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Jonathan A. Dantzig and Charles L. Tucker III
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MODELING IN MATERIALS PROCESSING

Mathematical modeling and computer simulation have been widely embraced in industry as useful tools for improving materials processing. Although courses in materials processing have covered modeling, they have traditionally been devoted to one particular class of materials, that is, polymers, metals, or ceramics. This text offers a new approach, presenting an integrated treatment of metallic and nonmetallic materials. The authors show that a common base of knowledge – specifically, the fundamentals of heat transfer and fluid mechanics – provides a unifying theme for these seemingly disparate areas. Emphasis is placed on understanding basic physical phenomena and knowing how to include them in a model. Thus, chapters explain how to decide which physical phenomena are important in specific applications, and how to develop analytical models. A unique feature is the use of scaling analysis as a rational way to simplify the general governing equations for each individual process. The book also treats selected numerical methods, showing the relationship among the physical system, analytical solution, and the numerical scheme. A wealth of practical, realistic examples are provided, as well as homework exercises. Students, and practicing engineers who must deal with a wide variety of materials and processing problems, will benefit from the unified treatment presented in this book.

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Preface

After some years of teaching separate courses on metal solidification and polymer processing, we realized that the two subjects shared a substantial base of common material. All the models started with the same basic equations and were built by using the same general procedure. We began to teach a single course on materials processing, and we found that our unified treatment gave students a better overall perspective on modeling. We also discovered that we needed a new book, as existing texts were almost all devoted exclusively to polymers, or to metals, or to ceramics. In this book, we treat metal and polymer processing problems together, building around the transport equations as a unifying theme.

We were also dissatisfied with ad hoc model development, in which terms were arbitrarily dropped from the governing equations, or simplifications were made without a clear explanation. Simplifying the general governing equations is a critical step in modeling, but it is a skill, not an art. In this text we introduce scaling analysis as a systematic way to reduce the governing equations for any particular problem. Scaling provides a way for both novices and experts to simplify a model, while ensuring that all of the important phenomena are included.

After deriving the governing equations in their general form and introducing scaling analysis, we examine physical phenomena such as heat conduction and fluid flow. We work out many problems that include only a few of these phenomena – problems that can be solved analytically. One might call these "canonical problems." They allow the reader to study each phenomenon in isolation, and then to explore how that phenomenon interacts with others. Real processes frequently involve multiple physical phenomena, and the ability to isolate a single phenomenon and understand its role is one of the great benefits of modeling. Canonical problems help students place different phenomena in perspective, and give them the ability to anticipate which phenomena will be important in any particular process. We once overheard a student describe our materials processing course as "the place where you finally understand what they taught you in heat transfer and fluid mechanics." We hope so.

We present examples for many different materials and processes, including polymer extrusion and injection molding, as well as metal casting and microstructure development. In each example we begin with the governing equations, and we use scaling to arrive at the final set of equations to be solved. This systematic approach makes problems for many different materials accessible.

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Of course, most practical materials processing models require a numerical solution, and any accomplished modeler knows a great deal about numerical methods. We chose not to say much about numerical methods, preferring to give solid coverage to the governing equations and physical phenomena. However, our canonical problems provide excellent test cases for numerical solution methods, and we use them to demonstrate some of the pitfalls of numerical modeling. By showing examples in which numerical schemes may be inaccurate or unstable, we help the reader become a more intelligent user of modeling software.

There is a lot to learn here, and many of the exercises at the end of each chapter go beyond the examples in the chapter. These exercises are written in a way that guides the student through the problem, step by step. This style emphasizes the overall pattern of problem solving, and it allows students to do more complex problems than they could otherwise attempt. A full set of solutions is available to instructors who adopt the book as a course text. Please contact the authors for the Solutions Manual.

We started writing this book to distill the important lessons from our own experience, one of us in polymer processing and the other in metal solidification. We eventually found that knowing more about modeling of all types of materials made us better at modeling the materials and processes we were so familiar with. We hope you will have the same experience.

