conditions and b is the temperature coefficient of viscosity. For food materials, the viscosity is also a strong function of the moisture concentration c_m. In addition, chemical changes, that typically occur at the microscale level in the material, affect the viscosity and other properties. Other models, besides the power-law model, are also employed to represent different materials [27–29].

Glass is another very important material. It is a supercooled liquid at room temperature. The viscosity varies almost exponentially with temperature. Even a change of a few degrees in temperature in the vicinity of the softening point, T_m, which is around 1600°C for fused silica, can cause substantial changes in viscosity and thus in the flow field and the transport [30]. An equation based on the curve fit of available data for kinematic viscosity ν is written for silica, in S.I. units, as

$$\nu=4545.45\exp\left[32\left(\frac{T_m}{T}-1\right)\right] \tag{19}$$

indicating the strong, exponential, variation of ν with temperature. The heat transfer is further complicated by the fact that glass is a participating medium for thermal radiation. The absorption coefficient is a strong function of the wavelength λ and the radiation is absorbed and emitted over the volume of the material. A two-band spectral absorption model has been used extensively for studying the thermal transport in the neck-down region of a furnace-drawn optical fiber [31,32].

There are several other important considerations related to material properties, such as constraints on the temperature level in the material, as well as on the spatial and temporal gradients, for instance in the manufacturing of plastic-insulated wires [33]. Similarly, constraints arise due to thermal stresses in the material and are particularly critical for brittle materials such as glass and ceramics.

Link Between Transport Processes and Material Characteristics. Numerical and experimental investigation can lead to the prediction of the thermal history of the material as it undergoes a given thermal process. Similarly, the pressure, stress, mass transfer, and chemical reactions can be determined. The next and particularly critical step is to determine the changes in the structure or composition of the material as it goes through the system. But this requires a detailed information on material behavior and how structural or chemical changes occur in the material as a consequence of the temperature, pressure and other conditions to which it is subjected.

Nano, Micro, and Macro-Scale Coupling. The characteristics and quality of the material being processed are generally determined by the transport processes occurring at the micro or nanometer scale in the material, for instance at the solid-liquid interface in casting, over molecules involved in a chemical reaction in chemical vapor deposition and reactive extrusion, or at sites where defects are formed in an optical fiber. However, engineering aspects are generally concerned with the macroscale, involving practical dimensions, typical physical geometries and appropriate boundaries. It is crucial to link the two approaches so that the appropriate boundary conditions for a desired micro or nanostructure can be imposed in a physically realistic system. A considerable interest exists today in this aspect of materials processing. For instance, interest lies in understanding microscopic phenomena associated with solidification and intense current research work has been directed at this problem. The solidification front can be divided into various morphological forms such as planar, cellular and dendritic. Various models have been proposed and studied [34].

Similarly, detailed experimental work on the chemical conversion of starches has been carried out [18]. The order of the reaction m in Eq. (12) has been shown to be zero for starches and the rate of the reaction K given as a combination of thermal (T) and shear (S) driven conversion as

$$K=K_T+K_S \tag{20}$$

where

$$K_T=K_{To}\exp(-E_T/RT) \quad K_S=K_{So}\exp(-E_S/\tau\eta) \tag{21}$$

Here, τ is the shear stress, and η is a constant, which is obtained experimentally for the material, along with other constants in the equation. A simple approximation may be applied to model the degree of conversion defined in Eq. (13), as given by [35]

$$w\frac{d\tilde{X}}{dz}=K \tag{22}$$

Here, w is the velocity in the down-channel direction z in an extruder. Thus, numerical results on conversion in the channel are obtained by integrating this equation.

Another area in which the changes at the molecular level are considered is that of generation of defects in optical fiber drawing. The differential equation for the time dependence of the E' defect concentration was formulated by Hanafusa et al. [36] based on the theory of the thermodynamics of lattice vacancies in crystals. It was assumed that the E' defects are generated through breaking of the Si-O band, and, at the same time, some of the defects recombine to form Si-O again. If the concentration and activation energy of the E' defects are represented by n_d and E_d, and those of the precursors by n_p and E_p, the differential equation is given by

$$\frac{dn_d}{dt}=n_p\nu^*\exp\left(-\frac{E_p}{\tilde{k}T}\right)-n_d\nu^*\exp\left(-\frac{E_d}{\tilde{k}T}\right) \tag{23}$$

where, ν^* is the frequency factor for this reaction, and $\tilde{k}$ the Boltzmann constant. The first term on the right hand side of this equation expresses the generation of the defects while the second term expresses the recombination. Thus the distribution of these defects in the fiber may be calculated [37].

Inverse Problems. Material behavior can often be employed to determine the thermal cycle that a given material must undergo in order to achieve desired characteristics. Metallurgical considerations for steel, for instance, indicate the thermal process needed for annealing, which is an important process employed for relieving the stresses in the material and restoring the ductility. The thermal processing involves heating of the material to the annealing temperature of around 723°C for common sheet steel, maintaining the temperature at this value for a given time, known as soaking period, so that this temperature level is attained everywhere in the material and the internal stresses are relieved, initial slow cooling to allow the microstructure to settle down, and final rapid cooling to reduce total time [38].

Since our interest lies in determining the conditions that would yield the desired temperature variation in the material, this is an inverse problem. Analysis only yields the outputs on system behavior for given inputs, rather than solve the inverse problem of yielding the inputs needed for a desired behavior. This latter problem is fairly difficult and has to be solved in order to select the design variables. The solution is not unique and efforts have to be made to narrow the domain over which design parameters and operating conditions are to be chosen. Iteration is generally necessary to obtain a satisfactory design. Optimization strategies may be used to obtain an essentially unique solution [39].

Solution Techniques and Simulation

Analytical. Due to the complexity of the governing equations and the boundary conditions, analytical methods can be used in very few practical circumstances and numerical approaches are generally needed to obtain the solution. However, analytical solutions are very valuable since they provide results that can be used for validating the numerical model, physical insight into the basic mechanisms and expected trends, and results for limiting or asymptotic conditions.

Consider, for example, the complex flow in a screw extruder, as shown in Fig. 1(d). This flow can be simplified and transformed to a shear and pressure driven flow in a channel, as discussed earlier and as shown in Fig. 3. If a fully developed flow, for which the velocity field remains unchanged downstream, is assumed, analytical solutions can be obtained for Newtonian fluids. If the pressure gradient is zero, the velocity profile is linear and the dimensionless flow rate, or throughput, q_v, which is the flow rate divided by the product of wall speed and cross-sectional area, is simply 0.5. For a favorable pressure gradient, i.e., pressure decreasing downstream, the throughput exceeds 0.5 and for an adverse pressure gradient it is smaller than 0.5. Similarly, for fully developed flow in a die, the relationship between the pressure drop Δp, across a cylindrical region of length L and radius R, and the mass flow rate $\dot{m}$ was obtained by Kwon et al. [40] for a power-law non-Newtonian fluid as

$$\Delta p = \frac{2L}{R}\hat{C}(T)\left[\frac{3n+1}{4n}\,\frac{4\dot{m}}{\rho\pi R^3}\right]^n \tag{24}$$

where $\mu = \hat{C}(T)(\dot{\gamma})^{1-n}$ and $\hat{C}(T)$ is a temperature dependent coefficient. This expression can be used for several common dies and it also applies for relatively long cylindrical regions in practical dies [41].

Numerical. The numerical solution of the governing equations is based on the extensive literature on computational heat transfer [11,42], with the most commonly employed technique being the SIMPLER algorithm, given by Patankar [43], and the several variations of this approach. This method employs the finite volume formulation with a staggered grid and solves for the primitive variables, such as velocity, pressure, concentration and temperature. For two-dimensional and axisymmetric problems, the governing equations are often cast in terms of the vorticity and streamfunction by eliminating the pressure from the two components of the momentum equation and by defining a streamfunction to take care of the continuity equation [11]. This reduces the number of equations by one and eliminates pressure as a variable, though it can be calculated after the solution is obtained. This approach is generally advantageous, as compared to the primitive variable approach, for two-dimensional and axisymmetric flows. The latter approach is more appropriate for three-dimensional circumstances.

In materials processing, both transient and steady-state solutions are of interest, depending on the process under consideration. In the former case, time marching is used with convergence at each time step to obtain the time-dependent variation of the transport. For steady problems also, time marching may be used to obtain steady-state results at large time. The problem can also be solved by iteration or by using false transients, with large time steps. Though central differences are desirable for all the approximations, numerical instability with the convection terms is often avoided by the use of upwind, exponential or power-law differencing schemes [43]. Because of the inaccuracy due to false diffusion, second-order upwind differencing and third-order QUICK schemes have become quite popular for discretizing the convection terms [44]. Under-relaxation is generally needed for convergence due to the strong nonlinearities that arise in these equations mainly due to property variations. Finite element and boundary element methods have also been used advantageously to simulate these systems.

Experimental. Experimental work is particularly important in a study of thermal processing of materials. This is needed for enhancing the basic understanding of the underlying transport processes, providing physical insight that can be used in the development of mathematical and numerical models, determining important aspects and variables, providing results for validation of mathematical and numerical models, and yielding quantitative results that can be used to characterize processes and components in the absence of accurate and dependable models. There are many complex transport processes where experimental results are needed to guide the development of the model and also generate quantitative data that can be used as empirical inputs if accurate modeling is not possible. Many important techniques have been developed in recent years on the measurement of flow, temperature and concentration distributions in a given system, and are being used in a variety of materials processing applications.

Typical Results From Numerical Simulation

The numerical results obtained for a few important processes are presented here to illustrate the basic characteristics of thermal processing of materials and some of the relevant considerations. Even though extensive results have been obtained in various studies, only a few typical results are presented.

Polymer Extrusion. This is an important manufacturing process, which has been mentioned earlier and is sketched in Figs. 1(d) and 3. Interest lies in the control and prediction of the heat transfer and flow in order to predict, improve and modify physical and chemical changes undergone by the material as it moves down the extruder channel. Figure 4 shows typical computed velocity and temperature fields in an extruder channel for a single-screw extruder. Large temperature differences arise across the channel height because of the relatively small thermal conductivity of plastics. There is little bulk mixing, due to the high viscosity, which is typically more than a million times that of water at room temperature. Reverse screw elements, sudden changes in the screw configuration and other such sharp changes in the channel are often used to disrupt the well-layered flow and promote mixing. The extruded material temperature rises beyond the imposed barrel temperature due to viscous dissipation. Additional results and trends are presented in several papers [27,28].

