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THERMAL PROCESSING OF MATERIALS: FROM BASIC RESEARCH TO ENGINEERING

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ABSTRACT

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, control 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, crystal growth for semiconductor fabrication, 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 and boundary conditions 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. Among the processes discussed here are polymer extrusion, optical fiber drawing, casting, continuous processing, and chemical vapor deposition for the fabrication of thin films. 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 involved with practical processes and systems is discussed in detail.

NOMENCLATURE

b	temperature coefficient of viscosity, Eq. (17)
Bi	Biot number, $Bi = hL/k_s$
c_m	species concentration
C_p	specific heat at constant pressure
$\bar{e}$	unit vector in the direction of gravitational force
E	activation energy
Ec	Eckert number, Eq. (15)
f_l	liquid mass fraction
$\bar{F}$	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
$\bar{i}$	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
p_a	hydrostatic pressure
p_d	dynamic pressure due to fluid motion
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)
Sr	Strouhal 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
$\bar{V}$	velocity vector
$\bar{x}$	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

Subscripts

a	ambient
b	barrel; wall
i	initial; inlet
l	liquid
m	melting point
o	reference
s	solid, surface

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 optimize the present processing techniques and improve the quality of the final product. Also, 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 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 thermal processing 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 . A range of processes is considered in order to discuss the basic aspects that arise and their effect on the processed material and on the system. Thus, the two main aspects that are considered in this paper are:

1. Basic heat and mass transfer phenomena underlying materials processing, including non-Newtonian, free surface, and surface tension driven flows, moving surfaces, transport with phase change and chemical reactions, transport in sprays, heat transfer under microgravity conditions, and other basic transport mechanisms that are of particular interest in this field.
2. Engineering aspects of materials processing, including the influence of thermal transport on the characteristics of the final product, in terms of consistency, uniformity, and quality, the rate of fabrication, and on the design and optimization of the system for the fabrication of traditional and advanced materials.

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 to develop, modify and improve systems to achieve desired goals, preferably under optimum conditions such as minimum cost.

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. The choice of an appropriate material for a given application is a very important consideration in the design and optimization of processes and systems, as discussed by Jaluria [1]. Thus, new techniques have been developed and are used along with the classical techniques of materials processing, such as heat treatment, forming and casting, to obtain the desired properties in the chosen material.

A few important materials processing techniques in which heat transfer plays a very important role are listed in Table 1.

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

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.

A few of these processes, in which heat transfer is of particular importance, 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 are available in the area of manufacturing and materials processing. However, most of these discuss important practical considerations and manufacturing systems relevant to the various processes, without a detailed consideration of the underlying thermal transport and fluid flow. See, for instance, the books by Schey [2] and Kalpakjian [3]. A few books do focus on the fundamental transport mechanisms in materials processing, for instance, the books by Szekely [4] and by Ghosh and Mallik [5]. The former considers fluid flow in metals processing and presents both the fundamental and applied aspects in this area. Specific manufacturing processes, as considered from a fundamental standpoint, are also presented in a few books, for instance, those by Altan et al. [6] and by Fenner [7]. In addition, there are several review articles and edited books on fluid flow and thermal transport in materials processing. Examples of these are the books edited by Hughel and Bolling [8], Kuhn and

Lawley [9], Chen et al. [10], Li [11], and Poulikakos [12], and the review article by Viskanta [13].

BASIC RESEARCH VERSUS ENGINEERING

Research in thermal materials processing is largely directed at the basic processes and underlying mechanisms, physical understanding, effect of different transport mechanisms, dominant considerations, effect of 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 and information on 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 control and 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. Automation and control are important for the satisfactory and safe performance of the given system. The results from the detailed design and optimization process are finally communicated to groups involved with the fabrication, sales and marketing. Several of these aspects, such as modeling, simulation and optimization, are discussed in greater detail later in this paper.

Basic Transport Considerations. Many important considerations arise when dealing with the thermal transport in the processing of materials, as given in Table 2.

TABLE 2
Some of the important considerations in heat transfer associated with 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

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. Also, experimental results are of critical value in validating mathematical and numerical models, as well in providing the physical insight needed for model development.

It must be noted that it is necessary for heat transfer researchers to thoroughly understand the concerns, intricacies and basic considerations that characterize materials processing in order to make a significant impact on the field. 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. This is the only way that research on heat transfer can stay at the cutting edge of technology in materials processing and significantly affect the future developments in this field.

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.

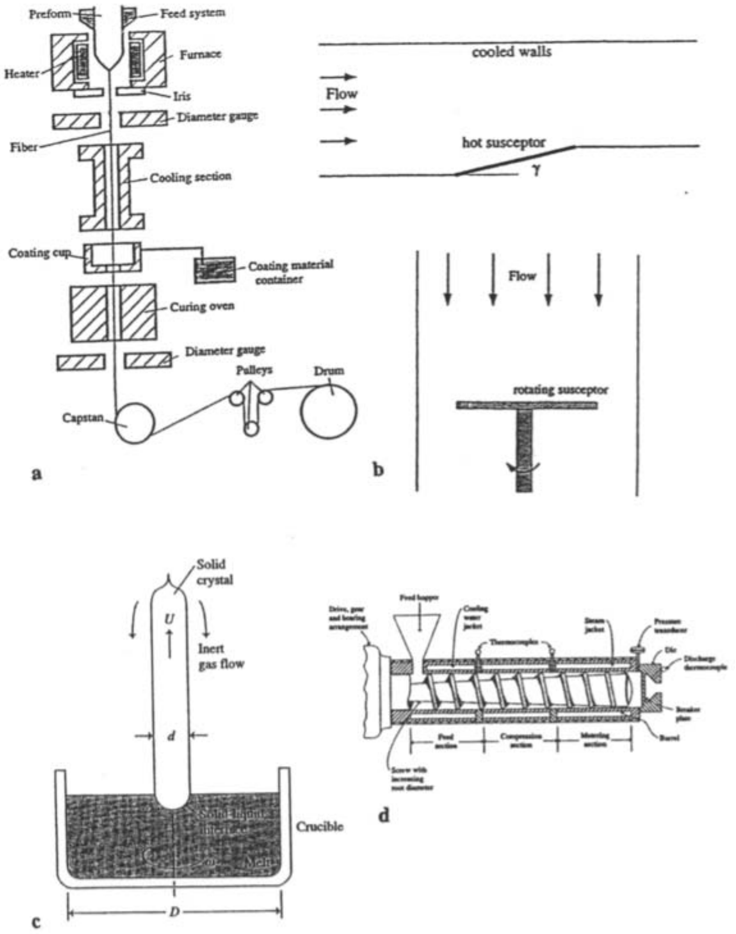


Fig. 1 Sketches of a few common manufacturing processes that involve thermal transport in the material being processed.
(a) Optical fiber drawing
(b) Chemical vapor deposition
(c) Czochralski crystal growing
(d) Plastic screw extrusion

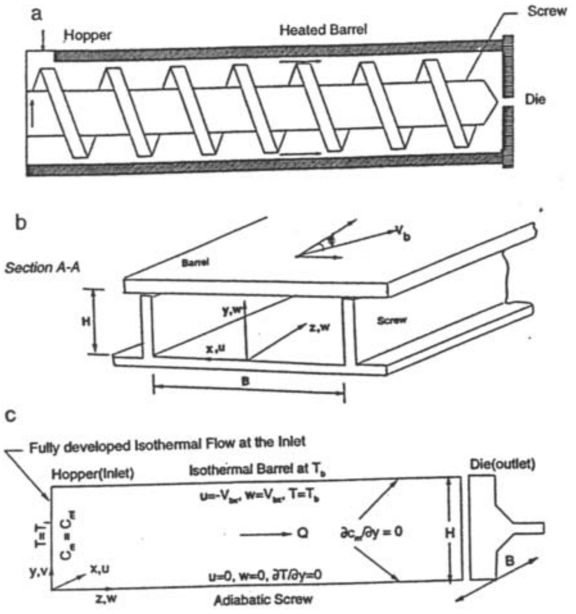


Fig. 4 Screw channel and simplified computational domain for a single-screw extruder.

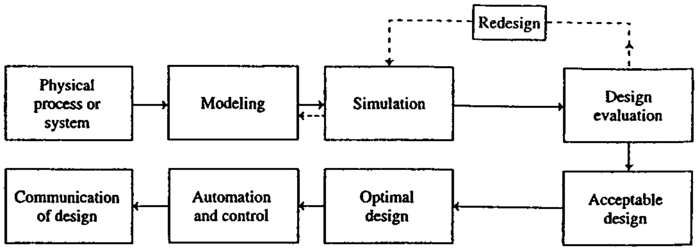


Fig. 2. Various steps involved in the design and optimization of a thermal system and in the implementation of the design.

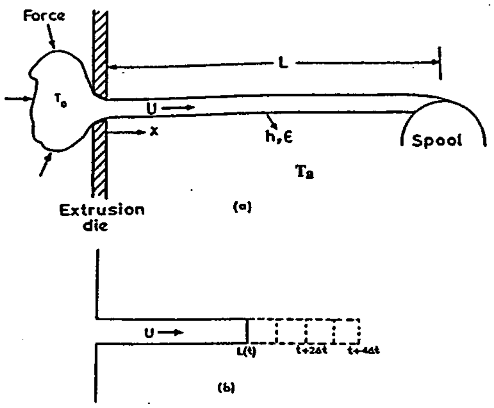


Fig. 3 (a) Sketch of the extrusion process for a heated material, (b) Moving material at different time intervals.

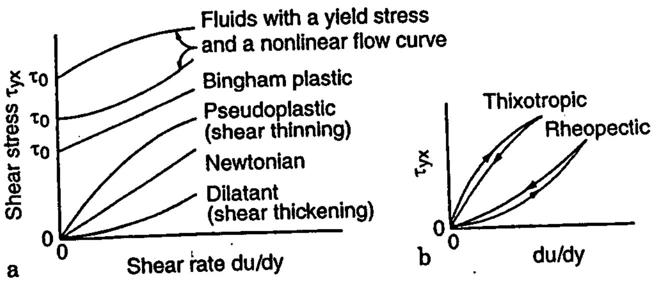


Fig. 5 Plots of shear stress versus shear rate for viscoinelastic non-Newtonian fluids. (a) Time-independent, and (b) time-dependent fluids.

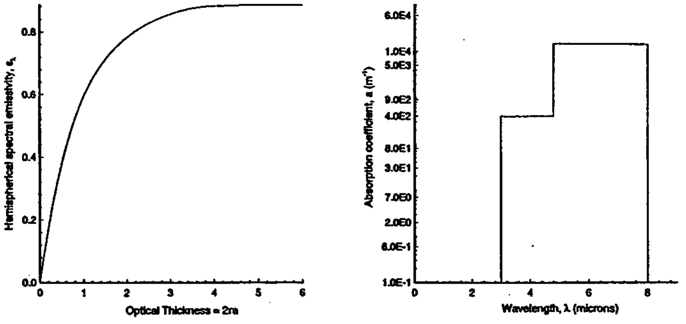


Fig. 6 Dependence of (a) hemispherical spectral emissivity on optical thickness and (b) absorption coefficient on wavelength for a two-band spectral model for silica glass.

