Thermal Issues in Materials Processing

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This paper considers the thermal aspects that frequently arise in practical materials processing systems. Important issues such as feasibility, product quality, and production rate have a thermal basis in many cases and are discussed. Complexities such as property variations, complex regions, combined transport mechanisms, chemical reactions, combined heat and mass transfer, and intricate boundary conditions are often encountered in the transport phenomena underlying important practical processes. The basic approaches that may be adopted in order to study such processes are discussed. The link between the basic thermal process and the resulting product is particularly critical in materials processing. The computational difficulties that result from the non-Newtonian behavior of the fluid, free surface flow, moving boundaries, and imposition of appropriate boundary conditions are important in several processes and are discussed. Some of the important techniques that have been developed to treat these problems are presented, along with typical results for a few important processes. Validation of the model is a particularly important aspect and is discussed in terms of existing results, as well as development of experimental arrangements to provide inputs for satisfactory validation. The importance of experimentation and linking the micro/nanoscale transport processes with conditions and systems at the macroscale are discussed. Future trends and research needs, particularly with respect to new materials and new processes, are also outlined.
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Introduction

An important area, which has been of considerable interest to engineers over several decades, if not centuries, is that of manufacturing, which refers to the industrial transformation of raw materials to useful products on a relatively large scale. Processes such as casting, welding, and forging have been used since the middle ages. In recent years, with the emergence of a wide variety of new materials such as ceramics, composites, advanced polymers, specialized alloys, semiconductor and optical materials, and nanomaterials, the transformation of materials, which is often referred to as materials processing, has become particularly important because of applications that demand specific characteristics, fabrication consistency, reduced costs, and high quality in the product. New materials and processes have been developed in order to meet the constraints and requirements of emerging areas in energy, environment, communications, transportation, biotechnology, and other engineering fields. Most of these materials processing applications involve thermal energy transport, which is governed by flow, heat and mass transfer, and thermodynamics. The thermal transport plays a critical role in the quality and characteristics of the final product and in the prediction, operation, control, and design of the associated thermal system [1–3].

The transformations in the material characteristics due to the thermal transport undergone by the material largely occur at micro- or nanometer length scales, whereas the operating condition and design parameters of the system that give rise to the desired thermal variation in the material are at macro or engineering length scales. Also, many practical devices involve these length scales, as well as similarly short time scales. Thus the governing transport phenomena at micro/nanoscale are crucial to an improvement in existing processes and development of new systems [4,5]. The mathematical and numerical modeling of these processes must include multiple length and time scales in many problems of practical interest. Experimental results are also important for validation, physical insight, and for providing inputs that are often not easily obtained by modeling.

In materials processing, many important basic and applied issues arise that need a detailed study and possible solution. Among the most critical ones are [6]

- process feasibility
- product characteristics
- product quality
- production rate
- system efficiency and cost
- appropriate operating conditions
- design of relevant system
- system optimization and control
- new products and methods

Thermal considerations are important in all these aspects. For instance, temperature distributions affect product characteristics and quality, heat transfer rates determine the production rate, feasibility may be determined by material flow and temperature or pressure limitations, efficiency is related to energy input, and so on.

This paper reviews the underlying thermal transport phenomena for a range of traditional and emerging materials processing applications, such as casting, forming, thin film deposition, optical fiber drawing, crystal growth for semiconductor fabrication, and polymer processing. Besides discussing the basic thermal issues in materials processing, the paper also outlines solution strategies using numerical and experimental approaches, how the transport processes affect the product, how multiple scales are treated, and the important considerations in optimization. It also discusses the current and future trends, as well as research needs in this important area.

Since the field of materials processing is quite extensive, only a few important aspects and techniques can be considered in detail, along with a few characteristic examples. The references given in each case may be consulted for further details. The basic thermal issues in important processes are presented and related to other

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materials processing systems where thermal aspects are of particular concern. Figure 1 shows the sketches of a few processes which are considered in some detail in this paper. These include mold casting, polymer extrusion, optical fiber drawing, and chemical vapor deposition for thin film fabrication. A list of common manufacturing or materials processing techniques in which thermal issues play a major part is given below [7–9].

Common traditional manufacturing processes:

1. Casting: mold casting, continuous casting
2. Heat treatment: annealing, hardening, surface treatment
3. Forming: hot rolling, wire drawing, metal forming, extrusion, forging
4. Bonding: soldering, welding, brazing
5. Glass processing: glass blowing, forming, annealing
6. Chemical processing: cooking, drying, curing, baking
7. Coating: spray coating, polymer coating
8. Machining: cutting, grinding, drilling
9. Other processes: gas flame heating, cutting, welding

Heat transfer is a critical component in all the traditional manufacturing processes given above, though heat removal is the main concern in machining. In other cases, heat transfer is essential to carry out the process. For instance, heating of the materials is necessary in polymer and glass processing and heat input is needed to melt materials for casting. Many other manufacturing or materials processing techniques have been developed in recent years due to the new materials and applications of interest. A list of some of the common processes is given below.

New and emerging materials and processing methods:

1. Polymer processing: extrusion, injection molding, thermoforming
2. Reactive processing: food processing, rubber manufacture
3. Powder processing: powder deposition, sintering, sputtering, nanopowders, and ceramics
4. Semiconductor materials: crystal growing, silicon deposition
5. Optical materials: optical fibers, silica glass, devices

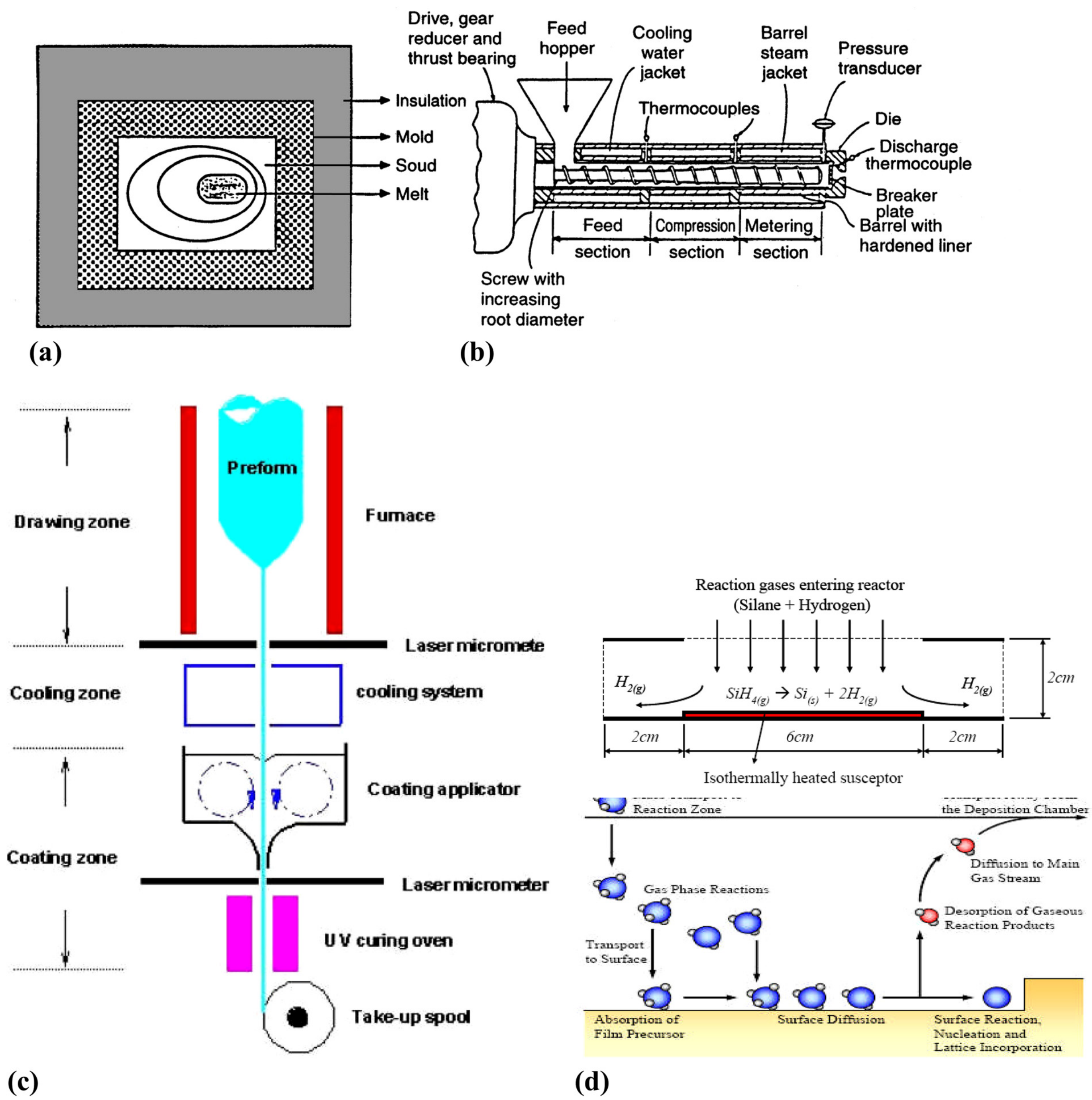


Fig. 1 Sketches of a few materials processing applications that involve significant thermal issues: (*a*) casting, (*b*) polymer single-screw extrusion, (*c*) optical fiber drawing, and (*d*) chemical vapor deposition