Jonathan A. Dantzig
Charles L. Tucker III
Urbana, Illinois
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Principal Nomenclature

Symbol	*Quantity Represented*
A	area
a	parameter in exponential model for temperature-dependent viscosity
$\mathbf{b}$	vector of body force per unit mass
C_A	mass fraction of species A
C_ℓ	mass fraction of solute in liquid
C_s	mass fraction of solute in solid
$\hat{C}_A$	concentration (mass per unit volume) of species A
c_0, c_1, etc.	constants of integration
c_p	specific heat at constant pressure
c_v	specific heat at constant volume
D	mass diffusivity of solute; diameter
D_{AB}	intrinsic mass diffusivity of species A in B
$\tilde{D}$	interdiffusion coefficient of species A in B
$\mathbf{D}$	rate-of-deformation tensor $= (\mathbf{L}+\mathbf{L}^T)/2$
E	internal energy of a system
E_η, E_D	activation energies for viscosity, diffusion
$\mathbf{e}_1$, $\mathbf{e}_x$, etc.	unit vectors
$\mathbf{F}$	deformation gradient tensor, $F_{ij} = \partial X_i/\partial x_j$
f_ℓ	mass fraction of liquid
f_s	mass fraction of solid
g	acceleration that is due to gravity $= 9.82$ m/s^2
G	temperature gradient; magnitude of pressure gradient
h	heat transfer coefficient; height above a reference level; half-gap height
H	gap height; specific enthalpy
$\mathbf{I}$	unit tensor (identity tensor); the ij component is δ_{ij}
I_D, II_D, III_D	scalar invariants of the tensor $\mathbf{D}$
i	$\sqrt{-1}$
$\mathbf{J}_A$	mass fraction flux for species A, equal to $\hat{\mathbf{J}}_A/\rho$
$\hat{\mathbf{J}}_A$	mass flux vector for species A (mol/area $\times$ time)
J	Jacobian $=$ det $\mathbf{F}$

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J_0, J_1	Bessel functions of the first kind, of order zero and one
$\mathbf{k}$	thermal conductivity (tensor)
k	thermal conductivity (scalar)
k_0	partition coefficient
L	length
L_d	primary dendrite arm length
L_f	latent heat of fusion
L_p	latent heat of pressure change
L_v	latent heat of volume change
$\mathbf{L}$	velocity gradient tensor, $L_{ij} = \partial v_i / \partial x_j$
ℓ	filled length of a mold
m	material constant in the power law model
m_ℓ, m_S	slopes of the liquidus and solidus lines
M	mass of a system; morphological number
n	power law index
$\mathbf{n}$	unit vector normal to a surface
P	power input to a system
p	pressure
$\hat{p}$	modified pressure $= p + \rho_0 g h$
$\mathbf{q}$	heat flux vector
Q	volume flow rate; power of a point heat source; heat input to a system
$\mathbf{Q}$	rotation matrix
R	radius; gas constant = 8.31 J/mol K
$\dot{R}$	specific heat generation rate
R_A	generation rate of species A
$\mathcal{R}$	thermal resistance
r, θ, z	cylindrical coordinates
r, θ, ϕ	spherical coordinates
S	bounding surface; specific entropy; flow conductance
s	inverse of power law index $= 1/n$
T	temperature; torque
T_m	melting temperature
T_L	liquidus temperature
T_S	solidus temperature
t	time
$\mathbf{t}$	surface traction vector
$\hat{\mathbf{t}}$	unit vector tangent to a curve
$\mathbf{v}$	velocity vector
V	volume; average velocity
$\hat{V}$	specific volume
W	width
$\mathbf{W}$	vorticity tensor $= (\mathbf{L} - \mathbf{L}^T)/2$
$\mathbf{X}$	material coordinate vector
$\mathbf{x}$	position vector
x, y, z	Cartesian coordinates; also x_1, x_2, x_3

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α	thermal diffusivity $= k/(\rho c_p)$
β	volumetric thermal expansion coefficient
Γ	surface tension (interfacial tension)
$\dot{\gamma}$	scalar strain rate $= (2\mathbf{D}:\mathbf{D})^{1/2}$
δ	solidified layer thickness; boundary layer thickness
δ_{ij}	unit tensor in indicial notation (the Kronecker delta)
ε	specific internal energy
ϵ_{ijk}	permutation symbol
κ	curvature of a curve; ratio of an outer radius to inner radius
κ_m, κ_G	mean and Gaussian curvatures of a surface
Λ	magnitude of the pressure gradient
λ	dilatational viscosity, compressible Newtonian fluid
λ_2	secondary dendrite arm spacing
μ	viscosity, Newtonian fluid
ν	kinematic viscosity $= \mu/\rho$
η	viscosity, non-Newtonian fluid
π	3.14159...
ρ	density
ρ_0	density at reference temperature and pressure
θ	dimensionless temperature; angular coordinate
$\boldsymbol{\sigma}$	total stress tensor
$\boldsymbol{\tau}$	extra stress tensor
τ	scalar magnitude of $\boldsymbol{\tau}$
τ_Y	yield stress
Ω	angular velocity
$\boldsymbol{\omega}$	vorticity vector $= \nabla \times \mathbf{v}$
ξ	scaled length within a boundary layer
ζ	similarity variable

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