The model may be *descriptive or predictive*, the former being used to describe and explain various physical phenomena. Predictive models can be used to predict the performance of a given system and are of particular interest in engineering design. There are four main types of predictive models that are of interest in the design and optimization of thermal systems. These are:

1. Analog models
2. Mathematical models
3. Physical models
4. Numerical models

Analog models use available results from another area to solve the problem at hand by using the analogy between the two, such as the analogy between heat and mass transfer. 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 experimental models, if needed. A physical model is one that resembles the actual system and is generally used to obtain experimental results on the behavior of the system.

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. Only very simple cases can usually be solved by analytical procedures and numerical techniques are needed for most practical systems. Numerical modeling refers to the restructuring and discretization of the governing equations in order to solve them on a computer.

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

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

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

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

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

For a solid, the energy equation is written as

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

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 $\bar{V}$ if the material characteristics are known. For instance, if μ is taken as constant for a Newtonian fluid, the relationship between the shear stresses and the shear rates, given by Stokes, are employed to yield

$$\rho \frac{D\bar{V}}{Dt} = \bar{F} - \nabla p + \mu \nabla^2 \bar{V} + \frac{\mu}{3} \nabla (\nabla . \bar{V}) \qquad (5)$$

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

Buoyancy Effects. The body force $\bar{F}$ is also 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

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

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 [14] and Gebhart et al. [15]. 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 and the solution is more involved. The governing equations are coupled because of the buoyancy term in Eq. (6) and must be solved simultaneously [16].

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

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

Similarly, expressions for other coordinate systems may be obtained. This term becomes important for very viscous fluids and at high speeds. The former circumstance is of particular interest in the processing of glass, plastics, food, and other polymeric materials.

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 and appropriate discretization of the two regions may be carried out [12, 17]. This becomes fairly involved since the interface location and shape must be determined for each time step or iteration. The governing equations are the same as those given earlier for the solid and the liquid.

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

$$\rho \frac{DH}{Dt} = \rho \frac{\partial H}{\partial t} + \rho \bar{V} . \nabla H = \nabla.(k \nabla T) \qquad (8)$$

where each of the phase enthalpies H_i is defined as

$$H_i = \int_0^T C_i \, dT + H_i^o \qquad (9)$$

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

$$H_s = C_s T \qquad H_l = C_l T + [(C_s - C_l) T_m + L_h] \qquad (10)$$

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

$$H = H_s + f_l (H_l - H_s) \qquad k = k_s + f_l \ (k_l - k_s) \qquad (11)$$

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 [18-20]. 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 food materials and other chemically reactive materials substantially alter the structure and characteristics of the product [21, 22].

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 [23]

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

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

$$\tilde{X} = \frac{M_i - M_t}{M_i - M_f} \qquad (13)$$

Here M_i is the initial amount of unconverted material, taken as starch here in [23], M_f is the final amount of unconverted starch and M_t is the amount of unconverted starch 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 [24, 25]. The concentrations of the chemical species in the reactor affect the chemical kinetics, which in turn affect the deposition.

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. Some of these have been mentioned in the preceding section. A general procedure may be adopted to obtain the usual simplifications in analysis [1]. These include considerations of transient versus steady-state transport, number of spatial dimensions needed, possible lumped mass approximation, simplification of boundary conditions, neglecting relatively small effects, idealizations such as isothermal or uniform heat flux conditions, characterization of material properties and use of the relevant conservation laws.

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 the no-flow circumstance at the ambient temperature, representing the situation before the onset of the process. For periodic processes, the initial conditions are arbitrary. However, a few special considerations arise for certain materials processing techniques. Some of these are discussed here.

At a free surface, the shear stress is often specified as zero, yielding a Neumann condition of the form $\partial \bar{V} / \partial n = 0$, if negligible shear is applied on the surface. If the shear stress exerted by the ambient fluid is significant, it replaces the zero in this equation. Basically, 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. [26] 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 $\bar{V} \to 0$, $T \to T_a$ as $n \to \infty$. However, frequently the condition $\partial \bar{V} / \partial n \to 0$ 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 $\bar{V}$ [27]. The gradient conditions allow the flow to adjust to ambient conditions more easily, without forcing it to take on the imposed values at a chosen boundary. This consideration is important for simulating openings in enclosures, commonly encountered in furnaces and ovens.

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 [17]. For a stationary interface, as is the case in crystal growing shown in Fig. 1(c) and for continuous casting, the appropriate boundary condition has been given by Siegel [28, 29].

Other Simplifications. In the case of material flow in a moving cylindrical rod or plate for extrusion or hot rolling, as sketched in Fig. 3, 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, $x = 0$, i.e., for large time, and if the boundary conditions are steady. Transient problems arise for small lengths of the rod at a short time following the onset of the process, and for boundary conditions varying with time [30, 31].

Similarly, coordinate transformations can be employed to convert transient problems to steady state ones in other circumstances. For instance, a moving thermal source at the surface of an extensive material gives rise to a transient circumstance if the coordinate system is fixed to the material. However, a steady state situation is obtained by fixing the origin of the coordinate system at the source. If x is measured in the direction of the source movement from a coordinate system fixed on the material surface and U is the velocity of the point source, the transformation used is $\xi = x - Ut$, which yields steady transport in many practical circumstances, such as welding and laser cutting.

In the case of a single-screw extruder, shown in Fig. 4, 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 pressure and shear driven channel flow, with shear arising due to the barrel moving at the pitch angle over a stationary screw. This is similar to the shear and pressure driven channel flow available in the literature. Therefore, this approximation substantially simplifies the mathematical/numerical model.

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

$$Sr = \frac{L}{V_c\, t_c} \;,\; Re = \frac{V_c\, L}{\nu} \;,\; Gr = \frac{g\, \beta\, (T_s - T_a)\, L^3}{\nu} \;,$$

$$Pr = \frac{\nu}{\alpha} \;,\; Ec = \frac{V_c^2}{C_p\, (T_s - T_a)} \tag{15}$$

where V_c is a characteristic speed, L a characteristic dimension, and t_c a characteristic time. It is often convenient to apply different nondimensionalization to the solid and fluid regions. The dimensionless equations may be used to determine the various regimes over which certain simplifications can be made. For instance, highly viscous flow usually gives rise to very small Reynolds numbers, for which the creeping flow approximation is often employed. The Reynolds number Re is generally much smaller than 1.0 for plastic and food flow in a single screw extruder and the inertia terms are usually dropped. At large Re, boundary layer approximations can be made to simplify the problem. At very small Prandtl number Pr, the thermal diffusion terms are relatively large and yield the conduction-dominated circumstance, which is often applied to the flow of liquid metals in casting, soldering and welding. A small value of Gr/Re^2 implies negligible buoyancy effects, for instance, in continuous casting where the effect of buoyancy on the transport in the melt region may be neglected. A small value of the Eckert number Ec similarly implies negligible pressure work effects and a small value of Ec/Re can be used to neglect viscous dissipation. Therefore, the expected range of the governing parameters such as Re, Gr, Pr, Sr, and Ec can be employed to determine the relative importance of various physical mechanisms underlying the transport process. This information can then be used to simplify the relevant governing equations and the corresponding modeling.

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 [32, 33]. Similar approaches are used to interpret and characterize experimental data. However, such an approach is satisfactory only for small ranges of the process variables. 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. Figure 5 shows the variation of the shear stress τ_{yx} with the shear rate du/dy for a shear flow such as the flow between two parallel plates with one plate moving at a given speed and the other held stationary. 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. Viscoelastic fluids show partial elastic recovery on the removal of a deforming shear stress. Food materials are often viscoelastic in nature.

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 [34]

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

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 [34]

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

where

$$\dot{\gamma} = \left[\left(\frac{\partial u}{\partial y} \right)^2 + \left(\frac{\partial w}{\partial y} \right)^2 \right]^{1/2}$$

with $$\tau_{yx} = \mu \frac{\partial u}{\partial y}, \; \tau_{yz} = \mu \frac{\partial w}{\partial y} \qquad (18)$$

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. Other expressions for the viscosity may be used to consider other reactive and non-reactive polymeric materials. 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 [35-37].

Glass is another very important, though complicated, material. It is a supercooled liquid at room temperature. The viscosity varies almost exponentially with temperature. In optical fiber drawing, for instance, the viscosity changes through several orders of magnitude in a relatively short distance. Even a change of a few degrees in temperature in the vicinity of the softening point, T_m, which is around 1600 ^{o}C for fused silica, can cause substantial changes in viscosity and thus in the flow field and the neck-down profile. This can lead to a significant effect on defect generation in the fiber and thus on fiber quality [26, 38, 39]. An equation based on the curve fit of available data for kinematic viscosity ν is written for silica, in S.I. units, as

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

indicating the strong, exponential, variation of ν with temperature. The other properties vary much more gradually with temperature.

In glass, the heat transfer is further complicated by the fact that it 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, as shown in Fig. 6, has been used extensively for studying the thermal transport in the neck-down region of a furnace-drawn optical fiber [40, 41]. Since the process and the quality of the optical fiber are strongly influenced by the heat transfer and the temperature distributions in the material, it is critical to obtain accurate absorption coefficient data and use these in the modeling.

There are several other important considerations related to material properties. Constraints on the temperature level in the material, as well as on the spatial and temporal gradients, arise due to the characteristics of the material. In thermoforming, for instance, the material has to be raised to a given temperature level, above a minimum value T_{min}, for material flow to occur in order for the process to be carried out. However, the maximum temperature T_{max} must not be exceeded to avoid damage to the material. In polymeric materials, $T_{max} - T_{min}$ is relatively small and the thermal conductivity k is also small, making it difficult to design a process, which restricts the temperature to T_{max} while raising the entire material to above T_{min} for material structural changes to occur. An example of this process is the manufacturing of plastic-insulated wires, as considered by Jaluria [42]. Similarly, constraints arise due to thermal stresses in the material undergoing thermal processing. Such constraints are particularly critical for brittle materials such as glass and ceramics. The design of the manufacturing system is then governed by the material constraints.

Link Between Transport Processes and Material Characteristics

The preceding discussion brings out the importance of material properties in a satisfactory mathematical and numerical modeling of thermal manufacturing processes, as well as for accurate interpretation of experimental results. The properties of the material undergoing thermal processing must be known and appropriately modeled to accurately predict the resulting flow and transport, as well as the characteristics of the final product. However, this latter aspect is an area in which there is acute lack of data and critical work is needed in the future.