6. Chemical vapor deposition: GaN, TiN, GaAs, SiC, selective surfaces, storage materials
7. Laser processing: laser cutting, heating and welding
8. Alloy casting: specialized alloys, micro/macro segregation
9. Rapid prototyping: printing technology, net shaping, thermal sprays, microfabrication
10. Composite materials processing
11. Microgravity materials processing
12. Others: ultrasonic machining, electrochemical machining, fluid jet cutting

Detailed analytical/numerical and experimental studies are needed on these processes to obtain the temperature distributions, flow field, pressures, heat and mass transfer rates, and other relevant thermal variables in order to obtain the relevant conditions to achieve the desired product quality and characteristics, as well as high production rates. In this paper the mathematical and numerical modeling of several of these processes is discussed, along with the important mechanisms, the basic aspects that need further investigation, and the inputs frequently needed for modeling, design, and optimization of the various systems.

Mathematical Modeling

As mentioned above, thermal considerations are very important in many materials processing techniques. The processes of melting and solidification, involved in casting and crystal growing, are driven by heat transfer to and from the material. Buoyancy-driven flows arise in the molten material due to temperature and concentration differences and affect the microstructure of the product, as well as the characteristics of the solid-liquid interface. In food extrusion, hot rolling, thin film deposition, and soldering, the thermal transport determines the rate of fabrication and the product characteristics. It is important to mathematically model these processes to develop numerical models and generalize experimental and numerical results. However, there are a wide range of complexities that set these processes apart from many other basic and applied areas of heat transfer and that have to be included for an accurate and useful simulation. Some of the important ones are outlined here.

Variable Properties. Large material property changes typically occur in materials processing with respect to temperature, pressure, shear rate, concentration, and other parameters. Material properties are crucial in obtaining accurate results from any numerical simulation. Unfortunately, accurate property data are often not available, particularly in the parametric ranges of interest. For instance, these data may be available at atmospheric and room temperature conditions that are vastly different from those for the actual process, and thus severely limit the predictability of the simulation. In the manufacture of optical fibers, for instance, data on thermal properties, particularly on viscosity, are needed above the softening point T_{melt} of silica glass, which is around 1900 K. Similarly, dopants like GeO_2 and B_2O_3 are added to the glass preform to vary the optical properties of the fiber. The material properties are strong functions of the temperature T and also vary with composition and changes in the microstructure. However, the data on the effect of the dopants on radiation properties and on viscosity are very limited. Some typical results in the literature are shown here [10].

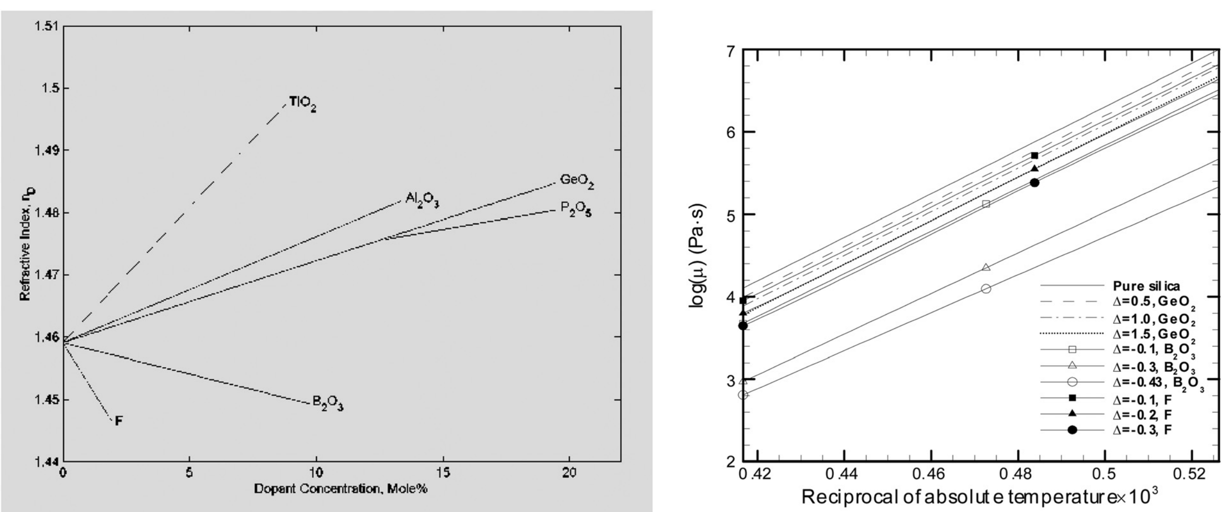
The variation in the viscosity is one of the most critical considerations for the flow since it varies exponentially with temperature. An equation based on the curve fit of available data for kinematic viscosity ν is written for silica, in SI units, as [11,12]

$$\nu = 4545.45 \exp\left[32\left(\frac{T_{\mathrm{melt}}}{T} - 1\right)\right] \quad (1)$$

Variations in all the other relevant properties of glass need to be considered as well, even though the variation with T is not as strong as that of viscosity. Unfortunately, very limited data are available on these as well as on the effect of dopants. Even though numerical models are available that can include strong variations in the properties, the lack of appropriate data is a major concern in generating accurate results. Figure 2 presents experimental results adapted from [10–12] on the effect of various dopants on the refractive index and viscosity of silica glass. The exponential variation of viscosity with temperature is also seen.

Thus, the material properties change as the material undergoes thermal processing. This includes changes in the material characteristics and structure because of chemical reactions. For instance, the transport processes in polymer processing involve large material property changes with temperature and species concentration, which may vary during the process such as extrusion. These materials are also generally non-Newtonian, i.e., the viscosity varies with the shear rate and thus with the flow. The fluid is often treated as a generalized Newtonian fluid with the viscosity given by expressions such as the one for a power-law variation written as [13]:

$$\mu = \mu_o(\dot{\gamma}/\dot{\gamma}_o)^{n-1} \exp(b/T) \quad (2)$$



(a) **(b)**

Fig. 2 Variation of silica glass properties with dopant concentration and temperature (adapted from [10–12])

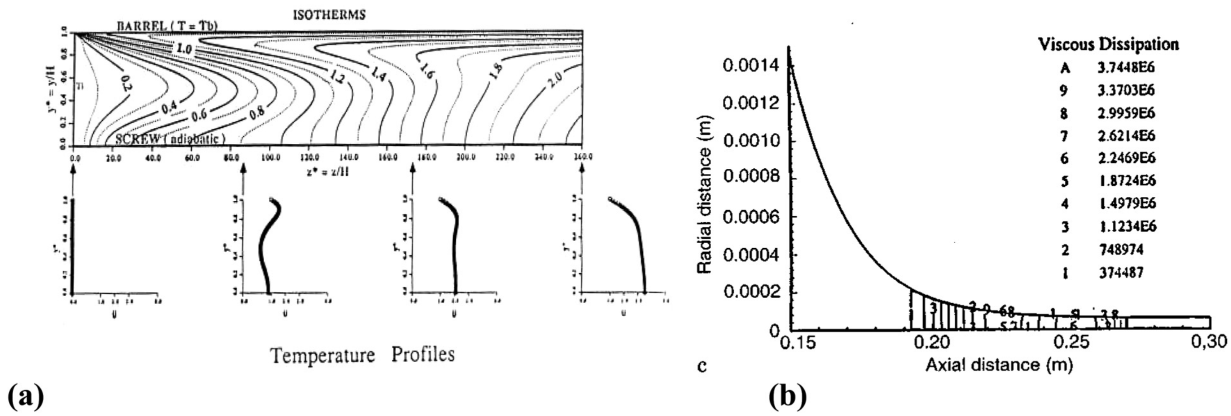


Fig. 3 (*a*) Isotherms and temperature distributions in a single-screw polymer extruder [15]. (*b*) Viscous dissipation in the neck-down region of an optical fiber drawing process [16].