The residence time distribution (RTD) is an important consideration in the extrusion process. The residence time is the amount of time spent by a fluid particle in the extruder from the inlet to the die. An excessive residence time can lead to over-processing or degradation. Similarly, a short residence time can result in under-processing. The final product is, therefore, strongly affected by the residence time distribution since structural changes due to thermal processing and chemical reactions are usually time-dependent. The RTD is a function of the flow field and can be numerically simulated by particle tracking. Several results are

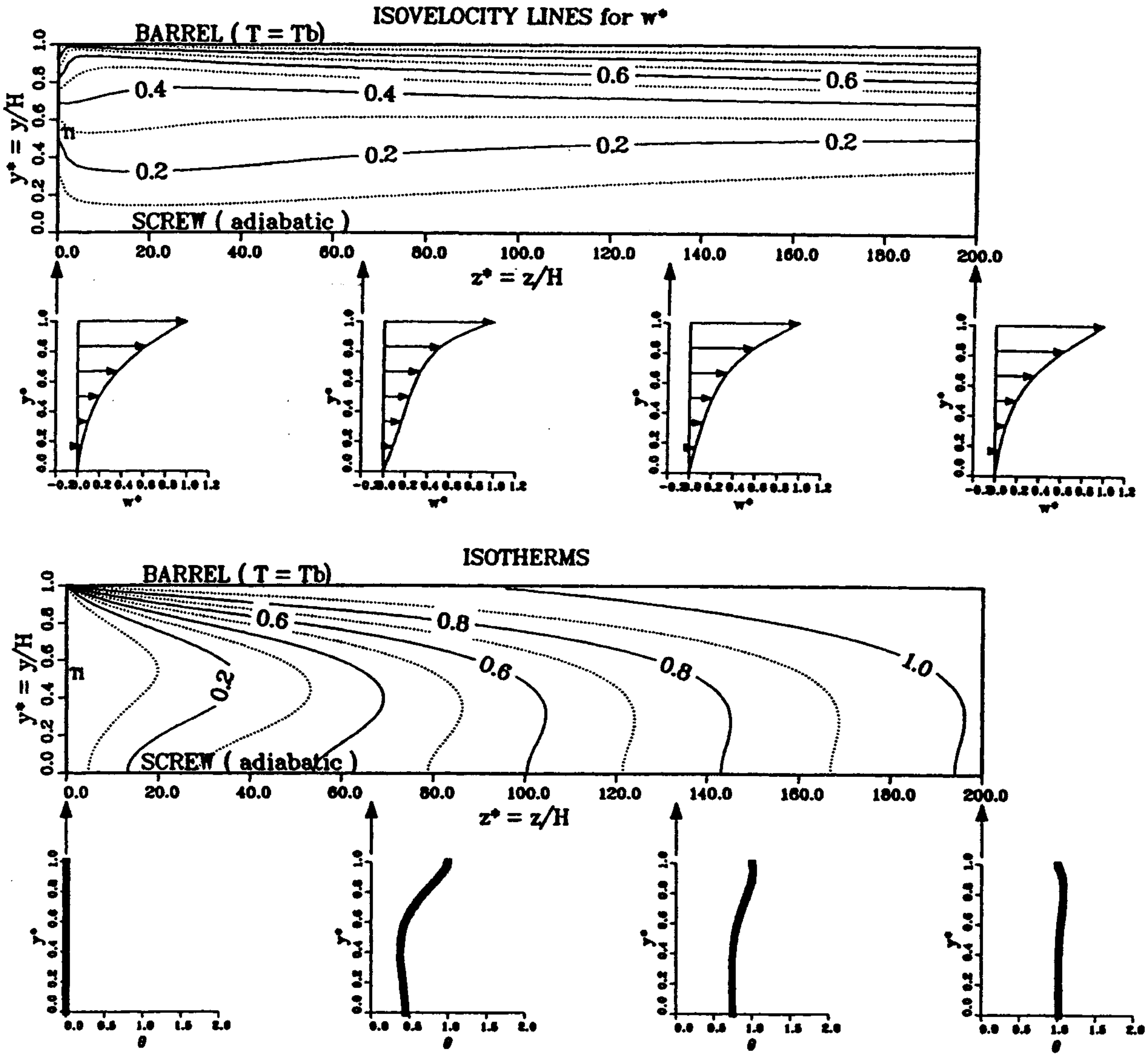

Fig. 4 Calculated velocity and temperature fields in the channel of a single screw extruder at $n=0.5$ and dimensionless throughput $q_v=0.3$, for typical operating conditions

given in the literature on RTD for different extruders [17,28,45]. It is experimentally obtained by releasing a fixed amount of color dye or tracer in the material at the inlet or hopper and measuring the flow rate of the dye material as it emerges from the extruder at the other end.

More recently, the use of twin-screw extruders for the processing of polymeric materials has increased substantially. The main advantages of twin-screw extruders, over single-screw extruders, are better stability, control and mixing characteristics. In twin screw extruders, two screws are positioned adjacent to each other in a barrel casing whose cross section is in a figure of eight pattern, see Fig. 5. Twin-screw extruders are of many types, such as, intermeshing, non-intermeshing, co-rotating, counter-rotating, to name a few.

The flow domain of a twin-screw extruder is a complicated one and the simulation of the entire region is very involved [46]. A major simplification in the numerical simulation is obtained by dividing the flow into two regions: the translation, or T region, and the mixing, or M region, as sketched in Fig. 5. This figure schematically shows sections taken normal to the screw axes of tangential twin screw extruders. Due to geometric similarity, the flow in the translation region is analyzed in a manner identical to that for a single screw extruder. The intermeshing, or mixing, region is represented by the geometrically complex portion of the extruder between the two screws. A hypothetical boundary is used to numerically separate the two regions [47]. The finite-element method is particularly well suited for the modeling of the complex domain in a twin-screw extruder. Figure 6 shows the finite element mesh used and some typical results on the transport in the mixing or nip region of the extruder. Large gradients arise in pressure, velocity and shear rate in the nip region, resulting in substantial fluid mixing, unlike the small recirculation in single-screw extruders. Similarly, other approximations and results on twin-screw extruders have been presented in the literature [48].

Optical Fiber Drawing. The optical fiber drawing process has become critical for advancements in telecommunications and networking. In this process, as sketched in Fig. 1(a), a cylindrical rod, which is known as a preform and which is specially fabricated to obtain a desired refractive index variation, is heated in a furnace and drawn into a fiber. Its diameter changes substantially, from 2–10 cm to around 125 μm in a distance of only a few centimeters. The radiative transport within the glass, which is a participating medium, is determined using the optically thick medium approximation or improved models such as the zonal method [49]. Interest lies in obtaining high quality optical fibers,

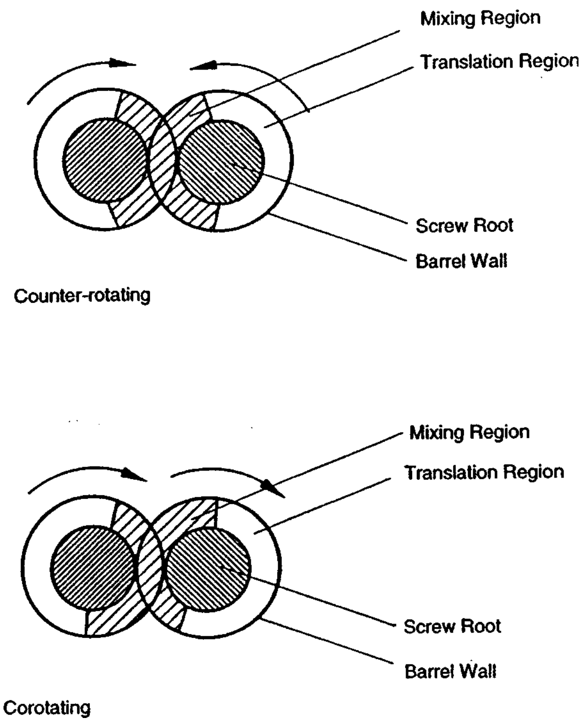

Fig. 5 Schematic diagram of the cross-section of a tangential twin screw extruder, showing the translation (*T*) and intermeshing, or mixing (*M*), regions

as indicated by low concentration of process-induced defects, diameter uniformity, desired refractive index variation, low tension, strength, and other important measures, at high draw speeds.

Typical computed results in the neck-down region, for a specified profile, are shown in Fig. 7 in terms of the streamfunction, vorticity, viscous dissipation and temperature contours. The flow is seen to be smooth and well layered because of the high viscosity. Typical temperature differences of 50–100°C arise across the fiber for preform diameters of around 2.0 cm. Larger temperature differences arise for larger preform diameters [37]. Viscous dissipation, though relatively small, is mainly concentrated near the end of the neck-down, in the small diameter region, and plays an important role in maintaining the temperatures above the softening point [30].

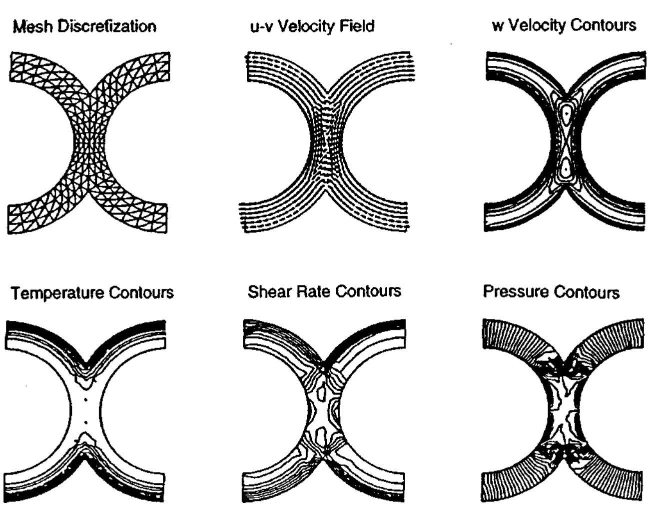

Fig. 6 Mesh discretization for the mixing region in a co-rotating tangential twin screw extruder, along with typical computed results for low density polyethylene (LDPE) at $n=0.48$, barrel temperature, $T_b=320°C$, inlet temperature, $T_i=220°C$, $N=60$ rpm, $q_v=0.3$

The determination of the neck-down profile of the glass preform as it is drawn into a fiber is a particularly difficult problem. Relatively simple models had been employed in the past to study the flow in this region [50]. More recently, a combined analytical and numerical approach, based on the transport processes and the surface force balance, was developed for the calculation of the neck-down profile [21]. Axisymmetric, laminar flows were assumed in the glass and in the circulating inert gases. A correction scheme was obtained for the neck-down profile using the radially lumped axial velocity, the normal force balance and the vertical momentum equations. The profile was then determined numerically by iterating from an initial profile and using this scheme for correcting the profile at intermediate steps, finally yielding a converged profile.

A typical example of the numerical generation of neck-down profile with a cosinusoidal starting profile is shown in Fig. 8(a). It is seen that, for the first few iterations, the neck-down profile is quite unrealistic, with a flat region and an abrupt change in radius near the end of neck down. But after a few iterations, the shape becomes quite smooth and monotonically decreasing, eventually reaching a steady, converged, profile, as indicated by the invariance of the profile with further iterations. For convergent cases, perturbations to the initial profile and different starting shapes lead to the converged neck-down profile, as seen in Fig. 8(b), indicating the robustness of the numerical scheme and the stability of the drawing process. The force balance conditions were also closely satisfied if convergence was achieved. However, convergence does not occur in every case, leading to infeasible drawing conditions, as discussed later. It was found that viscous and gravitational forces are the dominant mechanisms in the determination of the profile. Surface tension effects are small. The external shear and inertial effects are small, as expected. Later papers obtained the profile at higher draw speeds and for larger preform diameters [37,51].