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. Thus a study of the transport processes can, in principle, lead to a determination of the physical and chemical properties of the final product. 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. Additional diagnostics may also be undertaken to link important properties like strength, porosity, defects, and ductility of the product with the thermal transport.

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 nano-meter 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 nano-structure 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 experiments carried out to characterize such structures and growth [43, 44]. For instance, Fig. 7 shows equiaxed and columnar denritic crystals. Averaging volumes and dendrite envelopes that may be used for modeling of the microscopic phenomena are shown.

Similarly, detailed experimental work on the chemical conversion of starches has been carried out [23]. 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

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

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. (12), as given by [45, 46]

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

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. [47] 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, part of the defects recombine to form Si-O again. The net concentration of the E' defects is the difference between the generation and the recombination. 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, $\nu *$ 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. The values of E_p, E_d, $\nu *$ and $n_p(0)$ are all given by [47, 48] and may be used to calculate the distribution of these defects in the fiber [49].

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 for further machining and forming operations. The thermal processing involves heating of the material to the annealing temperature of around 723 ^{o}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 processing time [50, 51]. The typical temperature cycle undergone by a material is shown in Fig. 8.

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 is a fairly difficult problem, which 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. By generating extensive simulation results, an attempt is often made to solve the inverse problem by correlating the outputs with the inputs. An interesting inverse problem was solved by Issa et al. [52] to determine the furnace wall temperature distribution in an optical fiber drawing furnace, which would yield a measured temperature distribution in a glass or graphite rod in the furnace. An optimization strategy was used to obtain a solution that was in a very narrow range of the variables and could thus be taken as essentially unique.

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

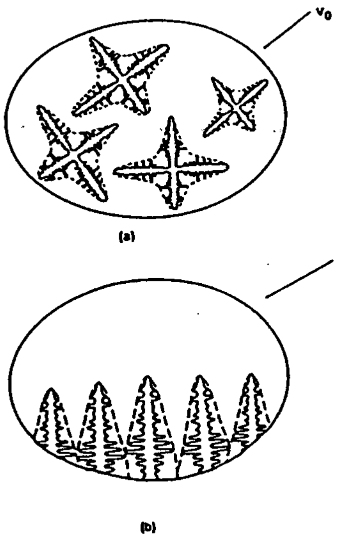


Fig. 7 Schematic illustration of the averaging volume and the dendrite envelopes for (a) equiaxed growth, and (b) columnar growth [43].

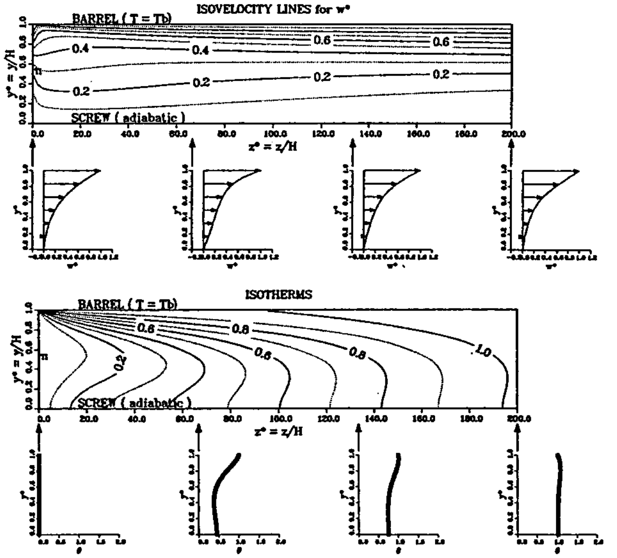


Fig. 9 Calculated velocity and temperature fields in the channel of a single screw extruder at n = 0.5 and dimensionless throughput $q_V = 0.3$, for typical operating conditions.

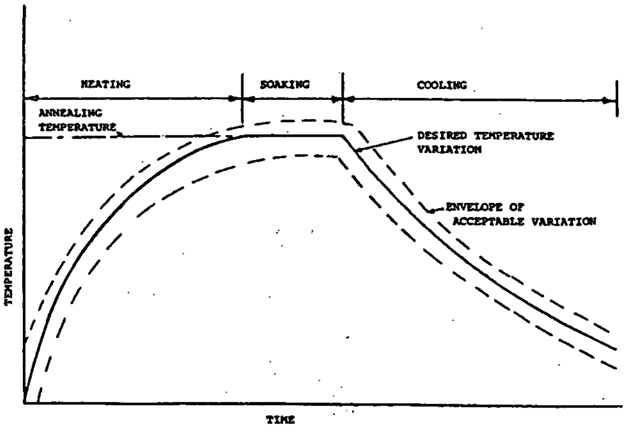


Fig. 8 Typical temperature cycle of the annealing process.

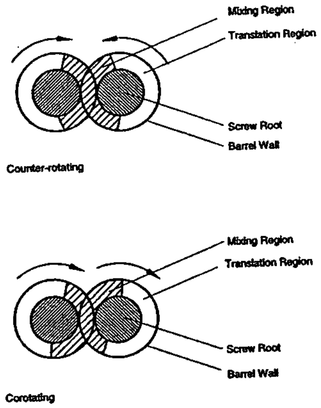


Fig. 10 Schematic diagram of the cross-section of a tangential twin screw extruder, showing the translation (T) and intermeshing, or mixing (M), regions.

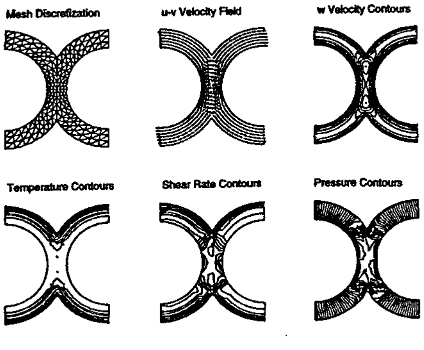


Fig. 11 Mesh discretization for the mixing region in a co-rotating tangential twin screw extruder, along with typical computed results for low density polyethylene (LDPE) at n = 0.48, $T_b = 320\ ^oC$, $T_i = 220\ ^oC$, N = 60 rpm, $q_V = 0.3$.

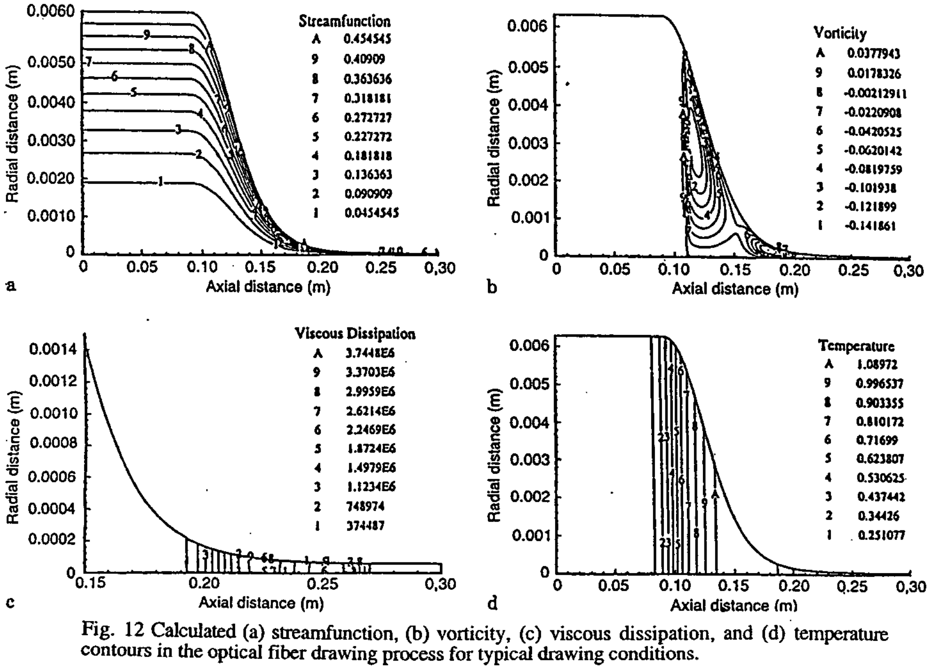


Fig. 12 Calculated (a) streamfunction, (b) vorticity, (c) viscous dissipation, and (d) temperature contours in the optical fiber drawing process for typical drawing conditions.

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. In addition, certain simple components can be idealized to obtain quantitative results by analysis.

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 seen in Fig. 4. 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 flow is known as drag, or shear-driven, flow and arises only due to the viscous effect of the wall moving at velocity U_s. For Newtonian fluids, 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, the fully developed flow in a die may be analyzed. 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. [53] for a power-law non-Newtonian fluid as

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

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, without significant error, for relatively long cylindrical regions in practical dies [54]. Expressions for a conical die and for an orifice were also given by Kwon et al. [53].

Numerical

The numerical solution of the governing equations is based on the extensive literature on computational heat transfer [16, 55], with the most commonly employed technique being the SIMPLER algorithm, given by Patankar [56], 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 [16]. 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 [57]. 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 [56]. 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 [58]. Under-relaxation is generally needed for convergence due to the strong nonlinearities that arise in these equations mainly due to property variations.

As mentioned earlier, major difficulties arise in material processing simulations due to the complexity of the computational domain as well as that of the boundary conditions. Finite element and boundary element methods have been used advantageously to simulate a wide variety of material processing systems. Finite difference and finite volume methods have also been used, often with coordinate transformations to convert the complex domains into much simpler forms so that the discretization is simplified.

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.

Though validation of mathematical and numerical models is often considered as the main reason for experimentation, 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. Also, there are many circumstances where experimentation is either the most convenient or the most dependable and accurate approach. This is particularly true for characterizing the material, determining the product quality, obtaining the characteristics of components like heat exchangers, pumps and blowers, and obtaining transport rates from complex bodies and surfaces.

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 4. The basic problem is complicated because of the strong variation of the viscosity with the temperature and the shear rate, complex geometry, large viscous dissipation, and the coupling between the momentum and energy equations. 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 9 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 [34, 35] .

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 residence time distribution is a function of the flow field and can be numerically simulated by particle tracking. Several results are given in the literature on RTD for different extruders [22, 35, 59]. 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. 10. 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 [60]. A major simplification in the numerical simulation is obtained by diving the flow into two regions: the translation, or T region, and the mixing, or M region, as sketched in Fig. 10. 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. For further details on this model for the twin screw extruder and on the numerical scheme, see [60-62]. The finite-element method is particularly well suited for the modeling of the complex domain in a twin-screw extruder. Figure 11 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 [63, 64]

Optical Fiber Drawing

The optical fiber drawing process has become critical for advancements in telecommunications and networking. As mentioned earlier, the viscosity of glass, which is a supercooled liquid, is a very strong function of temperature. At its softening point, the viscosity is still quite high, being of the same order as that of polymer melts considered previously. Thus, viscous dissipation is important and the momentum and energy equations are coupled. However, glass flow may be treated as Newtonian at typical draw speeds.