For food materials, the viscosity also varies with the moisture concentration C. One such constitutive relation for viscosity is of the form

$$\mu = \mu_o(\dot{\gamma}/\dot{\gamma}_o)^{n-1}\exp[-b(T-T_0)]\exp[-b_m(C-C_o)] \qquad (3)$$

The changes in the chemical structure due to chemical conversion can also be included as a factor in these equations if experimental data are available. One such equation multiplies the viscosity equation, such as the one given above by $(DG)^a$, where DG is the fraction of starch that has been converted and a is a constant obtained from a curve fit of the experimental data [14].

It is clear that material properties and their dependence on the local conditions like temperature and pressure are extremely important in manufacturing or materials processing. Limited data are available in the literature and a concentrated effort is needed in the future to obtain accurate data under appropriate conditions for various applications of interest in this area.

Viscous Dissipation. Due to the large viscosity of materials like plastics and glass, viscous dissipation effects are often important and must be included. An additional term $\mu\Phi$ arises in the energy equation, representing the irreversible part of the energy transport due to the shear stress. Viscous dissipation is thus a thermal source in the flow and is always positive. For a Cartesian coordinate system Φ is given by the expression

$$\Phi = 2\left[\left(\frac{\partial u}{\partial x}\right)^2+\left(\frac{\partial v}{\partial y}\right)^2+\left(\frac{\partial w}{\partial z}\right)^2\right]+\left(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial y}+\frac{\partial v}{\partial z}\right)^2+\left(\frac{\partial u}{\partial z}+\frac{\partial w}{\partial x}\right)^2-\frac{2}{3}(\nabla\cdot V)^2 \qquad (4)$$

Similarly, expressions may be obtained for other coordinate systems. Viscous dissipation is particularly important in polymer processing as seen in Fig. 3(*a*), which shows that the temperature in the fluid rises above the barrel temperature in extrusion due to this effect [15]. Though the overall effect of viscous dissipation in a process may be relatively small, it could play a substantial role in the temperature distributions in certain regions. In optical fiber drawing, for instance, viscous dissipation is a large effect in the narrow region of the flow, as shown in Fig. 3(*b*), and is critically important in the flow since, in its absence, the temperature could drop below T_{melt} and cause rupture [16]. Similarly, many other material processing applications involve significant viscous dissipation effects, which must therefore be included in the analysis.

Governing Equations. The basic equations that may be used to model the transport in materials processing may, thus, be written for a general three-dimensional process with variable properties as

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\bar{V})=0 \qquad (5)$$

$$\rho\left(\frac{\partial\bar{V}}{\partial t}+\bar{V}\cdot\nabla\bar{V}\right)=\bar{F}-\nabla p+\nabla\cdot[\mu(\nabla\bar{V}+\nabla\bar{V}^T)]-\frac{2}{3}\nabla(\mu\nabla\cdot\bar{V}) \qquad (6)$$

$$\rho C_p\left(\frac{\partial T}{\partial t}+\bar{V}\cdot\nabla T\right)=\nabla\cdot(k\nabla T)+\dot{Q}+\mu\Phi+\beta T\left(\frac{\partial p}{\partial t}+\bar{V}\cdot\nabla p\right) \qquad (7)$$

Here the viscous dissipation and compressibility effects are included, with the last term representing the latter. The general equations may be written or modified for specific applications and geometries, to include additional effects as needed. The stress terms in the momentum equation may also be written as $\nabla\cdot\tau$, where the stress τ may then be written in terms of the appropriate constitutive equations for Newtonian or non-Newtonian fluids [3]. These equations, which assume Stokes' relations and a zero bulk viscosity, are well known and, though analytical solutions are seldom possible in practical cases, numerical techniques can be employed to obtain the desired results on the physical variables for a variety of operating conditions and design parameters. However, several other challenges are commonly encountered in materials processing that make it difficult to use computational methods or to obtain accurate results. Some of these are outlined below.

Buoyancy Effects. In many manufacturing processes, such as casting, soldering, and crystal growing, buoyancy effects are important due to the temperature or concentration differences and these give rise to flows that can affect the quality of the product and the rate of production. The uniformity of the deposition in CVD can be significantly affected by buoyancy effects, which significantly change the flow field. Thus, the buoyancy term must be included in the momentum equations. For thermal buoyancy, body force and pressure terms in the momentum equation are replaced by the following terms, if Boussinesq approximations are employed [17],

$$\bar{F}-\nabla p=-\bar{e}g\rho\beta(\mathrm{T}-\mathrm{T}_a)-\nabla p_d \qquad (8)$$

This leads to the Grashof number Gr, which characterizes the buoyancy effects. The buoyancy term is more complicated if Boussinesq approximations cannot be used due to large changes in temperature. However, the buoyancy term couples the flow with the energy equation. Figure 4 shows a couple of cases where buoyancy effects are particularly important. The first one relates to solidification where buoyancy effects give rise to a flow in the melt and this, in turn, affects the solid-liquid interface. Instead of a vertical interface in the absence of buoyancy, a curved interface is seen to arise [18]. In CVD with a flow impinging on the heated susceptor, buoyancy effects give rise to a vertically rising flow that opposes the downward flow, resulting in the reacting gases not reaching the surface and lack of deposition, as seen in Fig. 4(*b*) for one half of the impingement region, from the center to the edge. In this figure the colors indicate the velocity level, going from red for the highest to blue for the lowest. Thus the flow is almost stagnant neat the center.

Complicated Geometry. In many cases, the process involves complicated geometry of the transport domain, including large changes in dimension. For instance, in optical fiber drawing, the preform diameter is of the order of 10 cm and the fiber of diameter 125 μm. Similarly, in solidification, as shown in Fig. 1, the molten region is quite irregular in shape. Transformations are often used to simplify the domain. For instance, both the glass and the gas regions in the optical fiber drawing furnace may be transformed by using Landau's transformation [19,20] to convert the computational domains to cylindrical ones, as shown in Fig. 5. Similarly, in single-screw extrusion, the geometry is very complicated and the rotation of the screw makes any simulation quite involved. But by locating the coordinate system on the rotating screw and neglecting curvature effects, a steady flow in a channel with the barrel moving at the pitch angle, as shown in Fig. 6 for two channel profiles, is obtained [21]. The grids are designed to capture the complicated geometry, with finite element methods being particularly suited to the generally intricate configurations encountered in many practical problems.

Combined Mechanisms. In most cases of practical interest, combined transport mechanisms arise. Among the most common are combined radiation and convection, operating at the surfaces or in participating media like glass. Combined heat and mass transfer also occurs in many processes such as chemical vapor deposition, drying, and food processing. The species conservation equation then must be solved for the concentration ω_i along with

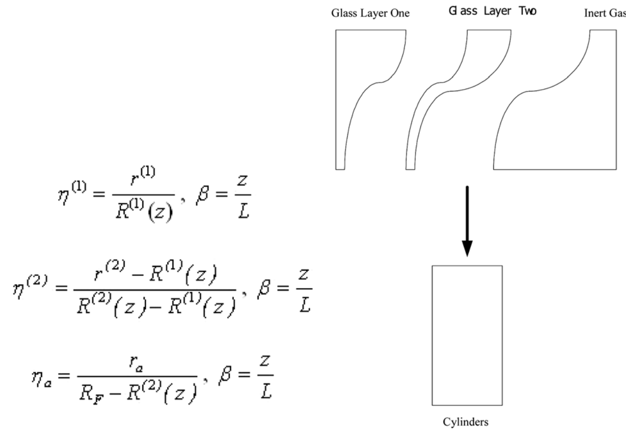


Fig. 5 Landau's transformations to convert axisymmetric complex shapes to cylindrical ones

the equations for the flow and temperature. A general form of the species equation is

$$\frac{\partial(\rho u_j \omega_i)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D_{ij}\frac{\partial \omega_i}{\partial x_j}\right) \tag{9}$$

where x_j represents the coordinate axes. Similarly, phase change processes like melting and solidification occur along with thermal transport in casting. Chemical reactions are the basis for material conversion in reactive polymers and for deposition in CVD reactors. Therefore, the governing equations have to be suitably modified to include such combined mechanisms that arise in the material or in the system.