There are several other processes involved in a typical optical fiber manufacturing process, as shown in Fig. 1(a). The fiber is cooled as it moves away from the furnace and is then coated with a jacketing material for protection against abrasion, to reduce stress induced microbending losses, and for increased strength. The temperature of the fiber entering the coating section is limited by the properties of the coating material used, being around 150°C for commonly used curable acrylates. The wet coating is then cured by ultra-violet radiation as it passes through the curing station [52–55].

Casting. Casting is an important manufacturing process, which involves solidification and melting [15]. The buoyancy-driven flow due to temperature and concentration differences in the liquid or melt region is coupled with the conduction in the solid. For casting in an enclosed region, the interface between the liquid and the solid moves away from the cooled walls for solidification till the entire material is solidified. However, the time-dependent location of this interface is not known and must be obtained from the solution. A coordinate transformation, such as the Landau transformation, may be employed to simplify the computational domains [12,14]. In continuous casting and crystal growing, as shown in Fig. 1(c), the interface between the solid and the liquid is essentially stationary, but it is not known a priori and an iterative procedure may be adopted to determine its shape and location. Transformations and body fitted coordinates may be employed to approximate the irregular shaped computational domains. If the enthalpy model is employed, the entire region is treated as one, considerably simplifying the computational procedure [14,56]. From an engineering standpoint, interest lies in obtaining high quality castings, with few voids and defects, good grain structure and low stresses, at high production rates.

The coupled conduction in the walls of the mold is an important

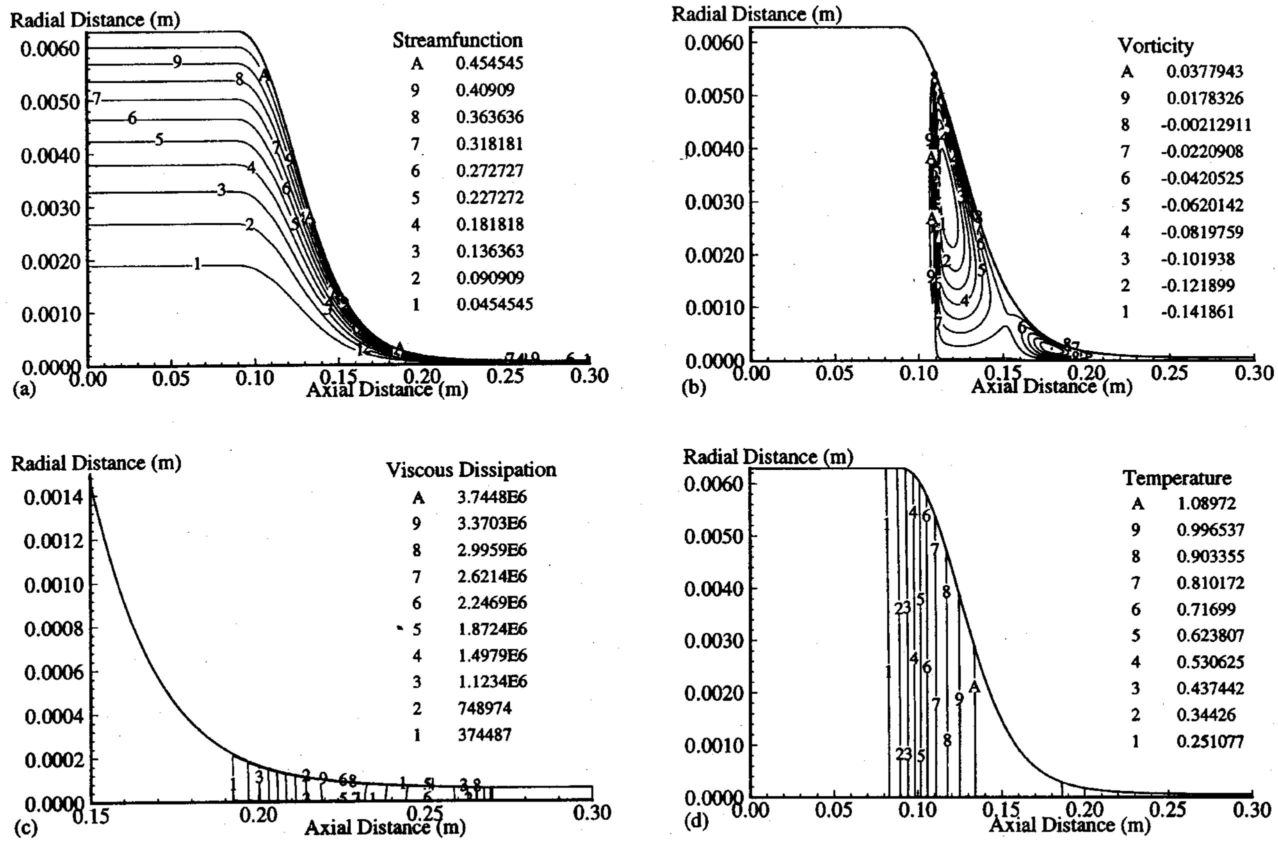

Fig. 7 Calculated (a) streamfunction, (b) vorticity, (c) viscous dissipation, and (d) temperature contours in the optical fiber drawing process for typical drawing conditions

consideration in these problems. The effect of the imposed conditions at the outer surface of the mold on the solidification process can be obtained by solving this conjugate problem, which yields the temperature distribution in the mold as well as that in the solid and the liquid. Banaszek et al. [57] carried out numerical simulations and appropriately designed experiments to demonstrate the importance of conduction in the wall, as shown in Fig. 9. Such numerical and experimental studies can be used to determine the movement of the solidification front with time and thus monitor the generation of voids and other defects in the casting. Experimental studies have been relatively few because of the complexity of the process. Detailed accurate experimental results are needed to critically evaluate the various models employed for simulation as well as to provide information on the characteristics of the interface for the development of microscale models.

Recent work on this problem has led to a much better understanding of the solidification process than before. The buoyancy-induced flow affects the heat and mass transfer processes, which in turn influence the characteristics of the melt-solid interface and the rate of melting/solidification. The transport also affects the quality of the product because of undesirable oscillations, generation of voids, and distribution of impurities. There has been a growing interest in the solidification of mixtures, particularly alloys, and polymers [58].

Continuous Processing. Continuously moving materials undergoing thermal processing are frequently encountered in manufacturing processes like hot rolling, wire drawing and extrusion. If the location of the moving surface is known, the continuous movement of the edge may be replaced by discrete steps and the numerical modeling carried out until results are obtained over a specified time or until the steady-state circumstance is obtained [22]. The corresponding initial and boundary conditions are obtained as:

$$t=0:\quad L(t)=0 \quad t>0:\quad \text{at } x=0,\quad T=T_o;$$

$$\text{at } x=L(t),\quad -k\frac{\partial T}{\partial x}=h_L(T-T_a) \tag{25}$$

where h_L is the heat transfer coefficient at the edge of the moving rod. The problem may be solved analytically [24] or numerically, the latter approach being more appropriate for two and three-dimensional problems and for practical circumstances. The length of the rod L increases with time and the temperature at the end decreases. At large time for steady ambient conditions, a steady temperature distribution arises over the rod and the temperature at the moving end reaches the ambient temperature.

In most practical circumstances, conjugate conditions arise at the surface and the convective transport in the fluid must be solved in conjunction with conduction in the moving solid. The region close to the point of emergence of the material usually has large axial gradients and requires the solution of the full equations. However, far downstream, the axial diffusion terms are small and boundary layer approximations may be made. Interest lies in controlling the local processing of the material in order to obtain uniformity, desired product characteristics and high productivity.

Figure 10 shows the typical calculated streamlines for a flat plate moving in a quiescent medium. The ambient fluid is drawn toward the moving surface because of large pressure gradients directed towards the origin. This effect decays downstream and

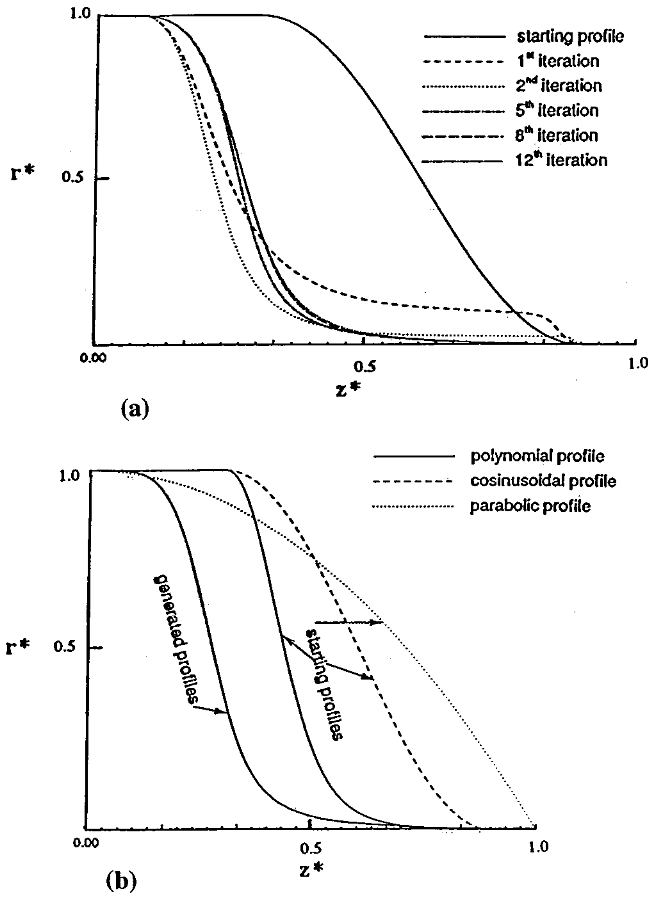

Fig. 8 (**a**) **Iterative convergence of the neck-down profile in optical fiber drawing;** (**b**) **results for different starting profiles. Here, $r^*=r/R$ and $z^*=z/L$, where R is the preform radius, and L the furnace length.**

the flow approaches the characteristics of a boundary-layer flow. The boundary-layer thickness increases in the direction of motion. If buoyancy effects due to the temperature differences are included, the maximum velocity in the flow is larger than the plate speed U_s, for an upward moving heated plate, as shown in the figure. This flow increases the heat transfer from the plate. Similarly, other orientations, the time-dependent flow at the initial stages of the process, and other important aspects have been investigated.

Chemical Vapor Deposition. Chemical vapor deposition involves the deposition of thin films from a gas phase on to a solid substrate by means of a chemical reaction that takes place during the deposition process. The activation energy needed for the chemical reactions is provided by an external heat source, see Fig. 1(b). The products of the reactions form a solid crystalline or an amorphous layer on the substrate. This technique has become quite important in materials processing and is used in a wide range of applications. The quality of the deposited film is characterized in terms of its purity, composition, thickness, adhesion, surface morphology and crystalline structure. The level of quality needed depends on the application, with electronic and optical materials imposing the most stringent demands. Much of the initial effort on this problem was directed at silicon deposition because of its importance in the semiconductor industry. However, recent efforts have been directed at the deposition of materials such as titanium nitride, silicon carbide, diamond, and metals like titanium, tungsten, aluminum, and copper.