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. This places stringent demands on the analysis and the numerical simulation. 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 [65]. Interest lies in obtaining high quality optical fibers, 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. 12 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 ^{o}C arise across the fiber for preform diameters of around 2.0 cm. Larger temperature differences arise for a larger preform diameter [49]. 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. Further details on this problem may be obtained from [38, 39, 66].

The determination of the neck-down profile of the glass preform as it is drawn into a fiber is a particularly difficult problem, since it involves modeling the free surface flow of glass under large variations in temperature, viscosity and cross-sectional area. Relatively simple models had been employed in the past to study the flow in this region [66]. 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 [26]. Axisymmetric, laminar flows were assumed in the glass and in the circulating inert gases. The transport equations were solved by finite difference methods. 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. 13 (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. 13 (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 [49, 67, 68].

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, and finally the fiber is spooled around a take-up drum at the base of the draw tower. All these processes have also been investigated in several studies with respect to providing adequate distance for cooling and controlling the thickness, quality and the concentricity of the coating layer [69-72].

Casting

Casting is an important manufacturing process, which involves solidification and melting. Several other materials processing techniques, such as crystal growing, welding, and polymer injection molding, involve phase change processes and, therefore, solidification and melting have been studied extensively, considering pure materials as well as mixtures such as alloys [73-75]. The buoyancy-driven flow due to temperature and concentration differences in the liquid or melt region is coupled with the conduction in the solid, though earlier studies neglected the convection effects. 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 [17, 19, 76]. Several other techniques have been developed to treat such moving boundary problems and the complicated domains that arise. 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 *apriori a*nd 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 [19, 77]. 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 consideration in these problems [78]. 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. [79] carried out numerical simulations and appropriately designed experiments to demonstrate the importance of conduction in the wall, as shown in Fig. 14. 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 [75]. Similarly, solidification in polymers is of interest in various processes [80]. For instance, in injection molding, the molten polymer is injected under pressure into a mold and, after the mold is filled, the material is allowed to cool and thus solidify. Solidification in extrusion dies and in channels leading to a mold must be avoided since it affects the polymer flow and the pressure due to the resulting blockage. Combined heat and mass transfer processes arise in these cases and significantly affect the thermal transport and the product quality.

Continuous Processing

Continuously moving materials undergoing thermal processing are frequently encountered in manufacturing processes like hot rolling, wire drawing and extrusion. The cooling of a moving optical fiber before coating is an example of such processing. If the location of the moving surface is known, as is the case for the circumstance of Fig. 3 (b), the continuous movement of the edge may be replaced by discrete steps, so that the length L is held constant over a time increment Δt, with the

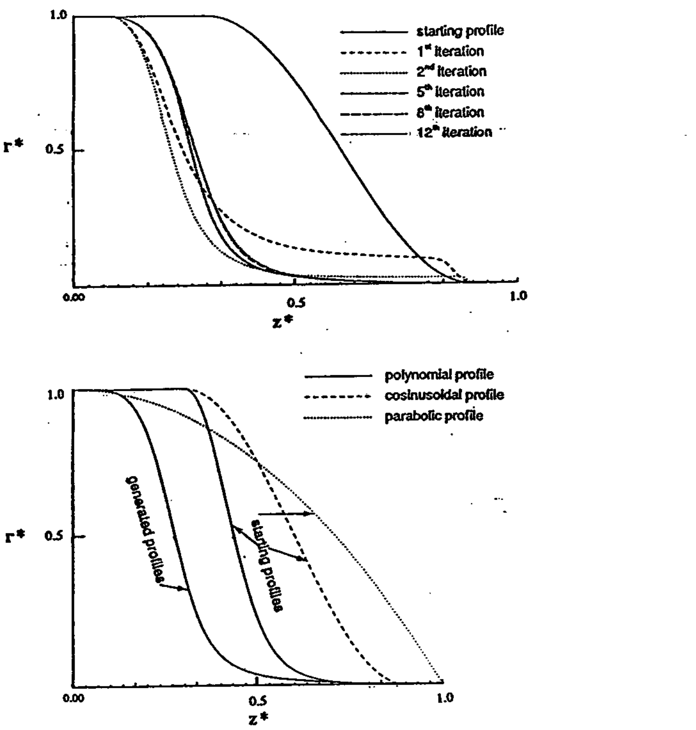


Fig. 13 Iterative convergence of the neck-down profile in optical fiber drawing. Here, r* = r/R and z* = z/L, where R is the preform radius and L the furnace length.

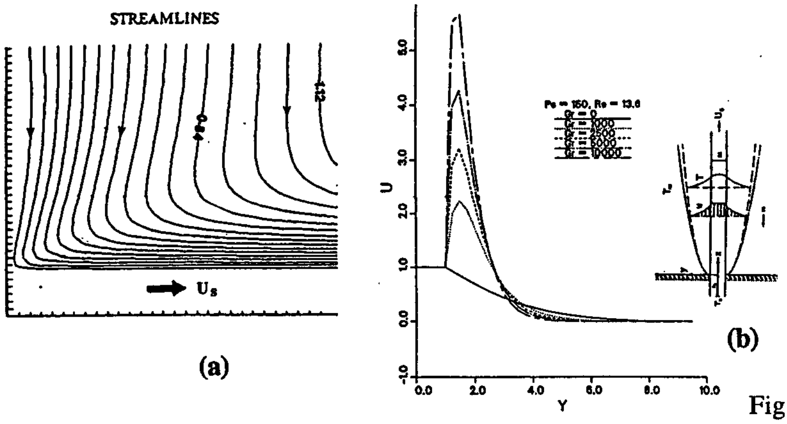


Fig. 15 (a) Flow in the ambient fluid due to a continuously moving material; (b) Dimensionless velocity (u/U_S) distribution in the fluid due to a vertically moving heated plate with aiding buoyancy effects.

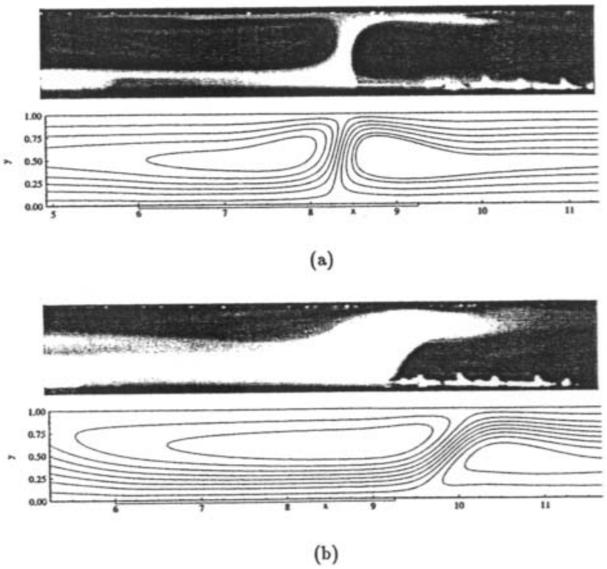


Fig. 17 Comparison between experimental observations and numerical predictions of streamlines at Re = 9.48 and Re = 29.7 for a ceramic susceptor.

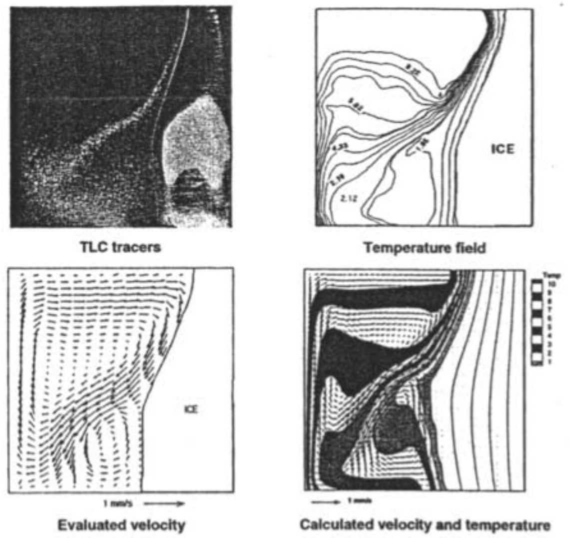


Fig. 14 Experimental and numerical results for water solidification driven by convection and conduction [79].

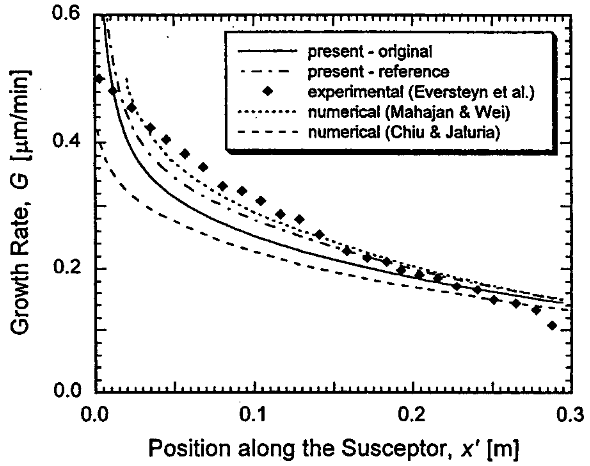


Fig. 16 Comparisons between the numerical results on predicted film growth rate and the experimental data of [87].

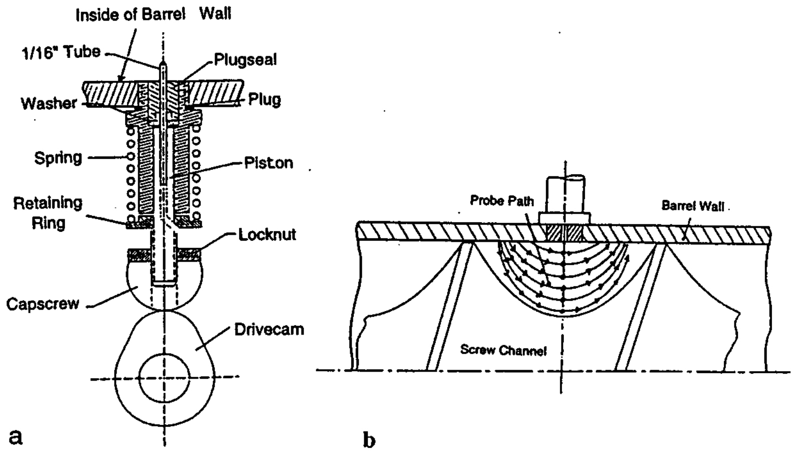


Fig. 18 (a) Cam-driven thermocouple for temperature measurements in the screw channel; (b) representation of the loci of points where temperature data are collected. [107, 108].

transient conduction problem being solved over this interval. The length L is then taken at the increased value for the next time interval, with the additional finite region adjacent to the base taken at temperature T_o, and the computation is carried out over this interval. The procedure is carried out until results are obtained over a specified time or until the steady state circumstance is obtained [27]. Then, the corresponding initial and boundary conditions are obtained as:

$$t = 0: \quad L(t) = 0$$

$$t > 0: \text{ at } x = 0, \; T = T_o; \;\; \text{at } x = L(t), \; -k\,\frac{\partial T}{\partial x} = h_L(T-Ta) \tag{25}$$

where h_L is the heat transfer coefficient at the edge of the moving rod. The problem may be solved analytically [31] 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. The problem may then also be solved as a steady, continuously moving, infinite rod.