Complex Boundary Conditions. The initial and boundary conditions in materials processes are often complicated due to combined transport mechanisms operating at the boundaries, as mentioned above, flow through openings, and surface motion. In several cases, free surfaces arise and have to be determined as part of the solution. This is the case in optical fiber drawing where the

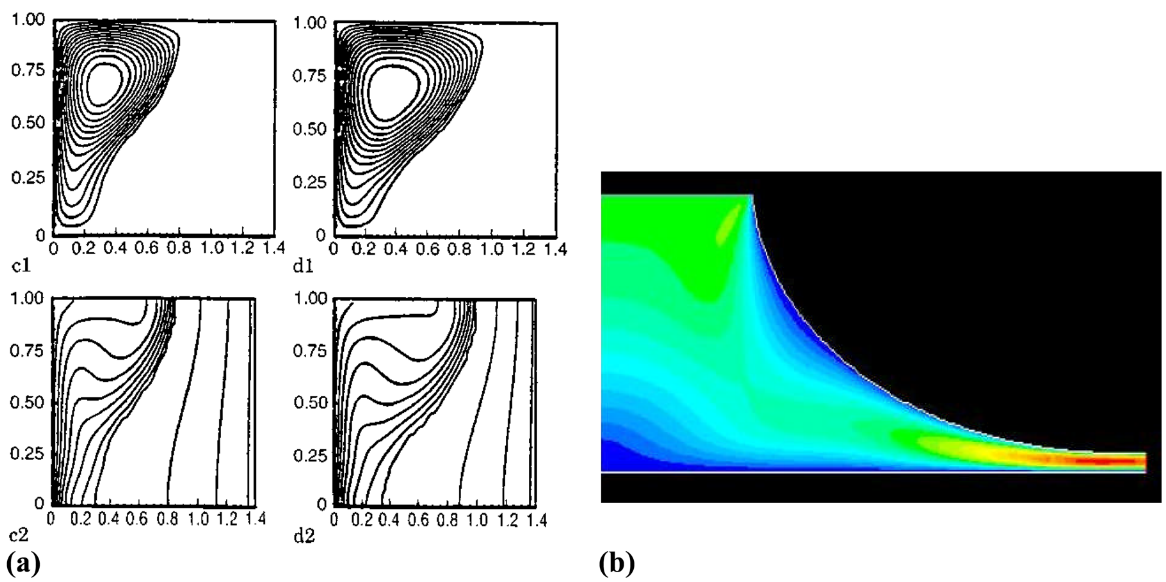


Fig. 4 (*a*) Streamlines (1) and isotherms (2) for melting of gallium in an enclosed region, with the left vertical boundary at a temperature higher than melting point, the right vertical boundary at a temperature lower than melting point, and the remaining two boundaries insulated, at dimensionless time *t* following the onset of melting of *t* = 1.5622 and *t* = 1.9789. (*b*) Calculated streamlines in an impingement CVD reactor showing the effect of buoyancy in the center [18].

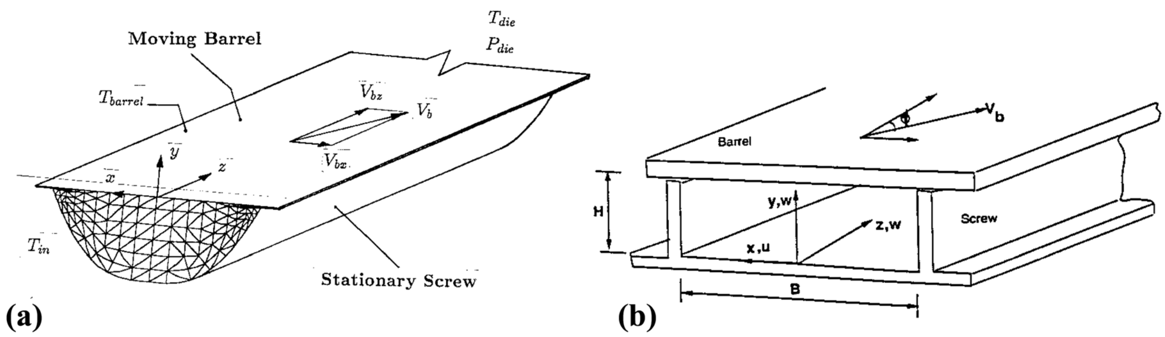


Fig. 6 Single-screw extruder with two difference channel profiles. The coordinate system is located on the barrel and curvature effects are neglected for the mathematical model.

neck-down profile is an important part of the solution. In this case, the feasibility of the process is determined by a stable neck-down profile, which is the result of the various forces such as viscous, gravitational, surface tension, and shear forces acting on the fiber. Coupled conduction and convection, or conjugate conditions, must be included in many cases, such as plastics extrusion due to conduction in the barrel and in the screw. Other interfaces and moving boundaries occur in phase change processes have to be appropriately modeled [22,23]. It is obviously very important to impose the boundary conditions accurately since the numerical results are strongly dependent on the transport at the boundaries.

Numerical Modeling and Simulation. A wide range of numerical methods, using finite difference, finite volume, finite element, or other approaches, is available to solve the differential equations that characterize materials processing. For two-dimensional and axisymmetric problems, it is often convenient to eliminate the pressure to obtain the vorticity equation. Then the vorticity and energy equations are solved using a nonuniform grid, with finer grids located in regions where large gradients are expected. Various other grids, including meshless methods, boundary-fitted coordinates, and adaptive grids, may be employed, depending on the problem being considered. For three-dimensional problems, it is more efficient to use the primitive variables. The strong variation of material properties, like viscosity, with temperature makes it imperative to employ fine grids, linearization and decoupling of the equations, and iterative procedures, using a variety of available and modified numerical techniques. For example, even a change of a few degrees in temperature in the vicinity of the softening point of glass or of the glass transition temperature of a polymer can give rise to substantial change in viscosity, which in turn affects the flow field and the thermal transport. Finite element methods are generally better suited to complicated domains and complex boundary. For further details on the appropriate numerical methods, many useful references are available [24–26].

Experimental Results

Experimental results are of particular importance in thermal materials processing, because of the complexity of the problem in most practical circumstances, as outlined above. Experimentation is needed for the following main reasons:

1. validation of the mathematical and numerical models
2. providing physical understanding of the underlying basic phenomena
3. providing inputs to simplify the simulation
4. providing inputs in cases where modeling is difficult, unavailable, or inaccurate

Validation of the models to ensure that the given physical process and system are simulated correctly and accurately is a critical concern in materials processing since various simplifying assumptions and idealizations are generally made to solve the problem [6,27]. Therefore, it is critical to verify the numerical model, ensuring that the results are essentially independent of the grid and other arbitrarily chosen numerical parameters, and validate the model to ensure that the results obtained are applicable, realistic, and accurate [28]. Among the approaches used are the physical behavior of the results obtained, comparisons with available analytical and numerical results, comparisons with benchmark solutions, and comparisons with experimental data. If experimental data are not available, well-designed experiments may need to be carried out. An example is a specially designed cam-driven thermocouple system to obtain the temperature profile in the channel of a rotating single screw polymer extruder to validate the model [29,30]. Similarly, a rotating cylinder experiment was designed and fabricated to test the model on the flow between two rotating screws in a twin-screw extruder [31].

Figure 7 shows two examples of validation by comparing numerical results with experimental data. Figure 7(*a*) gives the deposition rate in a horizontal CVD reactor for silicon as a function of location. The experimental data of Eversteyn et al. [32] are used for comparisons with several numerical studies [33–36], indicating close agreement in some cases and greater differences in others, though the basic trends are similar in all cases. An important problem, seen in this figure, is that very few experimental studies are typically available for many numerical studies, limiting the detailed validation that is often needed to establish the accuracy and validity of the numerical simulation. Figure 7(*b*) shows the case of melting of a pure metal, being tin here, in an enclosed region. A comparison between numerical results [18,37] and experimental data from [38] indicates fairly good agreement. However, because of the limited number of experimental studies, these data are used by several numerical studies for validation of the models. Clearly well designed and focused experiments are needed to satisfactorily validate analytical and numerical models and evaluate the accuracy of the results in many materials processing systems.

Because of the complexity of practical material processing systems, experimentation is often needed to understand the basic transport phenomena that govern the process. In food and polymer extrusion, for instance, experimental data on the product characteristics and on the residence time, i.e., time spent by the material in the extruder, are important in understanding the material transformation and the basic flow. Similarly, visualization of the flow in a transparent single or twin-screw extruder can be used to understand the mechanisms of mixing. In some cases, experimental data may be used to simplify the analysis as well. Continuing with extruders, temperature measurements in the barrel can be used to simplify the modeling by specifying the wall temperature distribution rather than solving the more complex conjugate problem.