Many different types of CVD reactors have been developed and applied for different applications. The quality, uniformity, and rate of deposition are dependent on the heat and mass transfer, and on the chemical reactions that are themselves strongly influenced by temperature and concentration levels [20,59]. The flow, heat transfer and chemical reactions in CVD reactors have been investigated by several researchers [59,60]. Some typical results obtained for silicon deposition are shown in Fig. 11, indicating a

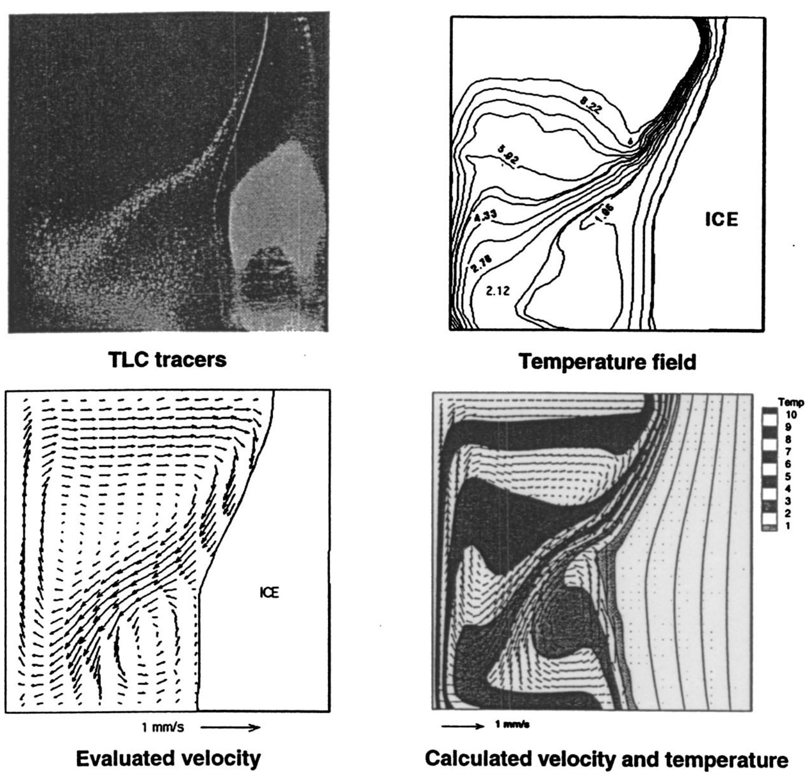

Fig. 9 Experimental and numerical results for water solidification driven by convection and conduction

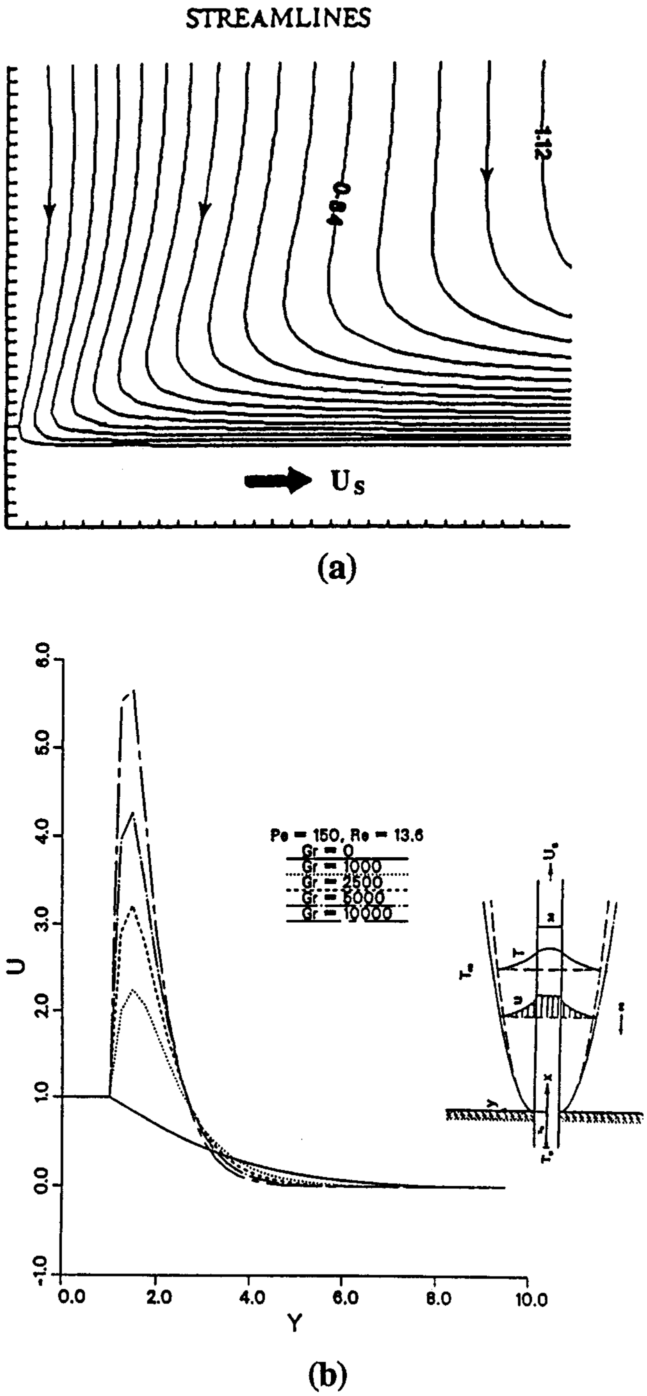

Fig. 10 (a) Flow in the ambient fluid due to a continuously moving material; (b) dimensionless velocity (u/U_s) distribution in the fluid due to a vertically moving heated plate with aiding buoyancy effects

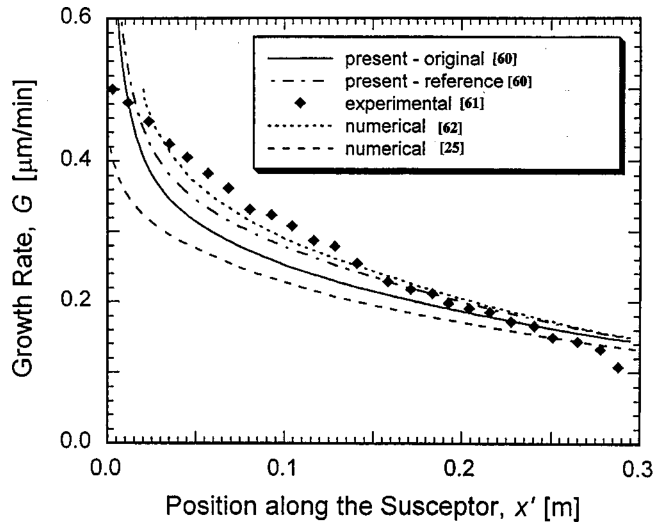

Fig. 11 Comparisons between the numerical results on predicted film growth rate and the experimental data of [61]

comparison between numerical and experimental results from [61]. A fairly good agreement is observed, given the uncertainty with material property data and with the chemical kinetics. The two results from [60] refer to two different values of the diffusion coefficient, the one labeled as the reference case employing the same values as those in [62].

Conjugate transport at the heated surface is also an important consideration, since in actual practice thermal energy is supplied to the susceptor, often at a constant rate, and the temperature distribution at the surface depends on the transport processes that arise. An experimental and numerical study was carried out by Chiu et al. [63] on the heat transfer in a horizontal channel with a finite heated region to approximate the susceptor. Figure 12 shows the typical results obtained, indicating good agreement between the experimental and numerical results. The characteristics of the flow, ranging from steady laminar to oscillatory and turbulent flow, were investigated and linked to the film uniformity.

Additional Processes. Only a few thermal processing techniques have been presented in the preceding section. There are many other processes in which the thermal transport is of crucial importance and which have been of particular interest in recent years. Among these are crystal growing, microgravity materials processing and thermal sprays. The Czochralski method, shown in Fig. 1(c), has dominated the production of single crystals for microelectronics and has been the subject of considerable research interest over more than three decades [64,65]. Other crystal growth techniques, including Bridgman crystal growing in which the furnace has an upper zone at temperature above the melting point and a lower zone at temperature below the melting point, have also been investigated [64]. Microgravity conditions are obtained, for instance, in laboratories orbiting in space, where the processing of materials can be carried out with reduced effects of the terrestrial gravitational field. Gravity determines the buoyancy-driven flows in the melt of a crystal growing system and thus affects the quality and characteristics of the crystal. Thus, by controlling the gravitational force, the resulting transport processes and the final product can be improved [66]. Thermal sprays may be used for the manufacture of near-net shape structured materials. Sprays containing droplets of the desired deposition material are directed at a specified substrate and the material is deposited by rapid solidification. Due to the elimination of several traditional processing steps, the process is fast and rapid solidification eliminates macrosegregation, which weakens traditionally cast materials [67–69]. Superior properties, associated with fine-grained microstructures and non-equilibrium phases, are usually obtained.

Validation

A very important consideration in modeling and simulation is that of validation of the models. This is particularly critical in thermal materials processing because of lack of accurate material property data, combined mechanisms and other complexities in the process. Validation of the models is based on a consideration of the physical behavior of the results obtained, elimination of the effect of arbitrary parameters like grid and time step, and com-

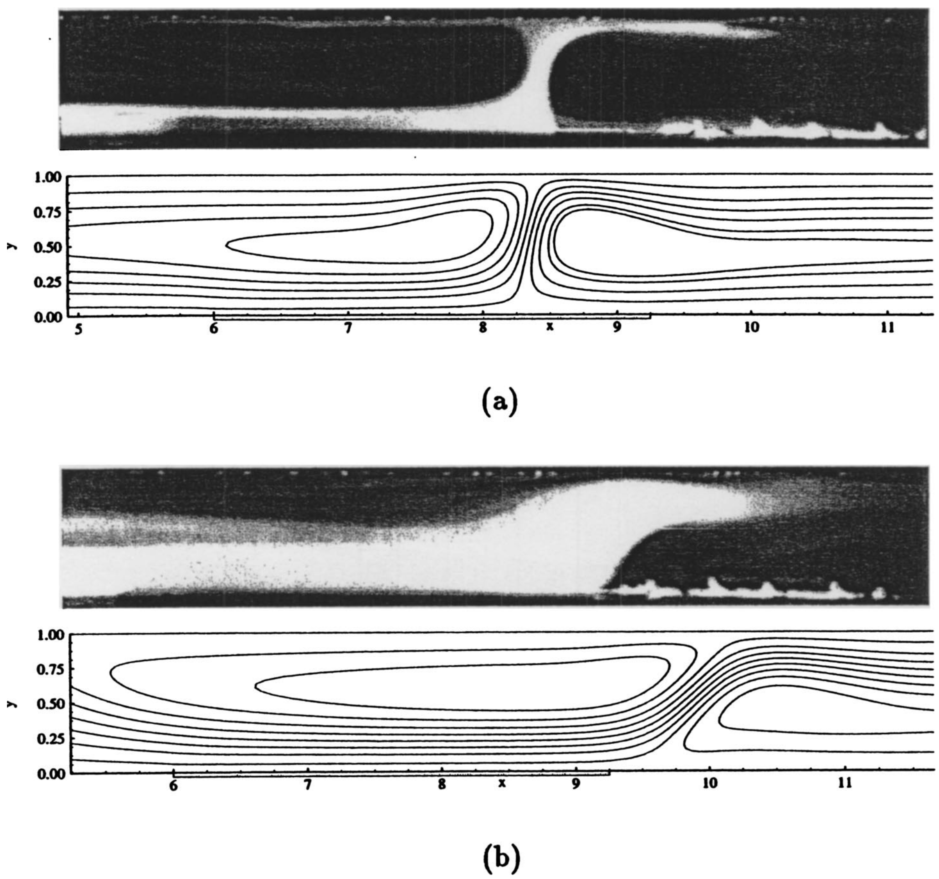

Fig. 12 Comparison between experimental observations and numerical predictions of streamlines at Re=9.48 and Re=29.7 for a ceramic susceptor

parisons with available analytical results for simpler configurations, with numerical results in the literature, and with experimental results on the process and on a prototype, if available [70,71]. A few examples are given here.