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 [81]. 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. In practical systems, interest lies in controlling the local processing of the material in order to obtain uniformity, desired product characteristics and high productivity.

Figure 15 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 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, addition of externally induced flow for enhanced cooling, 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 amorphous layer on the substrate. This technique has become quite important in materials processing and is used in a wide range of applications, such as those in the fabrication of microelectronic circuits, optical and magnetic devices, high performance cutting and grinding tools, and solar cells. 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 [25, 82, 83]. The flow, heat transfer and chemical reactions in CVD reactors have been investigated by several researchers [82-86]. Some typical results obtained for silicon deposition are shown in Fig. 16, indicating a comparison between numerical and experimental results from [87]. A fairly good agreement is observed, given the uncertainty with material property data and with the chemical kinetics. The two results from [86] refer to two different values of the diffusion coefficient, the one labeled as the reference case employs the same values as those in [88].

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. [89] on the heat transfer in a horizontal channel with a finite heated region to approximate the susceptor. Figure 17 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 uniformity of the deposition.

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.

Crystal growing is a very important area since most semiconductor devices are fabricated from single crystals grown from the vapor phase or from the melt. The former process generally involves sublimation and chemical transport in a sealed enclosure [90] and the latter was mentioned earlier, with the Czochralski process shown in Fig. 1(c). Several 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 been developed [91, 92]. The Czochralski method has dominated the production of single crystals for microelectronics and has been the subject of considerable research interest over more than three decades [91, 93, 94]. The transport phenomena involves buoyancy-driven convection in the liquid due to temperature and concentration differences, forced and mixed convection because of moving solid surfaces, thermocapillary flows because of surface tension gradients, phase change, and heat and mass transfer processes. The basic concerns are similar to those in casting and other phase-change processes. The transport processes affect the quality of the crystal through oscillations, instability, and distribution of impurities. Silicon crystals have been of particular interest in the fabrication of electronic devices. However, there has been growing interest in materials like GaAs, InP and other compounds because of their use in various electro-optic applications.

In the recent years, there has been considerable interest in thermal materials processing under microgravity conditions. Such an environment is 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. Similarly, gravity plays an important role in determining the shape of the meniscus in the fiber coating process and of the neck-down profile in optical fiber drawing. Thus, by controlling the gravitational force, the resulting transport processes and the final product can be improved [95, 96]. Many papers have focused their attention on crystal growing processes and additional aspects, such as bubble migration, film deposition and deforming interfaces, have also been investigated [97, 98]. Such efforts are in progress and are expected to lead to a much better understanding of materials processing under microgravity conditions.

Another area, which has received considerable attention, is that of thermal sprays 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 macro-segregation, which weakens traditionally cast materials [99]. Superior properties associated with fine-grained microstructures and non-equilibrium phases are usually obtained. Several materials, such as aluminum, tin, and different alloys have been employed in the droplet-based manufacturing process. The process involves generating the droplets, convective flow in the spray, droplet impact and deformation, and rapid solidification [100-102]. Plasmas are used for fabricating ceramics, particularly nanostructured ceramics [103].

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 simplifications and idealizations usually needed to make the problem amenable to a solution, lack of accurate material property data, uncertainly in material characterization, combined mechanisms that affect the transport and the product, and other complexities in the process. As discussed earlier, modeling is needed for a basic understanding of the processes involved, as well as for providing accurate inputs for system design, control and optimization. However, it is important to ensure that the numerical code performs satisfactorily for the chosen method and that the model is an accurate representation of the physical problem. These aspects are sometimes referred to as verification and validation, respectively, or simply as validation of the numerical model employed. Unless the models are satisfactorily validated and the accuracy of the predictions established, the models cannot be used as a basis for design and for choosing operating conditions for desired product characteristics. 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, comparisons with available analytical results for simpler configurations, comparisons with numerical results in the literature, and comparisons with experimental results on the process and on a prototype, if available [104]. Several international symposia have been devoted to the validation of numerical models [105]. Specific problems, such as buoyancy-induced flow in an enclosure and shear-driven cavity flow, have also been chosen as benchmark exercises and computational solutions obtained by different researchers on these problems have been compared to establish benchmark results. In several cases, it is necessary to design and carry out suitable experiments in order to validate the mathematical and numerical modeling of the given thermal material processing method. A few examples are presented here on experimental validation.

Polymer Extrusion. Measurements on the temperature and velocity distributions in an extruder channel is 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 inlet, residence time distribution, total heat input, characteristics of the extrudate, total torque exerted on the screw, and flow rate, are available in the literature [21, 34, 106]. 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. Sernas and co-workers [107, 108] have carried out innovative, well-designed, well-controlled, and accurate, experiments on single-screw extruders.

A specially designed single screw extruder was used for these experiments. A Plexiglas window was fitted at the measuring ports to provide optical access to the flow to observe if the screw channel was completely filled with the extrudate. The barrel was subdivided into three sections, which were maintained at different uniform temperatures. The pressure and temperature were measured at several down-channel locations. The measurement of the temperature profile in the screw channel is complicated because of the rotating screw. A cam-driven thermocouple system, as shown in Fig. 18 (a), was installed on the extruder in order to allow the thermocouple probe to travel in and out of the channel in a synchronized motion linked to the screw rotation. The probe moved a preset distance into the channel as the flights traverse due to screw rotation. The loci of points where data were taken are sketched in Fig. 18 (b). A considerable amount of effort and care was involved in extracting the appropriate data for the temperature profiles.

A few experimental results for Viscasil-300M, which is a non-Newtonian fluid, are shown in Fig. 19, along with numerical results from two-dimensional finite volume and three-dimensional finite element calculations [37, 109]. 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 needed to simulate this recirculation and the results are close to the experimental data. A good agreement between the experimental and predicted pressure and temperature at the die was also obtained, providing strong support to the model.

Similarly, experiments have been carried to validate models for twin-screw extrusion, particularly the approach of combining alternating translation and intermeshing regions, as sketched in Fig. 10 and discussed earlier. 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 [110]. Experimentally and numerically obtained streamlines in the region between two rotating cylinders, approximating a twin-screw, are shown in Fig. 20, indicating good agreement. Some of the fluid flowing adjacent to the left cylinder continues to flow along its surface, while the remaining flows over to the other cylinder. A flow division ratio x_f, defined as the fraction of the mass flow that crosses over from one channel to the other, is taken as a measure of mixing and is determined by using the dividing streamline that separates the two fluid streams. A comparison between experimental and numerical results is shown, indicating good agreement at the typically small Reynolds numbers encountered in extruders. A small difference, between numerical and experimental results, arises as Reynolds numbers increase beyond 1.0, because of significant inertia effects, which are neglected in the mathematical model.

Measurement of the velocity distribution in the channel is also very involved because of the complex geometry and rotating screws. Karwe and co-workers [111, 112] 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. 21 (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. 21 (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. Various other comparisons between experimental data and numerical predictions, particularly on pressure and RTD, can also be used to validate the model [113].

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 [52, 66]. Most efforts have been directed at the practical issue of fiber characteristics for different operating conditions such as furnace wall temperature, draw speed and applied tension. Only a few results are available that may be used for quantitative comparisons with numerical predictions. Paek and Runk [114] 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 [26] and compared with the experimental results, as shown in Fig. 22 (a). The analytical results obtained by Paek et al. [115] showed that the draw tension plotted on a 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. 22 (b). Similarly, other comparisons have been made on the profile and the draw tension. These comparisons with experimental results lend strong support to the mathematical and numerical model.

Casting. As mentioned earlier, very few detailed experimental results are available on the solidification process that can be used for validating the models. 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 23 shows the experimental results and corresponding numerical predictions on the liquid-solid interface location, for melting of pure tin, using the enthalpy model [116, 117]. Though these results are found to agree quite well, further detailed comparisons are needed to improve existing models.

Similarly, experimental validation of mathematical and numerical models for thermal processing of materials has been undertaken for various other manufacturing methods, such as chemical vapor deposition, continuous processing, heat treatment and coating. Even though validation is an expensive and time-consuming process, it is a critical step in the overall simulation and design process to improve existing processes, develop new techniques, and control product characteristics.

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. The numerical simulation of the system refers to the use of numerical modeling to obtain quantitative information on behavior and characteristics of the thermal materials processing system for given design parameters and set of operating conditions, as well as and for changes in these quantities.

Consider, for instance, a typical electrical furnace, which consists of the heater, walls, insulation, enclosed gases and the

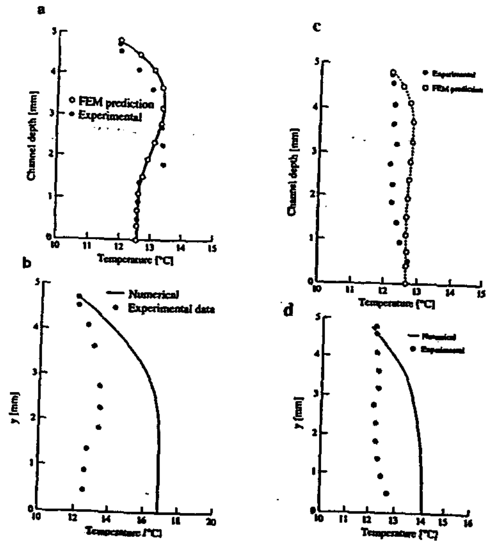


Fig. 19 Comparisons between numerical and experimental results on temperature profiles for Viscasil-300M, with (a) and (c) from the 3D (FEM) model and (b) and (d) from the 2D (FDM) model. For (a) and (b): T_i = 20.3 °C, T_b = 12.2 °C, N = 20. For (c) and (d): T_i = 18.8 °C, T_b = 22.3 °C, N = 35.