There are also cases where analysis is much too complicated or the basic mechanisms are not fully understood. An example is the coating of optical fibers by moving the fiber at high speed in a

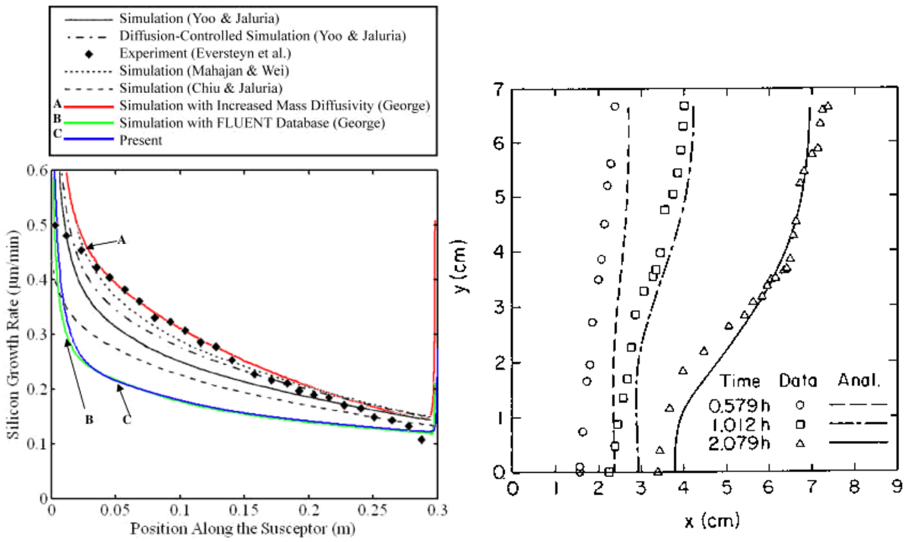


Fig. 7 Comparison between numerical results and measurements for (*a*) a horizontal CVD reactor for silicon [36] and (*b*) melting of tin in an enclosure [18]

coating die containing the desired coating material, such as acrylates which are cured at the next stage. The inlet meniscus that arises due to the fiber entering the liquid is the result of a dynamic contact angle, which arises due to a balance of surface tension, pressure, viscous, and gravitational forces. This is not a trivial problem and the surface properties play an important role. However, experimental results may be used to characterize the meniscus under a variety of operating conditions. Then the meniscus may be treated as given, rather than being obtained by a corresponding analysis [39–41]. This approach is demonstrated in Fig. 8, showing typical experimental results and the corresponding simulation results with a specified meniscus. Though the meniscus is critical in understanding bubble entrapment in the coating and other defects [42–44], the flow away from the meniscus is quite accurately predicted by the simulation.

Experimental results are rather limited in materials processing due to the various complexities such as high temperature and pressure, inaccessibility of a probe into the region of interest, changes in the material as it undergoes the given process, inconsistency of the raw materials, uncertainties in the imposed conditions, measurement difficulties in a production environment, and so on. Experiments on lab systems are often substituted for measurements on the full-scale systems; thus limiting the usefulness of the data. However, experimental data are crucial in the modeling of materials processing systems and thus in the design, development, and optimization of systems and processes.

Multiscale Simulation

In materials processing, the changes in the structure and characteristics of the material being processed are generally determined by the transport processes that occur at the micro- or nanometer scale in the material [45]. Examples are processes that occur at the solid-liquid interface in crystal growing, at the susceptor surface in a chemical vapor deposition reactor, or at sites where thermally induced defects are formed in optical fiber drawing. However, the product dimensions are generally at the commercial or engineering scale, involving dimensions of order of centimeters

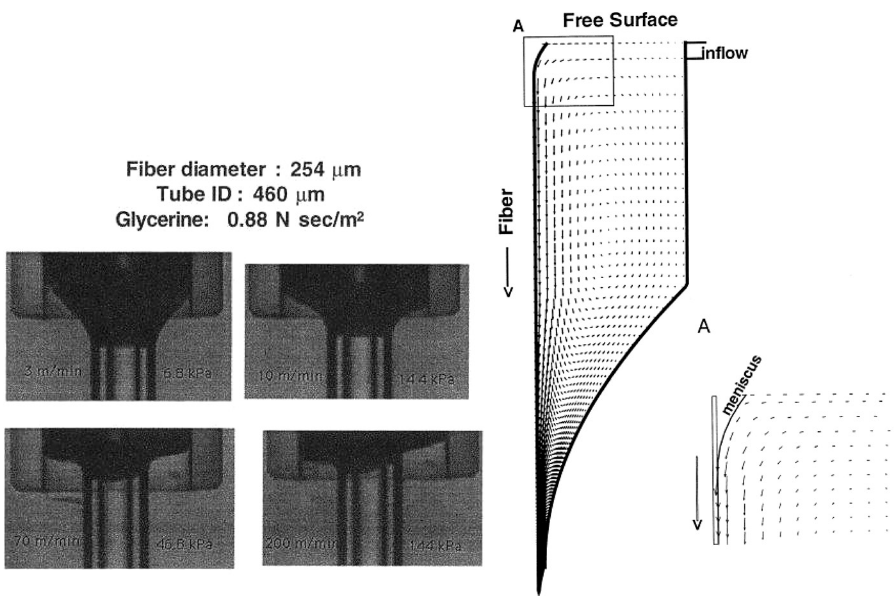


Fig. 8 (*a*) Observed meniscus for different operating conditions in optical fiber coating and (*b*) calculations on the flow with a specified meniscus

or meters. Also, the operating conditions are imposed at these macro length scales on systems that are also at these scales. Thus, very different length scales arise within the domain and need to be investigated by different methodologies to obtain the overall behavior.

In chemical vapor deposition, chemical kinetics plays a critical role in the deposition of material from the gas phase. The chemical kinetics for several materials is available in the literature and is often complicated by the large number of reactions and species involved. In addition, there are reactions at the surface as well as within the gas. Figure 7(*a*) presented the results for the fairly well known case for the deposition of silicon from silane (SiH_4) with hydrogen as the carrier gas. The chemical kinetics were given in a simple form by the expression [32]

$$K = \frac{K_o p_{SiH_4}}{1 + K_1 p_{H_2} + K_2 p_{SiH_4}} \tag{10}$$

where the p's are the partial pressures of the two species in the reactor, K is the surface reaction rate in mole of Si/m^2s, $K_o = A\exp(-E/RT)$, E being the activation energy, and A, K_1, and K_2 are constants which are obtained experimentally. Then, this equation is applied at the microscale level to obtain the reaction rates and the deposition, while the boundary conditions, in terms of velocity, temperature, concentration, etc., are imposed at the system level.

Figure 9 shows typical results for an impingement type CVD reactor for silicon, using silane and hydrogen with the above chemical kinetics [36]. The flow and temperature fields are shown, along with the deposition rate as a function of location. The green region represents acceptable uniformity and the red region unacceptable nonuniformity in film thickness. The nonuniformity of the deposited film is a major concern and efforts are made to achieve better uniformity by varying the operating conditions like susceptor temperature and inflow velocity and concentration. Similar considerations arise in the deposition of other materials like TiN, SiC, GaN, and GaAs, needed for different new and emerging applications like laser diodes, light-emitting diodes, and high-power transmitters.

Similarly, thermally induced defects are generated in optical fiber drawing at the nano and molecular levels. One such defect is the E' defect, which is a point defect that causes transmission loss and mechanical strength degradation in the fiber. A mechanism for the generation of these defects at high temperature during the drawing process was formulated on the basis of the thermodynamics of lattice vacancies in crystals by Hanafusa et al. [46]. The E' defects are generated through the breaking of the Si-O band and a fraction of the defects recombine to form Si-O again. The overall concentration of the E' defects is the difference between the generation and the recombination. Depending on the rate of fiber cooling after its emergence from the furnace, the final concentration of defects can be controlled. The equation for E' defect concentration is given as [46]

$$v\frac{dn_d}{dz} = n_p(0)v\exp\left(-\frac{E_p}{KT}\right) - n_d v\left[\exp\left(-\frac{E_p}{KT}\right) + \exp\left(-\frac{E_d}{KT}\right)\right] \tag{11}$$

where n_d and E_d represent the concentration and activation energy of the E' defect; while n_p and E_p represent those of the precursors. The initial values and constants were defined by [28].