Polymer Extrusion. Measurements on the temperature and velocity distributions in an extruder channel are very complicated because of the complex domain, rotating screw and generally opaque nature of the typical materials. However, the overall characteristics of the extrusion process, in terms of pressure and temperature at the die, residence time distribution, total heat input, characteristics of the extrudate, total torque exerted on the screw, and flow rate, are available in the literature [16,27]. These can be used to validate the main predictions of the models for the polymer extrusion process. However, detailed temperature, velocity and pressure distributions are needed to determine the accuracy, validity and predictability of the local behavior. Esseghir and Sernas [72] have carried out innovative and well-designed experiments on single-screw extruders, using a cam-driven thermocouple which allowed the probe to travel in and out of the channel in a synchronized motion linked to the screw rotation.

A few experimental results for Viscasil-300M, which is a non-Newtonian fluid, are shown in Fig. 13, along with numerical results from two-dimensional finite volume and three-dimensional finite element calculations [29,73]. The effect of fluid recirculation in the screw channel is seen as the temperature near the screw root being closer to the barrel temperature, than that predicted by the two-dimensional model which does not consider this recirculation. A three-dimensional model is thus needed to simulate this recirculation and the results are seen to be close to the experimental data. Similarly, an experimental study was carried out to investigate the characteristics of the flow and the basic features of the mixing process in the intermeshing, or mixing, region [74]. Experimentally and numerically obtained streamlines in the region between two rotating cylinders, approximating a twinscrew, were obtained and a good agreement between the two was observed.

Measurement of the velocity distribution in the channel is also very involved because of the complex geometry and rotating screws. Bakalis and Karwe [75] have carried out velocity measurements for heavy corn syrup, which is transparent. Employing a plexiglas window, a two-component Laser Doppler Anemometer (LDA) in the backscatter mode was used to measure the local velocities in the extruder, as shown in Fig. 14(a). The complicated, three-dimensional, flow field was studied and a comparison of the tangential velocity distribution in the translation region with the numerical predictions is shown in Fig. 14(b). A fairly good agreement is observed, lending support to the model. Similarly, different velocity components were measured in the intermeshing region and compared with numerical predictions, yielding good agreement.

Optical Fiber Drawing. Very little experimental work has been done on the thermal transport in the optical fiber drawing process because of the high temperatures encountered, high draw speeds, complex geometry, and difficult accessibility into the furnace [39,50]. Paek and Runk [76] experimentally determined the neck-down profile. Using the heat transfer coefficient values given by them and an appropriate parabolic furnace temperature distribution to obtain the experimental conditions, the neck-down profile was calculated in [21] and compared with the experimental results, as shown in Fig. 15(a). The analytical results obtained by Paek et al. [77] showed that the draw tension plotted on a

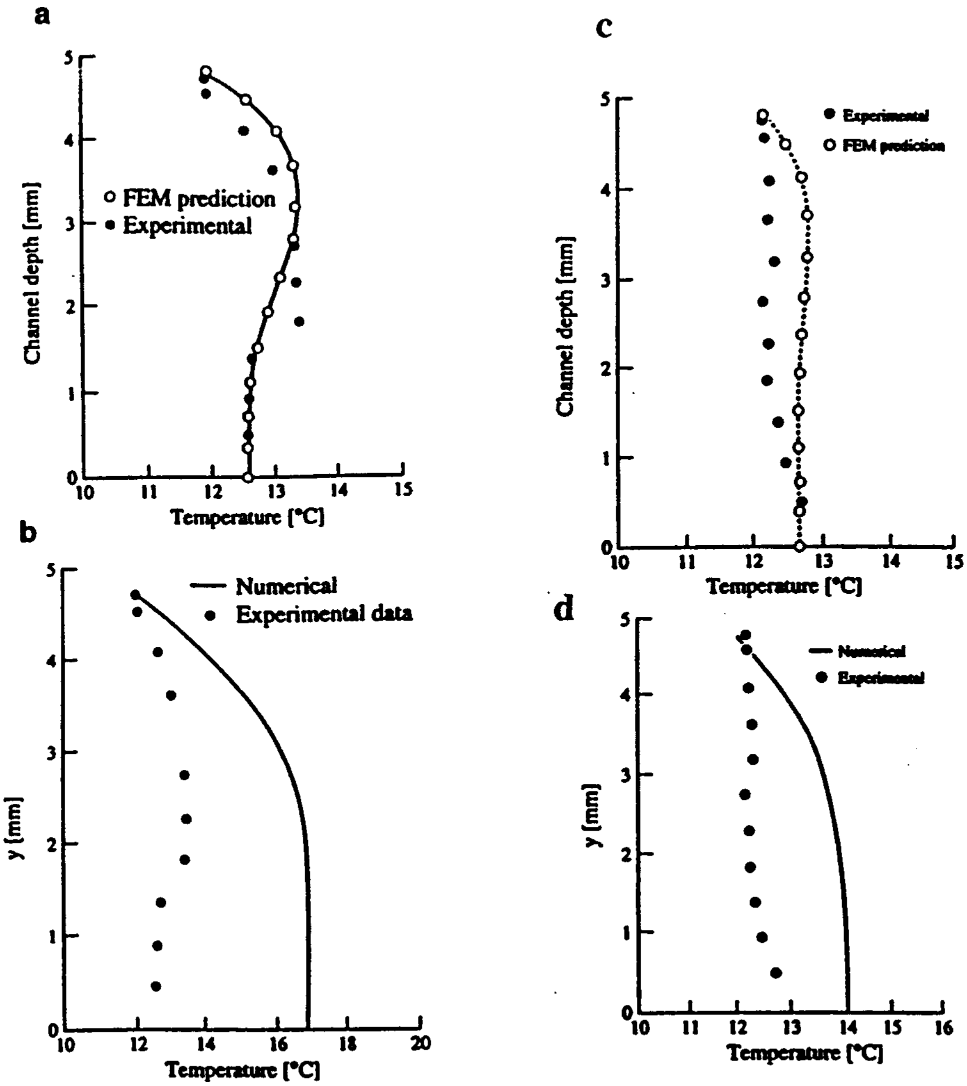

Fig. 13 Comparisons between numerical and experimental results on temperature profiles for Viscasil-300M, with (a) and (c) from the three-dimensional (FEM) model and (b) and (d) from the two-dimensional (FDM) model. For (a) and (b): T_i=20.3°C, T_b=12.2°C, N=20. For (c) and (d): T_i=18.8°C, T_b=22.3°C, N=35.

logarithmic scale varies linearly with the inverse of the furnace temperature. A comparison between the computed results and the experimental data show good agreement, as seen in Fig. 15(b).

Casting. Some numerical and experimental results were shown earlier for solidification of water, indicating good qualitative agreement. A benchmark problem, in which melting in a rectangular enclosed region is initiated by step changes in the temperatures at the left and right boundaries, the left being held at a temperature higher than the melting point and the right at a temperature lower than the melting point, has been used for validating the models. Figure 16 shows the experimental results and corresponding numerical predictions on the liquid-solid interface location, for melting of pure tin, using the enthalpy model [78,79]. Though these results are found to agree quite well, further detailed comparisons are needed to improve existing models.

System Simulation

In the preceding sections, we have discussed modeling and simulation of various processes and components that are of interest in the thermal processing of materials. However, there is another very important aspect that must be considered and that relates to the numerical simulation of the overall thermal system, which usually consists of several components, since the process undergone by the material results from the energy exchange with the various components of the system [1].

Consider, for instance, a typical electrical furnace, which consists of the heater, walls, insulation, enclosed gases and the material undergoing heat treatment. The transport mechanisms in all these components are coupled through the boundary conditions. Thus, the heater exchanges thermal energy with the walls, the gases and the material. Similarly, the material undergoing heat treatment is in energy exchange with the heater, the walls and the gases. The gas flow is driven by an externally imposed pressure difference, such as that due to a fan, by moving materials in continuous processing, and by buoyancy. Each individual component may first be mathematically modeled and numerically simulated as uncoupled from the others, by employing prescribed boundary conditions. Then, these individual simulations can be combined, employing the appropriate coupling through the boundary conditions. This procedure provides a systematic approach to the numerical simulation of the system, which may be a simple one or a complicated practical one [38]. Once the simulation of the system is achieved, with satisfactory experimental validation, the design and optimization of the process as well as of the system may be undertaken.