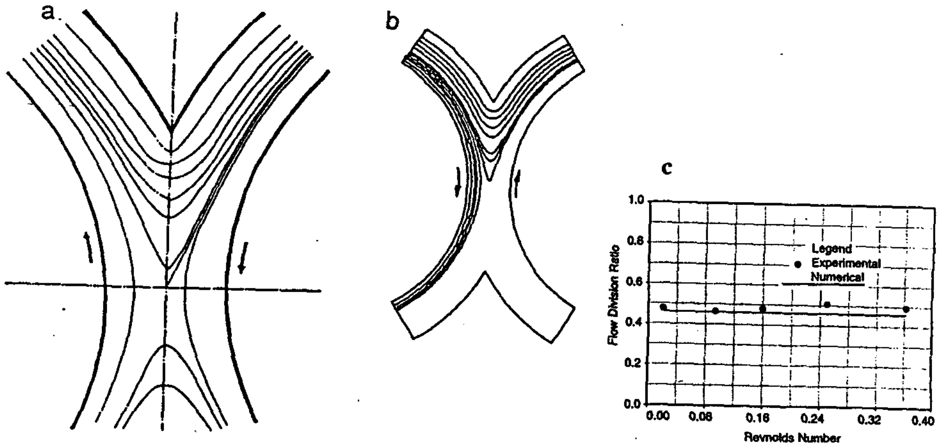


Fig. 20 Streamlines in the region between two rotating cylinders for CMC solution at 16 rpm. (a) Experimental results; (b) Numerical predictions for flow entering the region over one cylinder; (c) Comparison of flow division ratio x_f obtained from experimental and numerical results [57].

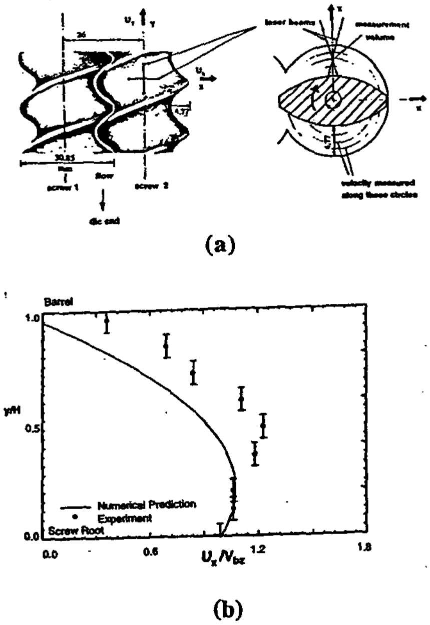


Fig. 21 (a) Experimental arrangement for velocity measurements in the flow of corn syrup a twin-screw extruder; (b) comparison between calculated and measured tangential velocity U_X profiles for isothermal heavy corn syrup at 26.5 °C, with mass flow rate of 6 kg/hr and screw speed of 30 rpm.

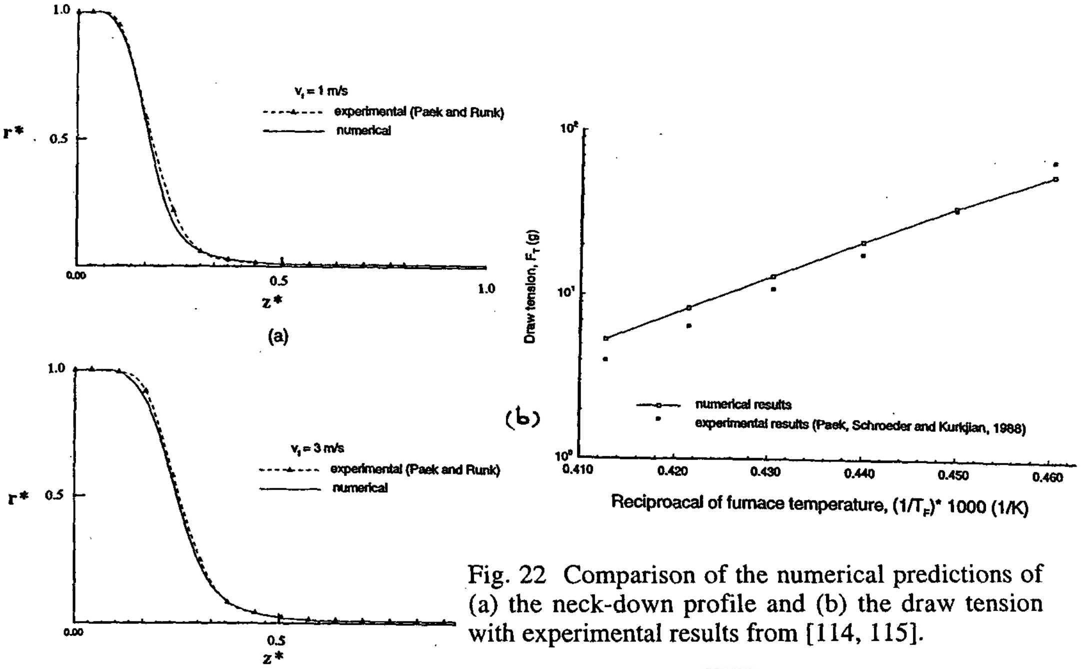


Fig. 22 Comparison of the numerical predictions of (a) the neck-down profile and (b) the draw tension with experimental results from [114, 115].

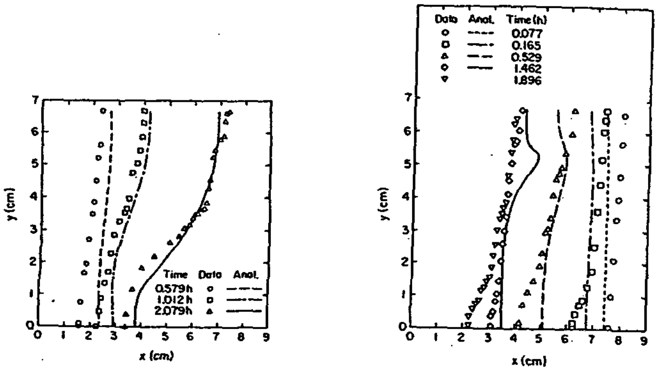


Fig. 23 Comparison between measured and predicted interface locations during (a) melting, and (b) soldification of pure tin from a vertical surface [116, 117].

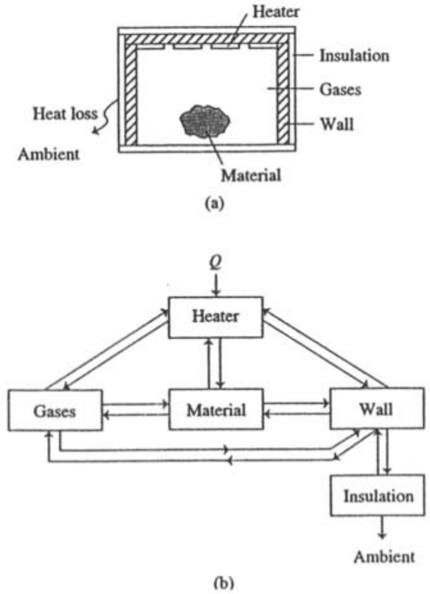


Fig. 24 (a) Sketch of an electric furnace; (b) Information-flow diagram showing the coupling between different parts of the system.

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. Figure 24 shows a sketch of this simple system and the information-flow diagram that indicates the coupling between the different parts. 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 [1, 16]. Similarly, Fig. 25 shows the components of a practical batch-annealing furnace for steel sheets. These components are used in developing the model for the entire system [50, 51]. Similarly, the different components in a polymer extrusion or an optical fiber manufacturing system may be considered. 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. The results obtained from the simulation provide the necessary inputs for improving existing designs, developing new designs, improving productivity, and improving the product quality for a given manufacturing process [1].

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 very significant role on this aspect since it can guide the selection of operating conditions and design parameters that can lead to a successful thermal processing. A few studies in the areas of polymer extrusion and optical fiber drawing are discussed here as examples. Similar concerns arise in other materials processing applications.

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. 26. An upper limit is obtained for the mass flow rate. Below this limit, practical operating conditions are found to occur and the simulation gives physically reasonable result in terms of pressure increase downstream. However, beyond the upper limit, though the numerical scheme converges, the results are not physical acceptable. In actual practice, for a given screw rotational speed, the mass flow capacity of the extruder is limited by the dimensions of the channel. With the assumption of constant density, 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. Higher screw speeds will yield higher flow rates. If one wants to achieve mass flow rates larger than these limitations, 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. With this physical limitation obtained by numerical simulation, one can provide guidelines for proper screw operation and choice of operating conditions [118].

For a specific screw speed, the simulation code also diverges for lower mass flow rates than the critical points shown in the figure. This is due to the marching numerical scheme employed in the translation region as well as the stability of the extrusion process itself. The velocity in the down-channel direction is a result of both shear due to the rotation and the pressure rise. The pressure acts in the direction opposite to that of the drag flow. When a narrow die is used and a low throughput is allowed, the pressure gradient in the down-channel direction becomes so large that the down-channel velocity becomes negative over a portion of the channel, in terms of the coordinate system fixed to the screw. The conventional marching schemes fail to simulate the flow in the translation region for this circumstance, since the downstream conditions are not known. However, other formulations, particularly the axial formulation, makes it possible to solve the problem to lower flow rates with the conventional marching schemes along the axial direction, since there is no back flow occurring in the direction parallel to the screw axis [119]. For the intermeshing region, the elliptic equations and the numerical scheme do not cause problems when back flow occurs. However, even with modifications in the numerical scheme, a lower limit on the mass flow rate arises in the feasible domain because of excessive pressures, temperatures and residence times.

These results and trends show good agreement with the observations on practical systems that suggest that a working domain exists in which a stable reactive extrusion process can be created [120]. The feasible domain and limitations obtained by simulation also agree quite well with experimental data. It is found that, as expected, the limitations on feasibility are more severe with chemically reactive materials, than those without chemical reactions.

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 [26, 121, 122]. 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 [123]. This is first indicated by the divergence of 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. Different operating conditions were studied to determine cases when drawing was feasible and those when it was not. Thus, as shown in Fig. 27, a region in which drawing is feasible can be identified. Beyond the boundaries of this region,

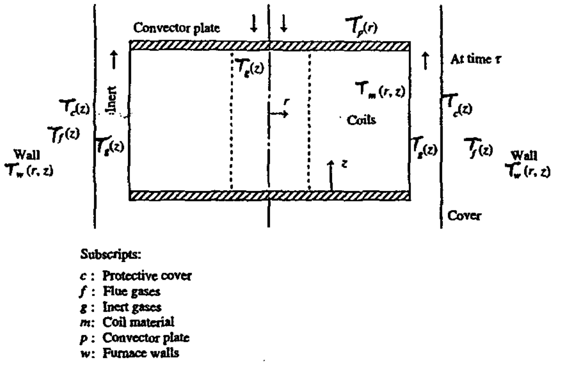


Fig. 25 Sketch of the different components of a batch annealing furnace for steel sheets, used for developing a mathematical model of the complete system.