Therefore, the transport processes in the silica preform/fibers are modeled to obtain the flow and thermal fields, along with the free surface which gives the neck-down profile. The governing equations that need to be solved for the axisymmetric fiber draw process are obtained from the general equations given earlier:

$$\frac{\partial v}{\partial z} + \frac{1}{r}\frac{\partial(ru)}{\partial r} = 0 \tag{12}$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial r} + v\frac{\partial v}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial z} + \frac{1}{r}\frac{\partial}{\partial r}\left[r\upsilon\left(\frac{\partial v}{\partial r} + \frac{\partial u}{\partial z}\right)\right] + 2\frac{\partial}{\partial z}\left(\upsilon\frac{\partial v}{\partial z}\right) \tag{13}$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial r} + v\frac{\partial u}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial r} + \frac{2}{r}\frac{\partial}{\partial r}\left(r\upsilon\frac{\partial u}{\partial r}\right) + \frac{\partial}{\partial z}\left[\upsilon\left(\frac{\partial v}{\partial r} + \frac{\partial u}{\partial z}\right)\right] - \frac{2\upsilon u}{r^2} \tag{14}$$

$$\rho C_p\left(\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial r} + v\frac{\partial T}{\partial z}\right) = \frac{1}{r}\frac{\partial}{\partial r}\left(rK\frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(K\frac{\partial T}{\partial z}\right) + \Phi + S_r \tag{15}$$

The radiative source term S_r is nonzero for the glass preform/fiber because glass emits and absorbs energy. The variation of the absorption coefficient with wavelength λ can often be approximated in terms of bands with constant absorption over each band. A two- or three-band absorption coefficient distribution has been effectively used. One of the methods that have been used successfully to model the radiative transport is the zonal model. The free surface is determined by a force balance, as mentioned earlier, and the defects are computed using the kinetics model given above. The changes in the local properties due to the presence of dopants are similarly incorporated. Figure 10 shows the calculated concentration of these defects at the exit of the draw furnace as a function of the furnace temperature and the concentration of different dopants [47]. Clearly the temperature is the most critical factor in the generation of this and other thermally induced

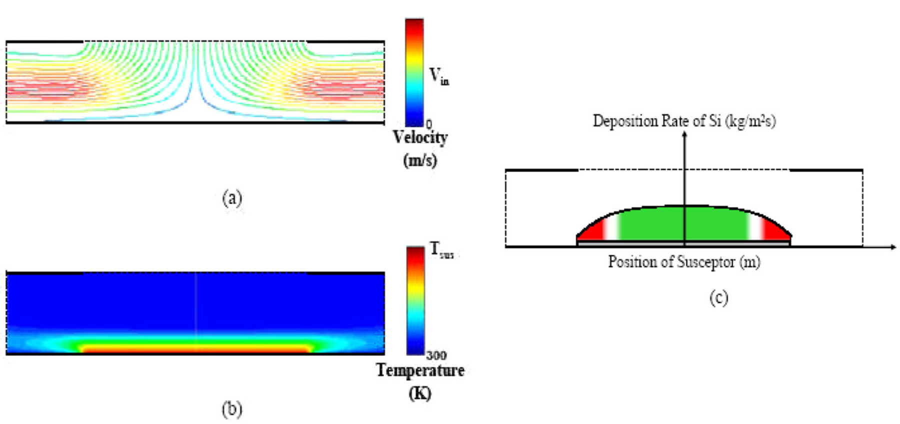


Fig. 9 Typical results on flow, temperature distribution, and deposition in a CVD reactor [36]

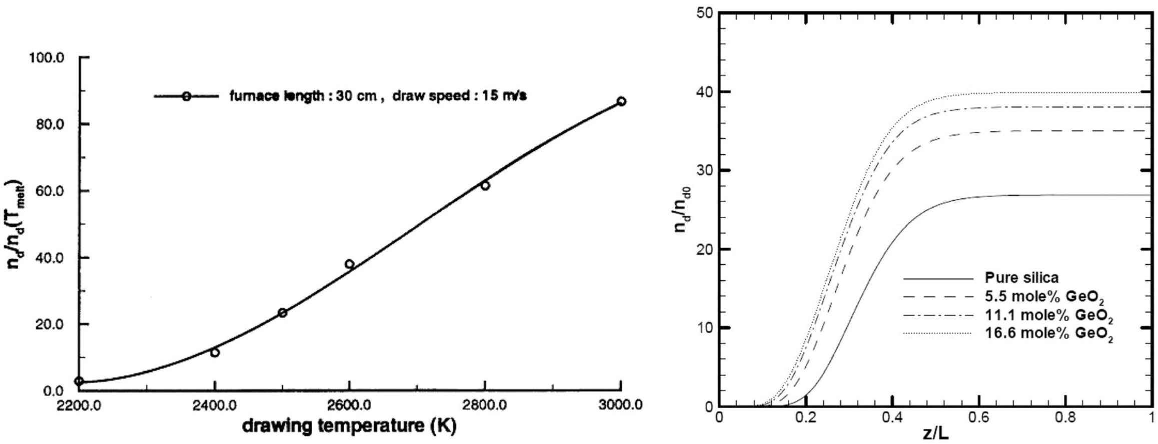


Fig. 10 Dependence of the thermally induced *E'* defects in optical fiber drawing on furnace temperature and dopant concentration [47]

defects. But annealing of the fiber, or slow cooling following the draw process, allows the defects to be reduced as recombination occurs to form the Si-O bond.

Similar considerations arise in other material processing applications. For instance, the chemical conversion of a reactive polymer like food occurs at the molecular or nanoscale level, whereas the boundary conditions are imposed at the macroscale, an example being the barrel temperature in extrusion or the applied pressure in injection molding. The conversion process in food depends on the shear as well as the temperature and, thus, the product is a strong function of the nature of conversion and the temperature and shear undergone by the material. Detailed studies have been carried out on the chemical kinetics and the conversion process, linking these with the product characteristics in food extrusion [5,14]. But, clearly a lot more needs to be done on linking the micro/nanoscale processes with the macro or engineering scale in order to accurately and realistically model the processes undergone by the material and the resulting characteristics.

System Design and Optimization

As discussed in detail in the preceding, analytical/numerical modeling and experimentation lead to a better understanding of the manufacturing process under consideration and of the basic thermal transport mechanisms that arise. The effects of various initial and boundary conditions are determined, providing a means to predict the transport process undergone by the material and the transformations that occur. However, one of the major goals of any simulation or experimentation is to employ the results obtained for designing an appropriate thermal system. Since a system is needed to provide the environment for the given process and since boundary conditions are imposed on the system, it is important to consider the design of the system and obtain an acceptable or feasible design that meets the given requirements without violating constraints, such as those arising from material, size, cost, energy, and other limitations. A feasible design is then followed by optimization of the process, in terms of the operating conditions, and of the system, in terms of the design parameters, to obtain high product quality, low cost, high efficiency, reduced environmental effect, high repeatability and consistency, and so on. Thus, the main engineering considerations involved in obtaining the desired thermal process are

- inverse problem to determine the appropriate boundary conditions
- feasibility of the process
- design of the thermal system
- optimization of the process with respect to operating conditions
- optimization of the system with respect to physical parameters and hardware
- sensitivity analysis
- effect of uncertainties

Inverse Problem. The imposition of boundary conditions and choice of governing parameters to achieve the desired thermal process is generally an inverse heat transfer problem, with multiple solutions. Effort must thus be directed at obtaining solutions in a narrow domain so that an essential unique result is achieved [48,49]. In many cases the direct solution, with given conditions, is solved and optimization techniques are used to converge to a solution to the inverse problem. An example is given in Fig. 11 for the optical fiber drawing furnace. The wall temperature is an unknown. However, by measuring the temperature distribution in a graphite rod placed at the center of the furnace and solving the inverse problem, the wall temperature distribution can be obtained [50]. Figure 11 shows the physical system, the measured centerline temperatures from the graphite rod, and the wall temperature distribution obtained, with two different rod diameters and cooled ends of the wall, from the inverse solution. Optimization was used to obtain an essentially unique result, which was found to agree closely with experimental data available from a temperature sensor used for control and that yielded the wall temperature at a specified location. Similar approaches have been used for other materials processing systems.

Feasible Design. The feasibility of the process is determined by the physical constraints, such as temperature, pressure and tension limitations, and availability and cost of resources and materials needed. This aspect is considered after a conceptual design has been selected. In terms of thermal issues, the boundary conditions are varied to ensure that the process is physically feasible. An example of this aspect is shown in Fig. 12, which gives the results for the drawing of a hollow optical fiber [51,52]. The neck-down profiles are shown for a few cases that are not acceptable due to the viscous rupture of the fiber or the central hollow collapsing, which results in a solid fiber rather than a hollow one. A feasibility domain is also shown for this process, along with the two main causes of infeasibility. Similar feasibility diagrams may be obtained through numerical simulation of various materials processing applications to determine the domain over which the design is feasible. Clearly this is a very important consideration in thermal processing of materials. However, not much work has been done on this aspect for the large variety of processes that have significant thermal issues.