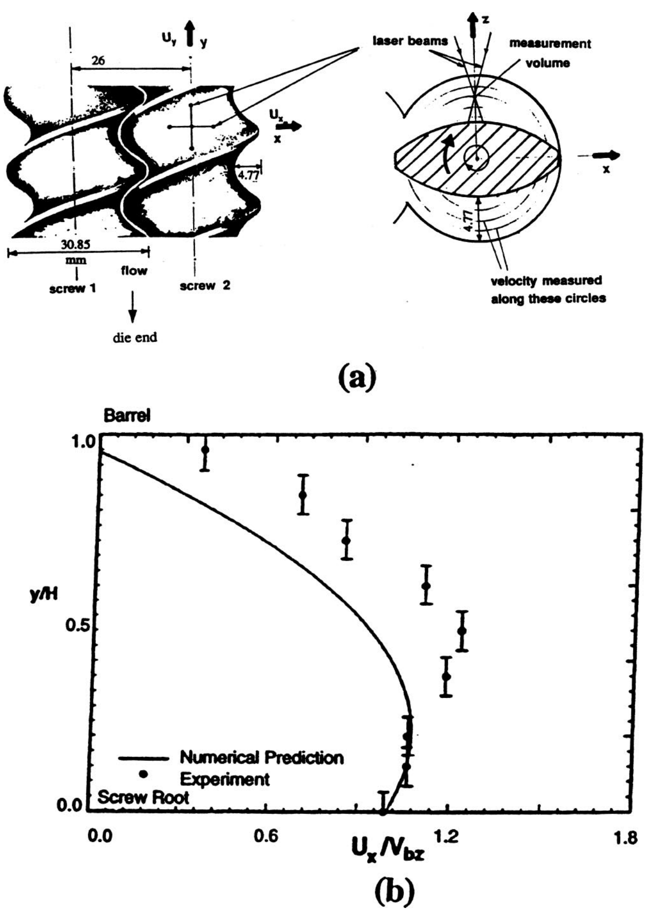

Fig. 14 (a) Experimental arrangement for velocity measurements in the flow of corn syrup in a twin-screw extruder; (b) comparison between calculated and measured tangential velocity U_x profiles for isothermal heavy corn syrup at 26.5°C, with mass flow rate of 6 kg/hr and screw speed of 30 rpm

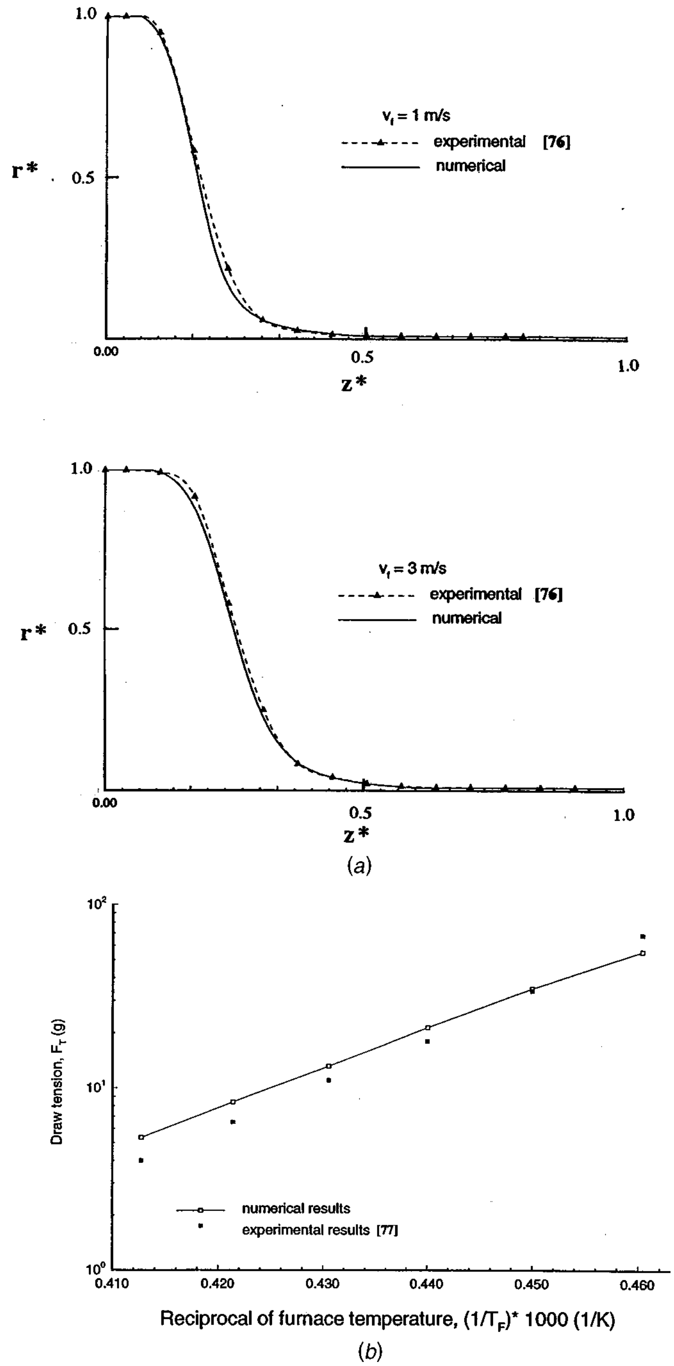

Fig. 15 Comparison of the numerical predictions of (a) the neck-down profile and (b) the draw tension with experimental results from [76,77]

Process Feasibility

An important consideration in the design of a system for materials processing is the feasibility of the process, since there is usually a fairly narrow domain of operating conditions in which the process is possible. Numerical simulation can play a significant role on this aspect since it can guide the selection of operating conditions and design parameters that can lead to successful thermal processing. A few studies in polymer extrusion and optical fiber drawing are discussed here as examples.

Polymer Extrusion. The feasibility of the process is determined largely by the flow and the pressure and temperature rise in the extruder. Using the modeling discussed earlier, the feasible domain for a self-wiping co-rotating twin-screw extruder is determined for the extrusion of Amioca, which is pure starch, as shown in Fig. 17. An upper limit is obtained for the mass flow rate. Beyond this limit, though the numerical scheme converges, the results are not physical acceptable. In actual practice, for a given screw rotational speed, each turn of the screw can move a specific maximum volume of material. Then the given mass flow rate can not exceed this limit given by the shear-driven flow. For higher mass flow rates, it is necessary to impose a favorable pressure gradient to push the material down the channel. Therefore, a negative pressure gradient along the axial direction will occur in the channel and that is not physically acceptable for an extruder [80]. For a specific screw speed, the simulation code also diverges for mass flow rates lower than the critical points shown in the figure because of flow instability and excessive pressures, temperatures and residence times. These results and trends show good agreement with the observations on practical systems that also yield a domain in which a stable reactive extrusion process can be created [81].

Optical Fiber Drawing. Using the mathematical and numerical models discussed earlier for optical fiber drawing, it has been shown that, for given fiber and preform diameters and for a given draw speed, it is not possible to draw the fiber at any arbitrary furnace wall temperature distribution [21,82,83]. If the furnace temperature is not high enough, it is found that the fiber breaks due to lack of material flow, a phenomenon that is known as viscous rupture [84]. This is first indicated by the divergence of

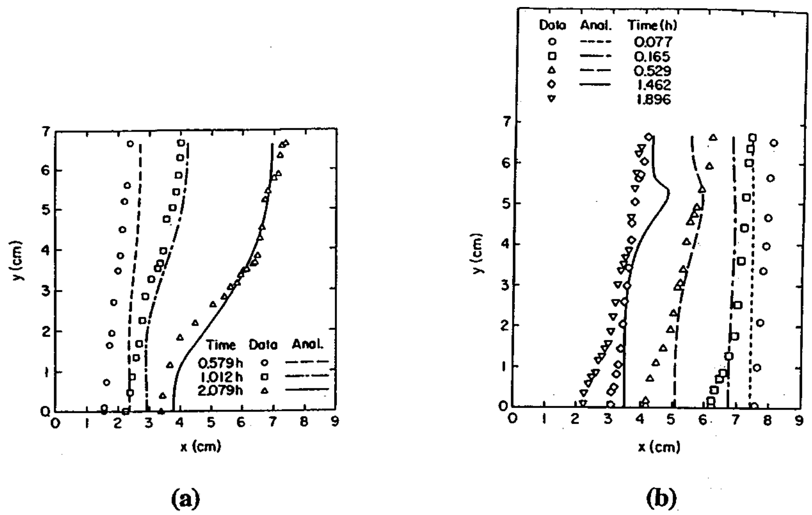

Fig. 16 Comparison between measured and predicted interface locations during (a) melting, and (b) solidification of pure tin from a vertical surface [78,79]

the numerical correction scheme for the profile and is then confirmed by excessive tension in the fiber. Similarly, it is determined that, for a given furnace temperature, there is a limit on the speed beyond which drawing is not possible, as this leads to rupture. Thus, as shown in Fig. 18(a), a region in which drawing is feasible can be identified. Beyond the boundaries of this region, drawing is not possible. For the domain in which the drawing process is feasible, the draw tension is calculated. The "iso-tension" contours are shown in Fig. 18(b). As expected, the draw tension is small at higher temperatures and lower speeds, which explains the positive slope of the iso-tension contours.

Similarly, different combinations of other physical and process variables, such as the inert gas flow velocity, furnace wall temperature distribution, furnace length and diameter, and preform and fiber diameters, may be considered to determine the feasibility of the process. Figure 18(c) shows the results when the furnace length and temperature are considered as the two main parameters. Again, the feasibility of the process is largely determined by viscous rupture, which is a direct result of high draw tension. It is seen that either a higher draw temperature or a longer residence time in the furnace, as regulated by its length, is needed to make fiber drawing possible at higher draw speeds. Using such results, the parameters in a fiber drawing system can be chosen to draw a fiber of desired diameter.

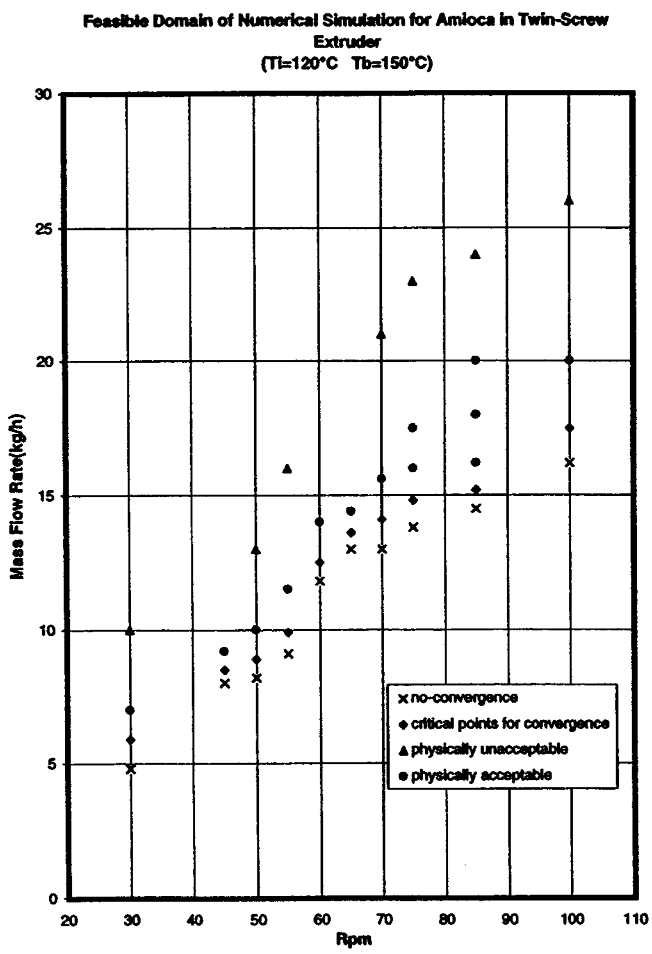

Fig. 17 Feasible domain for twin-screw extrusion of starch

Additional Engineering Aspects

Several important considerations in the design and operation of practical thermal materials processing systems were discussed in the preceding sections. These included issues like rate of fabrication, quality of the product, and feasibility of the process. However, there are obviously many other aspects that need to be considered in the design and optimization of the system and for the selection of the operating conditions. Some of these are outlined here.