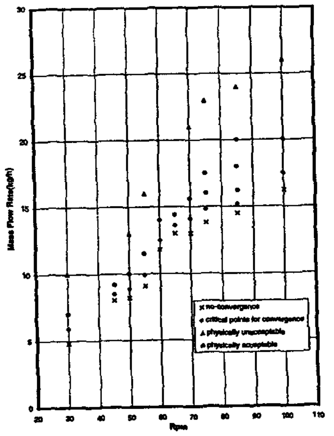
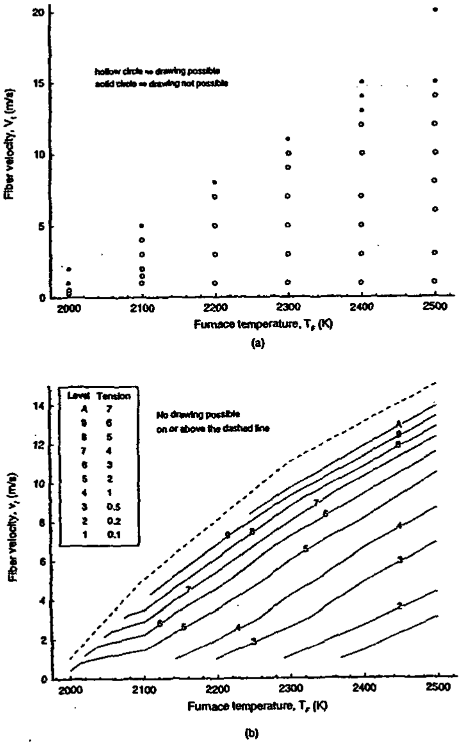


Fig. 26 Feasible domain for twin-screw extrusion of starch.



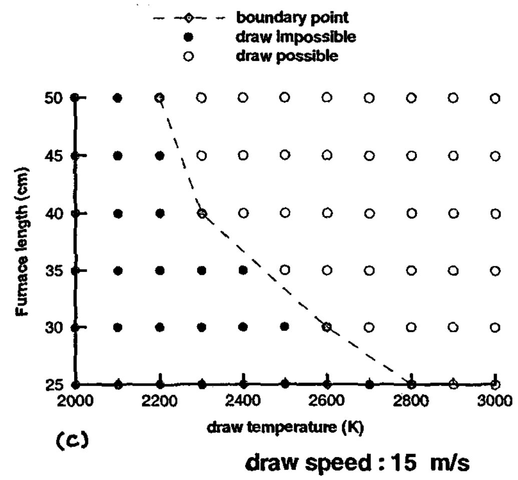


Fig. 27 Results obtained from a feasibility study of the fiber drawing process : (a) different cases studied, showing both feasible and infeasible combinations of parameters; (b) "iso-tension" contours for the feasible range of fiber drawing; (c) feasible domain at a draw speed of 15 m/s in terms of furnace length and temperature.

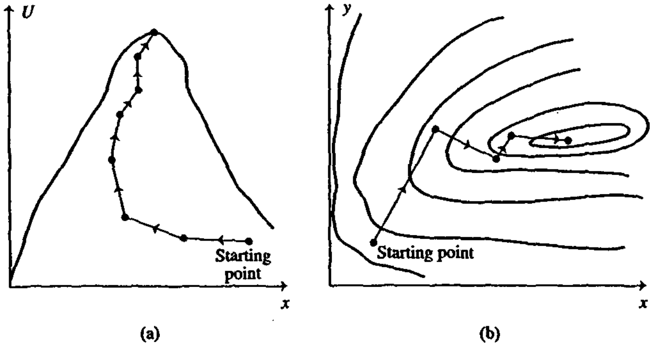


Fig. 28 Steepest ascent method, shown in terms of the climb towards the peak of a hill and also in terms of constant U contours.

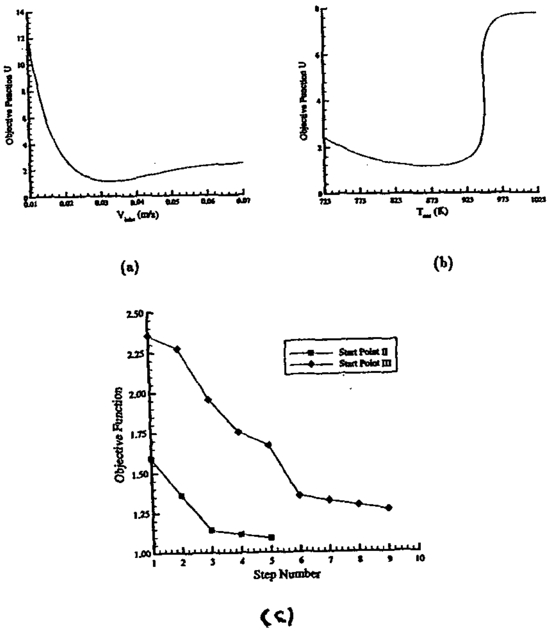


Fig. 29 Variation of the objective function U with (a) inlet velocity and (b) susceptor temperature. Also shown in (c) is the change in the value of the objective function with each step in the steepest descent method.

drawing is not possible. For the domain in which the drawing process is feasible, the draw tension is calculated. The "iso-tension" contours are also shown in the figure. 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, flow configuration, furnace wall temperature distribution, furnace length and diameter, and preform and fiber diameters, may be considered to determine the feasibility of the process. Figure 27 (c) shows the results when the furnace length and temperature are considered as the two main parameters. Clearly, the maximum draw speed at a given furnace temperature could be restricted by the heating-zone length due to the requirement that the temperature in the neck-down region must exceed the softening temperature. In all such cases, 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. These results are very important for a realistic fiber-drawing operation, since the parameters in a fiber drawing system can be determined so that a fiber of desired diameter can be drawn.

It must be pointed out that, in actual practice, fiber drawing may never reach the boundaries of the feasible domain due to unacceptably high draw tension. The numerical convergence, as well as the transport characteristics near the boundaries have been investigated to understand viscous rupture and other effects that arise. Also, there are other considerations that need to be taken into account to determine feasible and optimum drawing conditions. For example, a very high furnace temperature along with a small draw speed would result in a small draw tension due to the small value of viscosity. The fiber could break into drops because of the very mobile state of glass and the corresponding capillary instability [123]. Under these conditions, the process also becomes very sensitive to disturbances that are caused by variations in the drawing parameters. Similarly, the concentrations of various process-induced defects could be high at high draw temperatures, leading to unsatisfactory optical fibers. From these considerations, very high draw speeds or very high draw temperatures are not very desirable, even when drawing is feasible in terms of the transport process.

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. Some results on mixing, as given by the flow division ratio for flow between two rotating cylinders, were given earlier. The downstream motion of material particles may also be considered for a better understanding of the mixing process. Using the calculated three-dimensional velocity field in the extruder, one can consider specific particles inside the screw channel and follow their movement along the channel [124]. The particles undergo complicated spiral movements, except those near the barrel and screw surfaces. The spiral movement of the particles inside the screw channel promotes mixing within the single screw extruder. 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. These materials are followed with time as the fluid moves down the channel. The process is a slow one, though the materials are eventually mixed with each other. 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 [125, 126]. 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.

In optical fiber manufacture, the fiber has to be cooled rapidly in order to reach appropriate temperature levels before coating is applied. A lot of work has been done on this problem, because the height of the draw tower is significantly affected by the cooling process [66, 127]. The inert gases in the draw furnace play an important part in the thermal transport in the furnace. The convective flow is a strong function of the geometry, particularly of the locations of the inlet/outlet channels, and of the flow rate. The local transport rates affect the fiber quality as well as the draw process. The concentration of defects in the fiber is another important consideration, because it affect the quality of signal transmission and the distance one could go without enhancing the signal. Several defects are generated by the thermal process, and enhanced cooling could affect the distribution and retention of these defects. The glass flow also affects the distribution of these defects.

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 modeling and simulation in order to provide the appropriate inputs for system design and optimization. These relate to engineering issues like durability, maintenance and availability of different materials and components, as well as 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, or the best quality or performance per unit cost, with acceptable environmental effects. The need to optimize is very important in the design of the materials processing system 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

$$U (x_1, x_2, x_3, \ldots, x_n) \dashrightarrow U_{opt} \qquad (26)$$

with, $G_i (x_1, x_2, x_3, \ldots, x_n) = 0$, for i = 1, 2, 3, . . . , m (27)

and, $H_i (x_1, x_2, x_3, \ldots, x_n) \leq \text{ or } \geq C_i$, for i = 1, 2, 3, . . , l (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 since some constraints have to be discarded to make $m \leq n$. 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, such as the length of fiber drawn. 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 [128, 129].

Search methods constitute the most important optimization strategy for thermal systems. Many different approaches have been developed and are particularly appropriate for specific problems. 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. This is an important consideration with respect to thermal materials processing systems since each trial may take a considerable amount of computational or experimental effort. 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. It is a hill-climbing technique in that it attempts to move towards the peak, for maximizing the objective function, or towards the valley, for minimizing the objective function, over the shortest possible path. At each step, starting with the initial trial point, the direction in which the objective function changes at the greatest rate is chosen for moving the location of the point which represents the design on the multivariable space. Figure 28 shows this movement schematically on a hill as well as on a two-variable contour plot, the direction of the gradient vector ∇U being the direction in which U changes at the greatest rate. Since the search always moves in the direction of greatest rate of change of U, the number of trial runs needed to reach the optimum is expected to be small. However, it does require the evaluation of gradients in order to determine the appropriate direction of motion, limiting the application of the method to problems where the gradients can be obtained accurately and easily. Numerical differentiation may be used if an algebraic expression is not available for the objective function, which is often the case for thermal materials processing. Several other such gradient-based methods have been developed for optimization and are used for a variety of thermal processes [1, 130-132]. Genetic optimization algorithms, that are based on function evaluations instead of gradients, have also been developed and used, 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 processing systems, since the optimal design is a strong function of the chosen criterion for optimization. Frequently, optimization is carried out for different criteria and the final design is chosen by comparison and combination of results for different criteria. For illustration, let us consider a CVD system for deposition of TiN. As discussed in detail by Chiu et al. [133], the main qualities of interest include product quality, production rate, and operating cost. These three may be incorporated into one possible objective function, as given by

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

where U is to be minimized. 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. Chiu et al. [133] used two measurements of product quality, namely film uniformity and film resistivity. Film uniformity was defined as the maximum variation in film thickness across the susceptor surface. Thus, a minimum value of U implies greater film thickness uniformity. Similarly, operating costs were represented by heat input and gas flow rate. The production rate was expressed in terms of the deposition rate.

Obviously, the objective function may assume many possible forms. The preceding form is chosen because the magnitude of each aspect does not play a role in locating the optimal solution. It may be factored out as a constant during the minimization process. The change of each aspect in the objective function is of greater interest, since terms which exhibit significantly larger variations relative to others will drive the optimization. When a design incorporates effects with different sensitivities to the process variables, this problem may be circumvented by expressing the objective function as a sum of the log of the qualities. Another common form of the objective function expresses the effects as a sum or as the square root of the squared sums of the affects. All the aforementioned possibilities are possible forms for an objective function, but the proper form will strongly depend on the desired performance of a particular system.