Optimization. A feasible design would generally not be the best or optimal design, as judged on the basis of cost, efficiency,

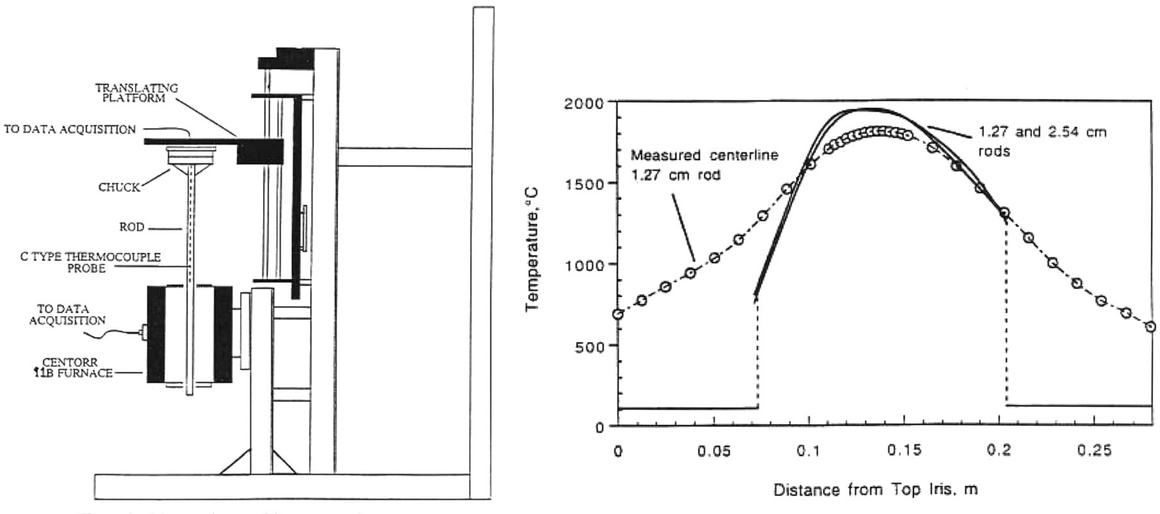


Fig. 11 Sketch of a fiber drawing furnace with an instrumented graphite rod at the center and the solution from an inverse problem to determine the furnace wall temperature distribution [50]

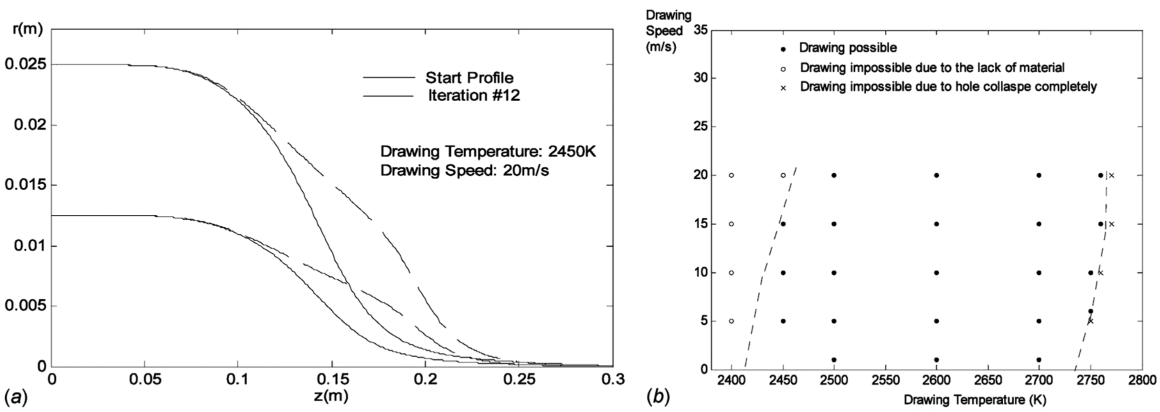


Fig. 12 Calculated neck-down profiles in hollow fiber drawing for infeasible draw conditions and the feasibility domain [52]

quality or performance per unit cost, or other such measures. In recent years, it has become crucial to optimize the process and the system due to growing global competition. An important consideration in optimization is the quantity or objective function U, which is to be minimized or maximized. Search methods are among the most important optimization strategies for materials processing. A number of designs are generated and the best among these is selected. The steepest ascent/descent method and other gradient-based methods are widely used for thermal systems [6].

The objective function is among the most critical and difficult aspects to be decided in the optimization of materials processing systems since the optimal design is often a strong function of the chosen criterion for optimization. In many cases, optimization is carried out for different criteria and the final design is chosen by comparison of results for different criteria. Each criterion leads to an optimization curve and the combination of these is known as a Pareto set obtained by considering different criteria in a multicriteria optimization problem. Then, the optimization is based on trading-off between different criteria.

As an example, let us consider a CVD system. The main qualities of interest include product quality, often characterized by the uniformity of the film, and the production rate, characterized by the deposition rate [53,54]. These may then be represented by the percentage working area (PWA), which gives the percentage acceptable from the film uniformity, and the mean deposition rate (MDR). Similarly, rms and kurtosis may be used to represent uniformity. These quantities may be combined to yield a single objective function, which is optimized with the given constraints, or each objective function may be considered separately to obtain the Pareto set [55,56]. In the first case, the composite objective function may assume many possible forms and the optimal design will generally depend on the function chosen. Some examples are

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

$$U = (\text{PWA}) \times (\text{MDR}) \quad (16)$$

We can also choose one of the quantities for maximization, while the other is specified by a given constraint. For example, we could

$$\text{Maximize } U = \text{PWA for given constraint on MDR} \quad (17a)$$

$$\text{Maximize } U = \text{MDR for given constraint on PWA} \quad (17b)$$

Then, we could specify that the deposition rate should not be lower than a given value while we maximize the percentage working area, and vice versa. This approach was found to be quite definitive and to yield useful and consistent results.

On the basis of simulation and experimental results, response surfaces may be generated to represent the overall behavior of the process or the system. Response surfaces of different orders can be generated, though lower order surfaces, such as second and

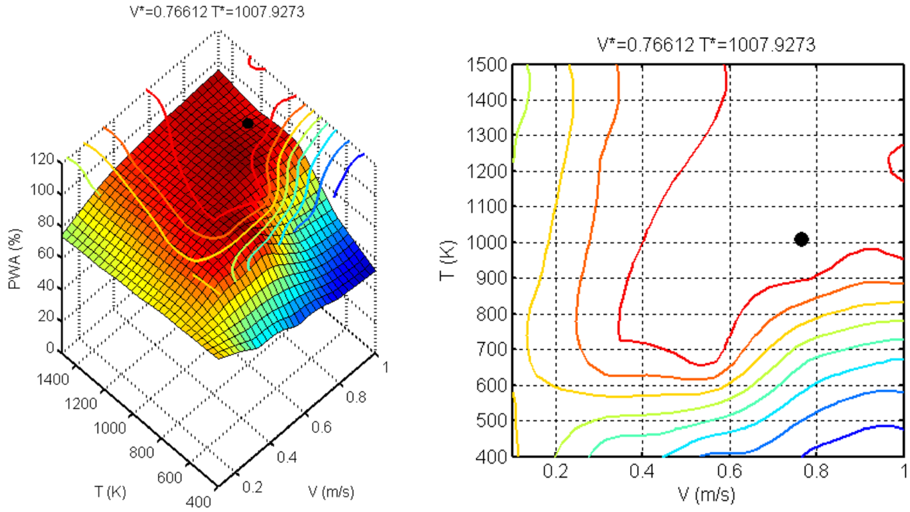


Fig. 13 Response surface for the percentage working area (PWA) and the optimal conditions in terms of susceptor temperature and average inlet flow velocity for an impingement CVD reactor for the deposition of silicon [36,54]

third order, are desirable for ease in optimization [57]. Figure 13(*a*) shows a typical response surface obtained from numerical simulation for the deposition of silicon [36,54]. Generally, effort is made to use a relatively small number of simulation runs since each is expensive in complicated systems. This figure is based on only 25 runs selected to cover the feasible domain. The figure, thus, indicates the dependence on the operating conditions and the existence of an optimal circumstance, which is shown on a two-dimensional plot in Fig. 13(*b*). Many such cases were investigated and the optimal processing conditions determined. Similar approaches can be used for other processes, though the effort has generally been relatively small so far. Also, several recent advances, such as genetic algorithms, concurrent experimental and numerical methods to obtain the inputs, and knowledge based methodology, can be used to make the optimization process more efficient.