An important consideration in polymer extrusion is the mixing inside the screw channel since it determines the homogeneity of the processed material. The downstream motion of material particles may be considered for a better understanding of the mixing process. Similarly, the distributive mixing inside the channel may be considered in terms of mixing between two different types of materials, with each initially occupying one half of the channel. Several other measures of mixing have been considered in the literature. Substantial work has also been done on mixing in twin-screw extruders, including the use of chaos introduced by changes in the geometry and the boundary conditions [85]. Similarly, melting and solidification of the material, leakage across screw flights, instability in the flow, unfilled screw channels, and conjugate transport due to conduction in the barrel are other important engineering issues in polymer extrusion. Transient effects are also important, both for the start-up of the process and for changes in the operating conditions.

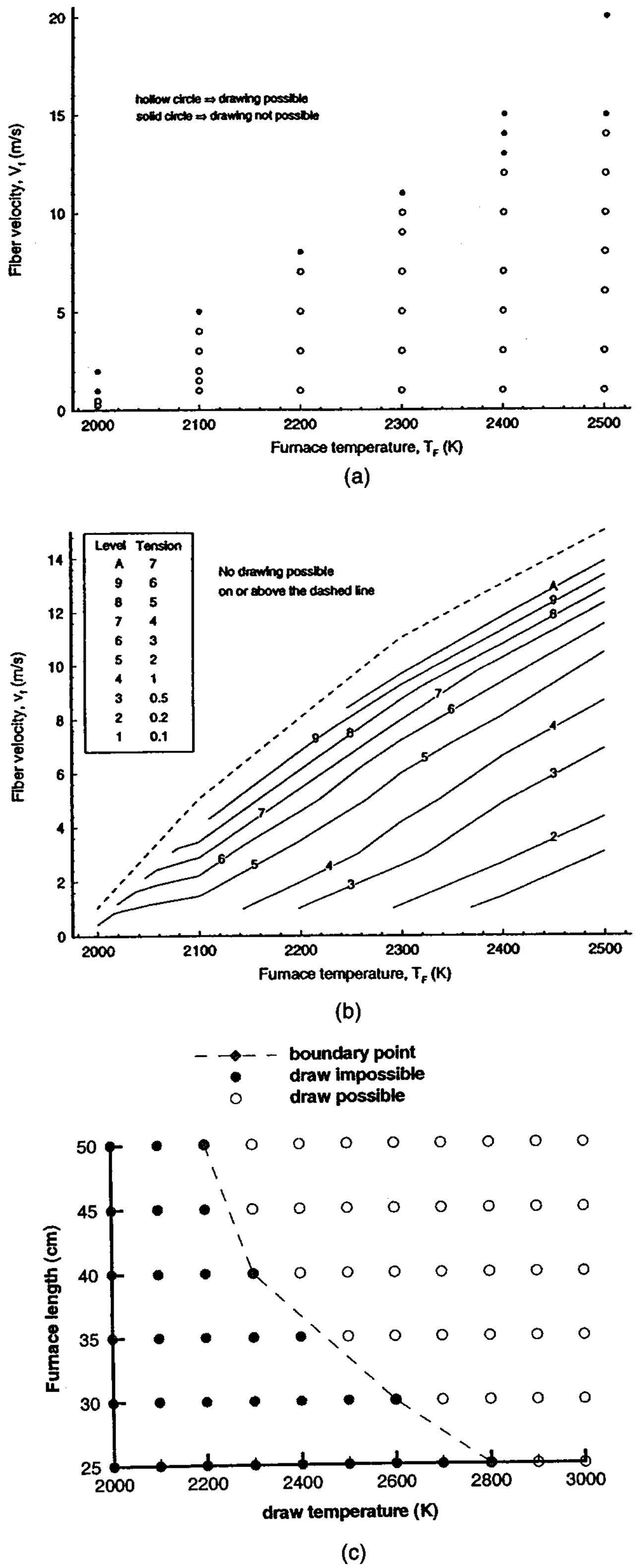

Fig. 18 Results obtained from a feasibility study of the optical fiber drawing process: (a) different cases studied, showing both feasible and infeasible combinations of parameters; (b) "iso-tension" contours for the feasible range of fiber drawing; (c) feasible domain at a draw speed of 15 m/s in terms of furnace length and temperature

Similarly, in other thermal materials processing systems, important aspects that are particularly relevant to the process under consideration arise and must be taken into account by the simulation and experimentation in order to provide the appropriate inputs for system design and optimization. These relate to engineering issues like durability, maintenance, availability of different materials and components, and the convenience and practical range of operating conditions.

Optimization

We have so far largely considered workable or acceptable design of a system. Such a design satisfies the requirements for the given application, without violating any imposed constraints. However, the design would generally not be the best or optimal design, as judged on the basis of cost, performance, efficiency, performance per unit cost, or other such measures, with acceptable environmental effects. The need to optimize is very important in the design of the materials processing systems and has become particularly crucial in the recent times due to growing global competition.

Any optimization process requires the specification of a quantity or function U, known as the objective function and which is to be minimized or maximized. The general mathematical formulation for the optimization of a system may be written as

$$U(x_1,x_2,x_3,\ldots,x_n)\rightarrow U_{\text{opt}} \tag{26}$$

with,

$$G_i(x_1,x_2,x_3,\ldots,x_n)=0, \quad \text{for } i=1,2,3,\ldots,m \tag{27}$$

and,

$$H_i(x_1,x_2,x_3,\ldots,x_n)\leqslant \text{or} \geqslant C_i, \quad \text{for } i=1,2,3,\ldots,l \tag{28}$$

where x_i represent the design variables and operating conditions, G_i represent equality constraints, and H_i inequality constraints. If the number of equality constraints m is equal to the number of independent variables n, the constraint equations may simply be solved to obtain the variables and there is no optimization problem. If $m>n$, the problem is over constrained and a unique solution is not possible. Some constraints have to be discarded to make $m\leqslant n$. If $m<n$, an optimization problem is obtained.

For thermal materials processing, the objective function U could be taken as the number of items produced per unit cost, product quality, or the amount of material processed. The constraints are often given on the temperature and pressure due to material limitations. Conservation principles and equipment limitations restrict the flow rates, cutting speed, draw speed, and other variables. The second law of thermodynamics and entropy generation can also be used to optimize systems so that exergy, which is a measure of the availability of energy from a thermal system, can be maximized [86].

Search methods constitute the most important optimization strategy for thermal systems. The underlying idea is to generate a number of designs, which are also called trials or iterations, and to select the best among these. Effort is made to keep the number of trials small, often going to the next iteration only if necessary. The steepest ascent/descent method is an important search method for multivariable optimization and is widely used for a variety of applications including thermal systems. However, it does require the evaluation of gradients in order to determine the appropriate direction of movement, limiting the application of the method to problems where the gradients can be obtained accurately and easily. Several other such gradient-based methods have been developed for optimization and are used for a variety of thermal processes [1,87,88]. Genetic optimization algorithms, that are based on function evaluations instead, have also been developed, though these methods are often less efficient than gradient-based methods.

The objective function is among the most critical and difficult aspects to be decided in the optimization of thermal materials

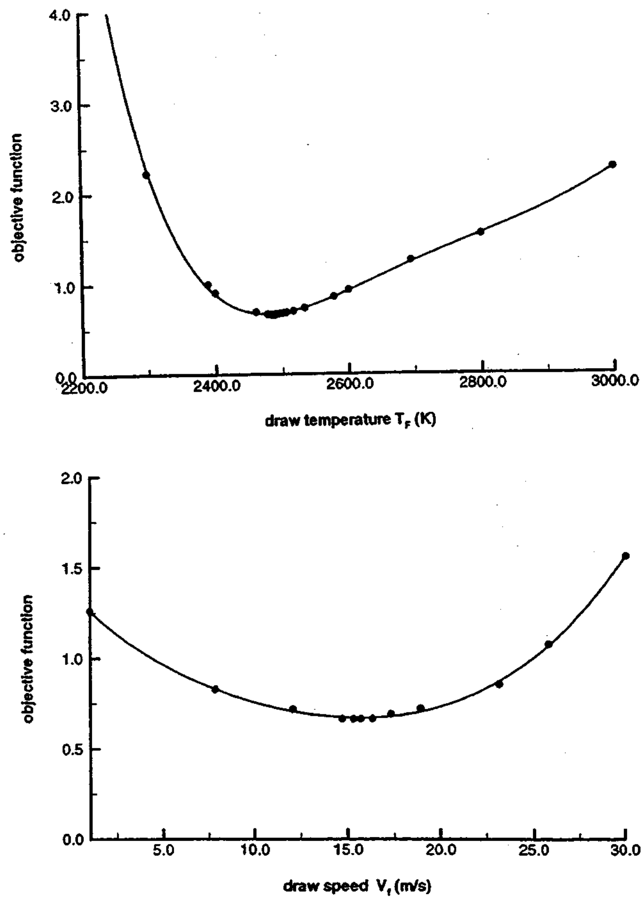

Fig. 19 Evaluation of optimal draw temperature at a draw speed of 15 m/s and the optimal draw speed at a draw temperature of 2489.78 K, obtained in the first part, by using the golden-section search method

processing systems, since the optimal design is a strong function of the chosen criterion for optimization. For illustration, let us consider a CVD system for deposition of TiN. As discussed in detail by Chiu et al. [88], the main qualities of interest include product quality, production rate, and operating cost. These three may be incorporated into one possible objective function *U*, which is to be minimized and is given by

$$U=\frac{(\text{Product Quality Deficiency})\times(\text{Operating Cost})}{\text{Production Rate}} \tag{29}$$

Here, the product quality is defined in terms of uniformity of film thickness and other properties which quantify the desired attributes. Since the objective function is minimized, maximum production rate is achieved by placing it in the denominator. The objective function represents equal weighting for each design quality. Obviously, the objective function may assume many possible forms. Using the steepest ascent method, Chiu et al. [89] obtained the optimal design.

A similar study was carried out by Cheng [90] on the optical fiber drawing process, considering the numerical simulation of the draw furnace. The objective function could again be taken as the general form given by Eq. (29). Because of the complexity of the process and lack of information on operating costs, the effort was directed at the fiber quality, taking the tension, defect concentration and velocity difference across the fiber, all these being scaled to obtain similar ranges of variation, as the main considerations. The objective function *U* was taken as the square root of the sum of the squares of these three quantities and was minimized. Several search methods, such as golden-section for single variable and univariate search for mutivariable cases, were employed. Figure 19 shows typical results from golden-section search for the optimal draw temperature and draw speed. The results from the first search are used in the second search, following the univariate search strategy, to obtain optimal design in terms of these two variables. Several other results were obtained on this complicated problem.