A detailed study of the design space was carried out by Chiu et al. [133] to determine the domain of acceptable designs and the effects of various parameters on the objective function. Using the steepest ascent method, the optimal design was obtained considering different combinations of parameters. Some typical results are shown in Fig. 29, indicating the variations of the objective function with the inlet velocity V_{inlet} and the susceptor temperature T_{sus} and also with each iteration step for two different starting points. The variation of U with the different parameters can also be employed for univariate search, which involves optimizing with respect to one variable at a time and alternating the variables [1, 132].

A similar detailed study was carried out by Cheng [134] 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 for multivariable cases, were employed. Figure 30 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, particularly on furnace dimensions and operating conditions to achieve optimal drawing.

KNOWLEDGE BASE

An important consideration 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. It is obviously important to use this knowledge base in developing acceptable and optimal designs, and in the selection of operating conditions for given product characteristics. Some effort has been directed in recent years at streamlining the design process, improving the design methodology, automating the use of existing information and developing strategies for rapid convergence to the final design [135]. The basic concept behind knowledge-based systems is the storage and use of this knowledge to take logical decisions for selection, diagnostics and design [136]. 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.

A very important element in the development and use of knowledge-based methodology is object-oriented programming. All the information needed to use an object are stored in the object itself. The methods embedded or encapsulated in each of the objects are unique to that object. Therefore, encapsulation makes different objects reusable and reduces duplication within a program. Inheritance gives each object access to the features of the methods from the class above it on a tree structure. This aspect allows any system to be easily modified by adding an object, or subroutine, without affecting any other object. With the use of these features of object-oriented programming, it is easy to store and retrieve expert knowledge. A couple of examples are discussed here to illustrate the use of the knowledge-based strategy for design.

Knowledge-based design methodology is particularly useful in selecting an initial design for a polymer extrusion die. Die design is an important consideration in plastic extrusion since the operation of the extruder system and the quality of the final product are strongly influenced by the die. Even though a die is often treated as a component of the extruder, practical dies are usually subsystems consisting of different parts, such as entrance, flow channel and exit regions, which are attached to each other through couplings and screws, and the heating/cooling arrangement to maintain a desired temperature [34, 35, 106, 137]. 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 is based on expert rules for die design. Employing knowledge and experience used by an expert, rules may be set down to generate a design for the given requirements and constraints [138]. Preliminary evaluations and estimates are used to develop a possible design that is used as initial design. 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. Figure 31 shows a sketch of the initial design module giving these different strategies.

The knowledge base is also used in the redesign module to evaluate a given design and, if this is not satisfactory, to generate a new design. Expert rules are written on the basis of earlier experience and knowledge from an expert. These 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 the results of the design process up to the given instant. Thus, the efficiency of the iterative process is substantially improved. Figure 32 shows the advantage of selective search which avoids local minima that are physically unacceptable, as compared to an exhaustive one, in the drive toward the optimum given by a minimum value of the objective function.

Another problem that may be considered is 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

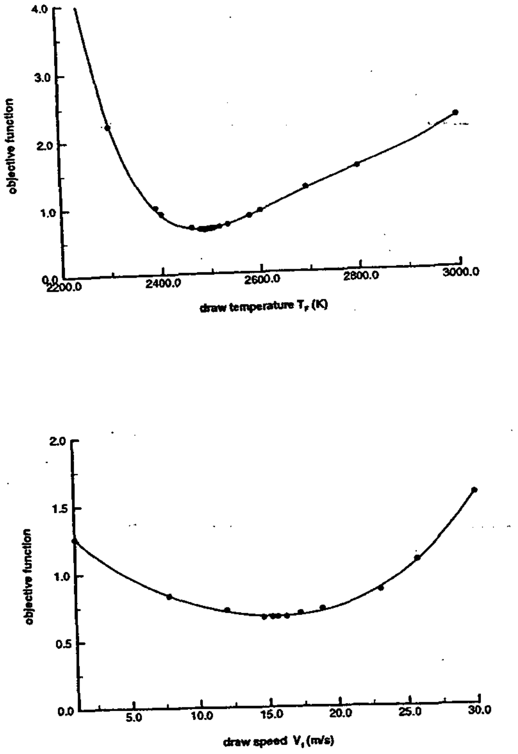


Fig. 30 Evaluation of optimal draw temperature at a draw speed of 15 m/s and the optimal draw speed at a draw temperature of 2489.78 K by using the golden-section search method.

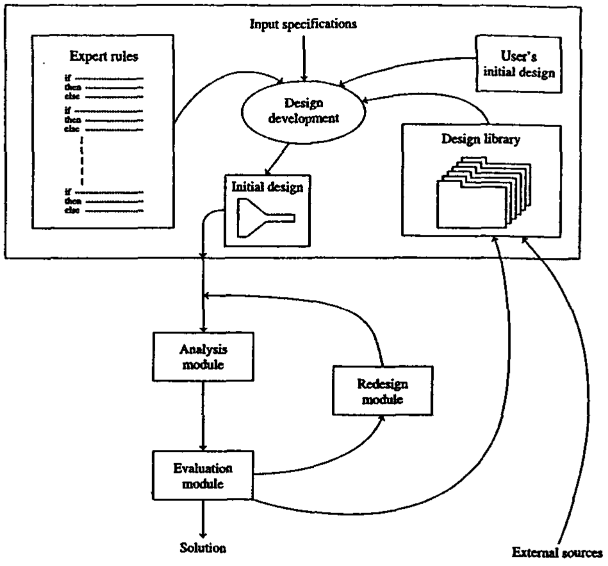


Fig. 31 Initial design module using knowledge-based methodology [138].

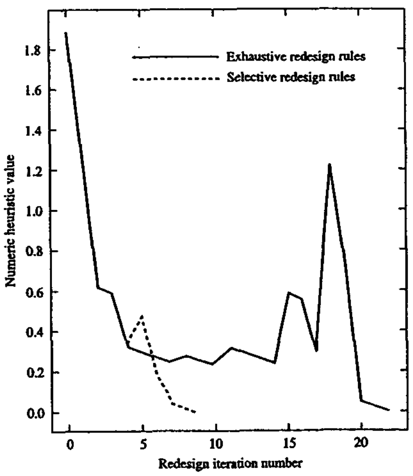


Fig. 32 Comparison of redesign strategies for a 1 cm circular die for extruding low density polyethylene (LDPE) at 400 kg/hr [138].

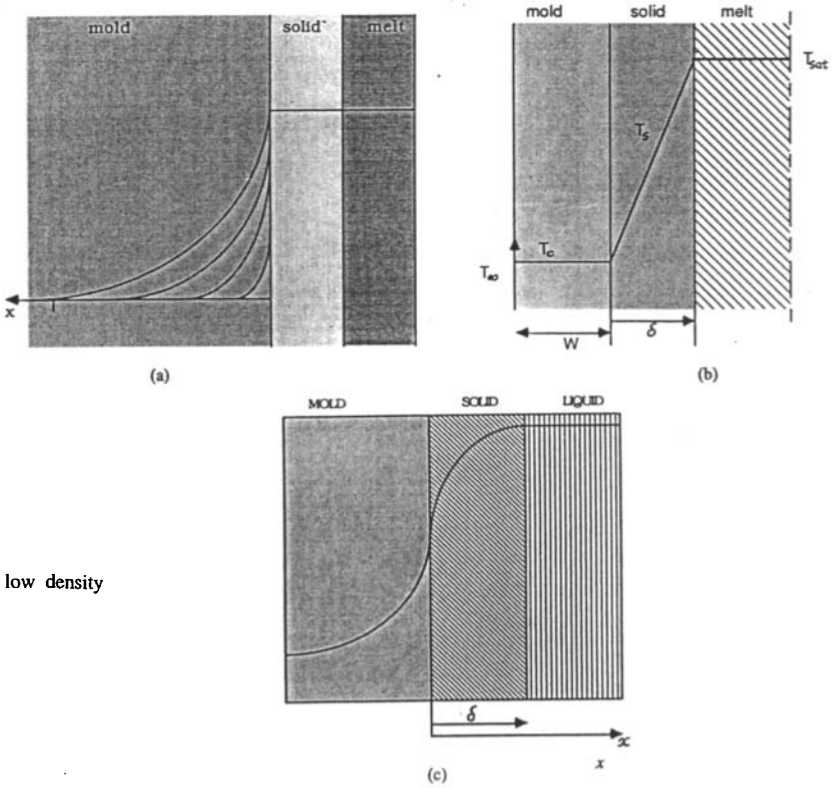


Fig. 33 Different mathematical models for ingot casting. (a) Chvorinov model; (b) lumped mold model; (c) semi-infinite model.

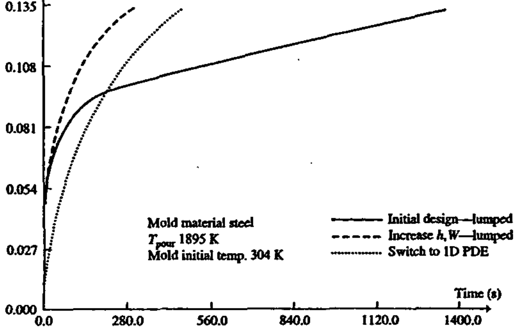


Fig. 34 Results for design of an ingot casting system, showing solid-liquid interface movement with time and switching to a more complex model after many design trials.

process, using modeling and simulation, to obtain inputs for design and to evaluate the nature of the casting.

Viswanath [139] and Viswanath and Jaluria [140] considered this problem, using knowledge-based methodology for design. Several models are available for the study of solidification. These may be listed 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 and energy balance is used.
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 distribution is assumed in the mold, solid and melt.
5. *Two- and three-dimensional models:* Natural convection flow in the melt is included.
6. *More sophisticated models:* Needed for alloys, generation of voids and defects, complicated geometries, etc.

Three models among these are sketched in Fig. 33. 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, 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 for a given casting being chosen as the objective function and employing constraints from the expert knowledge to avoid unacceptable thermal stresses and defects in the casting. We can start with relatively simple models and move to more complicated models if the desired details are not obtained. We may also 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. Figures 34 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. This is the process of improving the system through learning from past experiences.

Clearly, the use of the available knowledge base on the process is important in the design, optimization and operation of the system, as well as in choosing the operating conditions for a desired product. In actual practice, this knowledge, which may simply be called experience, is used all the time by engineers and workers involved with materials processing. Decisions are often made on the basis of what is known about existing processes, past trials and other similar systems. Therefore, it is desirable to build this knowledge base into the design, control and operation of the system.

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 transport instability mechanisms. 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 thermal processing needs further work.

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