Uncertainties. Essentially all the design parameters and operating conditions are subject to uncertainties, which must be considered because the failures of a given thermal system can be dangerous and expensive. A review paper by Lin et al. [36] presents a systematic strategy of thermal system modeling and optimization including the effects of uncertainties. An impingement CVD reactor is taken as an example. Some of the major uncertainties that arise in this process are

Uncertainties in Operating Conditions

- inlet velocity or flow rate
- susceptor temperature or heat flux input
- inlet mass fractions of reactive gases
- initial conditions
- ambient conditions

Uncertainties in System Design

- dimensions
- inlet and susceptor concentricity
- geometric symmetry
- material and gas properties

Focusing on objectives such as percentage working area and mean deposition rate, the reliability-based design optimization (RBDO) algorithms are employed. Probabilistic constraints are established with respect to either normally or non-normally distributed random variables and optimal solutions are obtained subject to the allowable level of failure probability. Figure 14 shows a sample of results for different constraints, with normal distribution of the variables. The failure is brought down to less

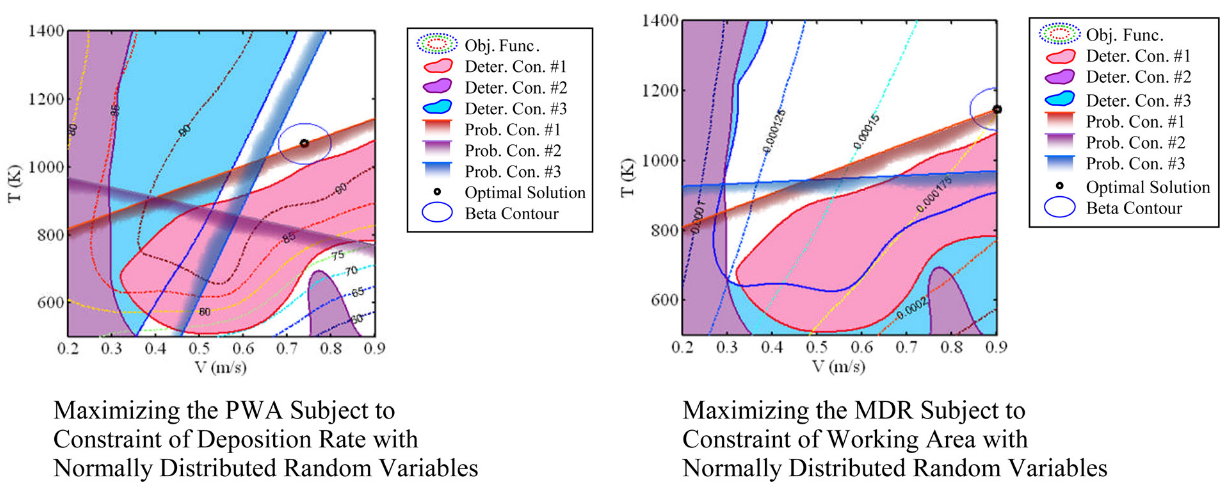


Fig. 14 Optimization with deterministic and probabilistic constraints for normally distributed variables, indicating the optimization with variables with given uncertainties to achieve a specified level of reliability [36]

than 0.13%, which is the accepted level in RBDO. Due to the uncertainties, the optimal point moves to satisfy this condition. Without uncertainties, the failure rate was over 40% in both the cases shown in the figure and, by including uncertainties, a more realistic and practical optimal design is obtained. Further details are given in [33] and other references on reliability-based design are also given in this paper. This aspect has only recently been incorporated in design and optimization of thermal systems. Clearly much work is needed for the materials processing systems to obtain optimal designs that are more reliable and realistic.

Future Research Needs

Throughout the discussions in the preceding, some applicable approaches and characteristic results on materials processing were presented. The need for future work on various aspects was also pointed out. To summarize these comments, the following list may be given as the areas that need detailed and focused future research to further understand the underlying thermal issues and model, simulate, design, and optimize systems for materials processing.

1. There is strong need for information on material characteristics and property variations since the accuracy of the model, as well as of the predictions from experimental data, depend on these.
2. A better quantitative understanding of the effect of the micro/nanoscale transport processes on material changes is needed in order to control the operating conditions in order to obtain the desired product characteristics.
3. A better coupling is needed between micro/nanoscale and macroscale processes since the material changes occur at the former scales and operating conditions are imposed at the latter scales.
4. Model validation is critical for obtaining accurate and dependable results for the design, prediction, and control of the process. Validation is needed at both micro/nanoscale and macroscale levels.
5. Further detailed and well planned experimentation is critical for validation, physical insight, and inputs to improve existing processes and develop new ones.
6. In many cases, special instrumentation is needed to study the basic processes involved, particularly with respect to changes undergone by the material subjected to the thermal process.
7. Since experimental data and simulation results are both important in understanding and developing the manufacturing process, further work is needed on combined analytical/ numerical and experimental approaches.
8. Further work is crucial on feasibility, control, design, and optimization if the existing processes are to be improved and new techniques are to be developed.
9. Future work should focus on the thermal processing of new materials and devices, particularly for new and emerging applications in biological, energy, transportation, and environmental systems.
10. It is important to study the sensitivity of the results obtained to boundary conditions and important design parameters for existing and new manufacturing processes.
11. A detailed consideration of appropriate objective functions for different manufacturing processes is important and needed. This study must also be coupled with multiobjective optimization, using available methods as well developing new ones.
12. Since uncertainties invariable arise in physical variables, it is important to consider this aspect in typical manufacturing processes in order to obtain realistic designs.

Of these, the most critical are material properties, experimentation, and linking very different length and time scales that arise in materials processing. There is very limited information on these aspects, despite their importance in an accurate simulation and design of materials processing systems. The other issues are also important and demand further study to add to the existing information. Finally, only a selected number of processes have been considered here. There is a wide range of materials processing techniques that are currently in use for a variety of applications [58]. Though the basic considerations are similar to those presented here, there are obviously many additional aspects that arise with different processes and need detailed study.

Conclusions

Thermal aspects are crucial in a wide range of materials processing systems and determine the characteristics and quality of the product, as well as the production rate. The transformation of the material is largely driven by the thermal process undergone by the material in processes such as annealing, baking, and drying and heat input is needed to achieve the desired process in crystal growing, glass forming, soldering, and polymer extrusion. In other cases, heat removal and thermally induced defects are of concern. This paper focuses on processes where thermal issues are of particular significance. Some of the major complexities that arise are discussed, along with possible approaches to solve them. Typical experimental and numerical results are presented for a variety of processes.

Since material transformations often occur at the micro/nanoscale range, whereas the boundary conditions are imposed at engineering scales, a multiscale problem is generally of interest, linking the processes at different scales. Experimentation is needed for validation of the models, for physical insight, and for providing inputs to simplify the analysis as well as in cases where analysis is unavailable, difficult, or inaccurate. The design and optimization of the thermal system needed to achieve the desired process is an important consideration in this area. The paper considers inverse problems for choosing the appropriate boundary conditions, obtaining a feasible design and optimizing the process and the system. Several objectives are generally of interest, for instance, product quality and production rate, and a multiobjective optimization with trade-offs is often the best approach. These issues are discussed in detail. The optimization must also consider possible uncertainties in design parameters and operating conditions to obtain realistic and useful results. The paper presents current and future trends in materials processing and suggests areas in which further work is needed. Among the most crucial ones are material properties and characteristics, experimental results, coupling micro/nanoscale processes with those at macroscale, and optimization.

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Nomenclature

b = temperature coefficient of viscosity
b_m = concentration coefficient of viscosity
C = species concentration
C_p = specific heat at constant pressure
D_{ij} = mass diffusion coefficient of species i in j direction
$\bar{e}$ = unit vector in the direction of gravitational force
E = activation energy
$\bar{F}$ = body force vector
g = magnitude of gravitational acceleration
Gr = Grashof number
h = convective heat transfer coefficient
$\bar{i}$ = unit vector in x direction
k, K = thermal conductivity

K_c = consistency index for non-Newtonian fluid
L = characteristic length
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
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
S_r = radiative source
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
μ = dynamic viscosity of fluid
ν = kinematic viscosity
ω_i = concentration of species i
Φ = viscous dissipation function
ρ = density
θ = dimensionless temperature

Subscripts

a = ambient
b = barrel; wall
i = initial; inlet
melt = melting/softening point
o = reference
s = solid, surface

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