Knowledge Base

An important aspect in the design of systems for the thermal processing of materials is the use of the available knowledge base on the process to guide the design and operation of the system. The knowledge base typically includes relevant information on existing systems and processes, current practice, knowledge of an expert in the particular area, material property data, and empirical data on equipment and transport, such as heat transfer correlations. Some effort has been directed in recent years at streamlining the design process and improving the design methodology [91]. The basic concept behind knowledge-based systems is the storage and use of this knowledge to take logical decisions for selection, diagnostics and design [92]. Empirical data, heuristic arguments and rules for making decisions are all part of this knowledge-based methodology. The expert knowledge is obviously specific to a given application and represents the knowledge and experience acquired by the expert over a long period of work in the area of interest.

Knowledge-based design methodology is particularly useful in selecting an initial design for a given system. Two strategies may be used for generating an initial design. The first is based on a library of designs built using information from earlier design efforts and from existing systems. The design closest to the given problem may be selected by comparing the designs in the library with the desired specifications. The second approach uses the knowledge and experience of an expert to generate a design for the given requirements and constraints [93]. Of course, the user can always enter his/her own initial design if the output from the library or the expert rules is not satisfactory.

The knowledge base is also used in the redesign process to evaluate a given design and, if this is not satisfactory, to generate a new design. Expert rules establish the relationship between a design variable and the objective function. Several efficient strategies can be developed for selecting the design variables to go from one design to the next. The selection of design variables for the new design are guided by expert rules as well as by the results of the design process up to the given instant.

This approach may be applied to the casting of a material in an enclosed region. The need for design and optimization of the system arises because of the desire to reduce the solidification time and improve the product quality. A large number of design parameters arise in this problem, such as materials, initial melt pour temperature, cooling fluid and its flow rate, and dimensions. The quality of the casting is determined by grain size, composition, directional strength, concentration of defects, voids, thermal stresses, etc. It is necessary to carry out a thermal analysis of the solidification process, using modeling and simulation, to obtain inputs for design and to evaluate the nature of the casting.

Viswanath [94] and Viswanath and Jaluria [95] considered this problem, using knowledge-based methodolgy for design. Several models are available for the study of solidification, such as

1. *Steady conduction in solid model*: Melt is taken at freezing temperature, mold at fixed temperature and steady conduction in the solid is assumed.
2. *Chvorinov model*: Entire thermal resistance is assumed to be due to the mold
3. *Lumped mold model*: Temperature in the mold is assumed to be uniform and time-dependent, melt is taken at freezing temperature and steady conduction in the solid is assumed.
4. *One-dimensional conduction model*: Transient 1D temperature distributions are assumed in the mold, solid and melt.

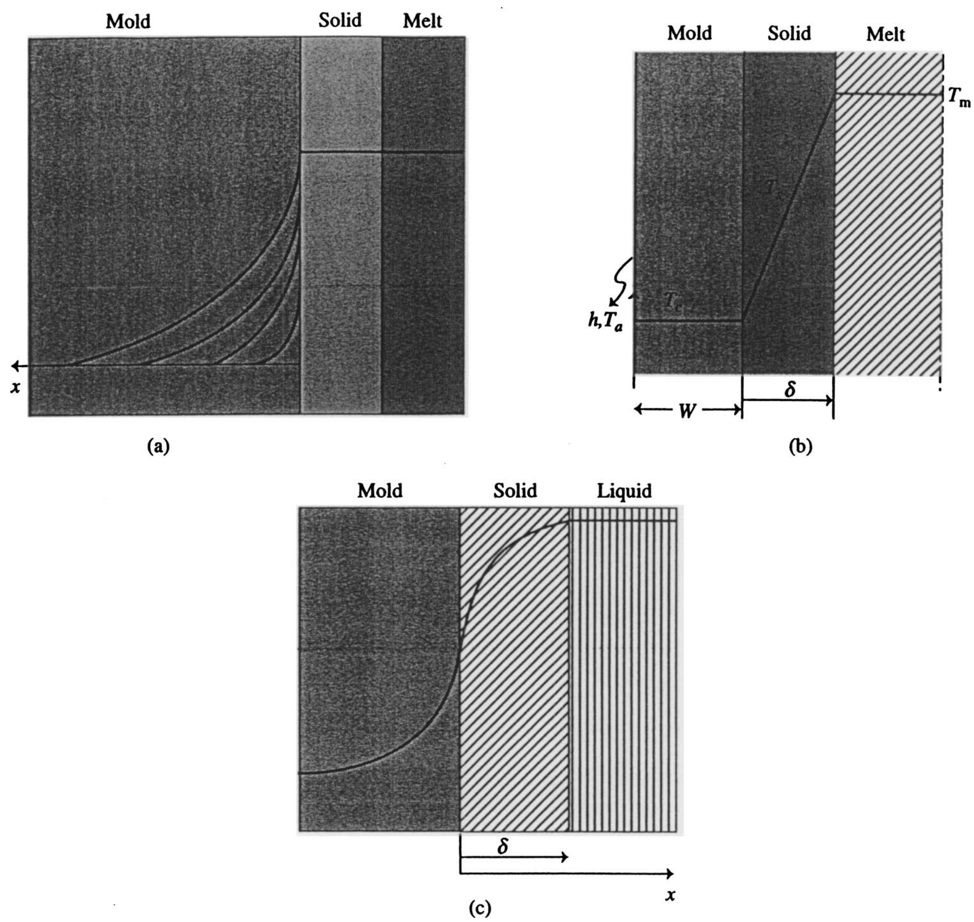

Fig. 20 Different mathematical models for ingot casting: (a) Chvorinov model; (b) lumped mold model; and (c) semi-infinite model

5. *Two and three-dimensional models*: Natural convection flow in the melt is included.
6. *More sophisticated models*: Needed for alloys, generation of voids, complicated geometries, etc.

Three models among these are sketched in Fig. 20. Each model has its own level of accuracy and validity. Different models may be chosen, depending on the application and materials involved. Expert knowledge plays a major role here. For instance, if an insulating material such as ceramic or sand is used for the mold,

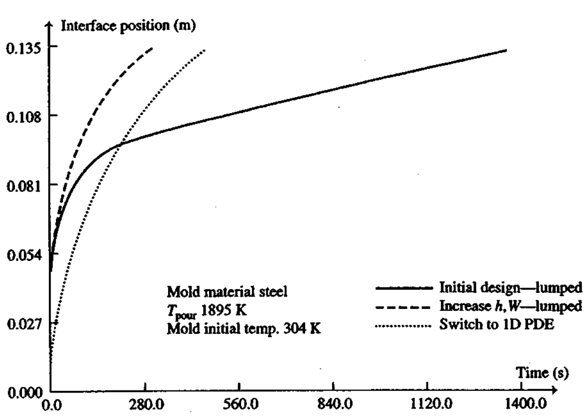

Fig. 21 Results for design of an ingot casting system, showing solid-liquid interface movement with time and switching to a more complex model after many design trials

the Chvorinov model may yield good results since most of the thermal resistance is in the mold. One-dimensional models are adequate for solidification near the boundaries. Sophisticated models are needed for alloy solidification and for considering the microstructure in the casting.

The optimal design may be obtained with solidification time being chosen as the objective function and employing constraints from the expert knowledge to avoid unacceptable thermal stresses and defects in the casting. We may start with the simplest model and keep on moving to models with greater complexity till the results remain essentially unchanged from one model to the next. Thus, models may be automatically selected using decision-making based on accuracy considerations. In a typical design session, the cooling parameters are first varied to reduce the solidification time. If the solidification time does not reach the desired value, the pour temperature of the melt may be varied. If even this does not satisfy the requirements, the thickness of the mold wall may be changed. The material of the wall may also be varied, if needed. Thus, by first varying the operating conditions and then the dimensions and materials, the solidification time may be minimized or brought below a desired value. Figure 21 show some a typical run for the design of the given system, indicating model change as the design proceeds. Each successful design may be stored for help in future designs.

Conclusions and Future Research Needs

This paper presents a review of the current status of the important field of thermal processing of materials. It focuses on the link between basic research on the underlying transport mechanisms and the engineering aspects associated with the process and the system. Several important processing techniques, such as optical fiber drawing, polymer extrusion and chemical vapor deposition, are discussed in particular detail to bring out the basic and applied issues in materials processing. These include modeling, validation, system simulation, process feasibility, and the design and optimization of the system. Important solution techniques, typical results in thermal materials processing and the implications for practical systems are discussed.

Our understanding of thermal processing of materials has grown significantly over the last three decades. Many new and improved techniques have been developed, along with new materials, new processing systems and better control on product quality and production costs. However, there are still many areas that need detailed further work. Among the most important ones are material properties and characteristics, experimental results, and coupling of micro or nano-scales, where materials processing occurs, and the macro-scale of interest in engineering. The measurement and availability of accurate material properties are crucial to a study in this area. Also, experimental results are strongly needed for validation of models and for providing inputs and insight for future model development.

In addition, work is needed on several other topics. Some of the main ones are transport in complex materials such as powders, particulates, and granules, characteristics of free surfaces and interfaces, accurate numerical modeling of combined mechanisms, multiple domains, and multiphase transport, and system instability. Experimental techniques are needed for practical materials which are often opaque and for measurements under high temperature and pressure. Similarly, numerical techniques are needed for large material property changes and for coupling the transport equations with the chemical kinetics which may involve several different reactions, with different reaction rates, activation energy, and other constants. Further development of new products, processes and systems on the basis of underlying thermal transport is needed. The design, control and optimization of the systems, as well as the selection of operating conditions, in order to achieve the desired processing needs further work.

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Nomenclature

b = temperature coefficient of viscosity, Eq. (17)
C_p = specific heat at constant pressure
$\underline{e}$ = unit vector in the direction of gravitational force
E = activation energy
Ec = Eckert number, Eq. (15)
f_l = liquid mass fraction
$\underline{F}$ = body force vector
g = magnitude of gravitational acceleration
Gr = Grashof number, Eq. (15)
h = convective heat transfer coefficient
H = enthalpy
H^o = enthalpy at 0 K
$\underline{i}$ = unit vector in x-direction
k = thermal conductivity,
K = bulk viscosity, reaction rate
K_c = consistency index for non-Newtonian fluid, Eq. (16)
L = characteristic length
L_h = latent heat of fusion
$\dot{m}$ = mass flow rate
n = power-law fluid index
N = speed in revolutions/min (rpm)
p = local pressure
Pr = Prandtl number, Eq. (15)
q = heat flux
q_v = dimensionless volume flow rate in a polymer extruder
$\dot{Q}$ = volumetric heat source
R = universal gas constant; radius
Re = Reynolds number, Eq. (15)
t = time
T = temperature
u, v, w = velocity components in x, y and z directions, respectively
U, U_s = speed of a moving solid or source
$\underline{V}$ = velocity vector
$\underline{x}$ = position vector
x, y, z = coordinate distances
X, Y, Z = dimensionless coordinate distances

Greek Symbols

α = thermal diffusivity
β = coefficient of thermal expansion
$\dot{\gamma}$ = strain rate
δ = location of interface between solid and liquid
ε = surface emissivity
λ = second viscosity coefficient
μ = dynamic viscosity of fluid
ν = kinematic viscosity
Φ = viscous dissipation function
ρ = density
θ = dimensionless temperature
τ = shear stress

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