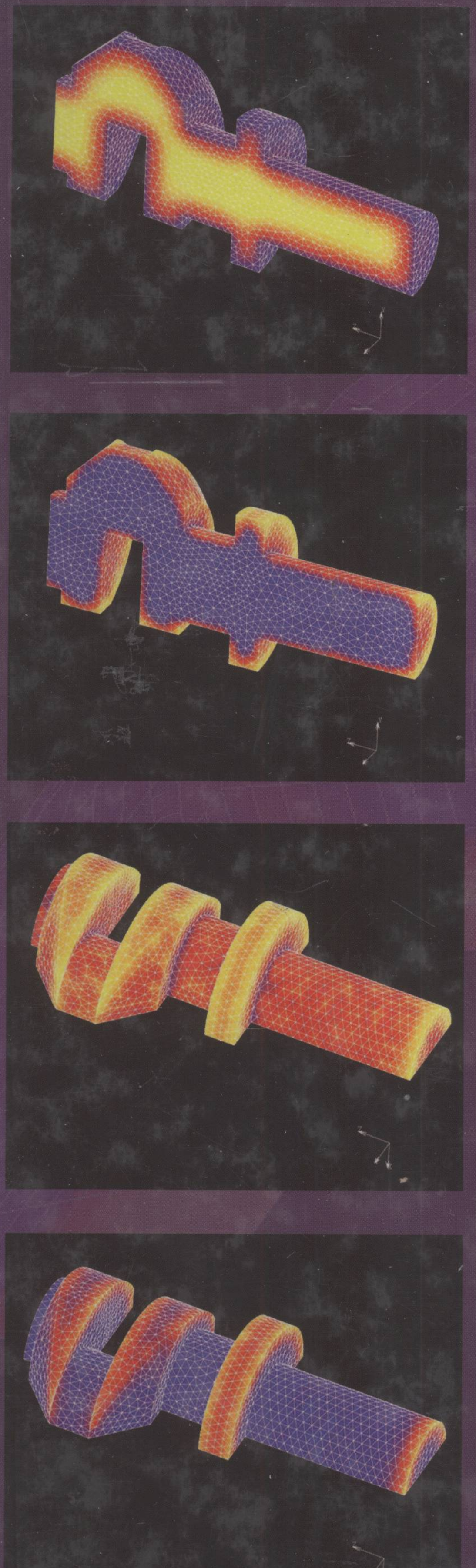


Handbook of

Thermal Process Modeling of Steels

EDITED BY
CEMIL HAKAN GÜR
JIANSHENG PAN

IFHTSE
INTERNATIONAL FEDERATION FOR HEAT TREATMENT AND SURFACE ENGINEERING

CRC Press
Taylor & Francis Group

Handbook of Thermal Process Modeling of Steels

Edited by
Cemil Hakan Gür
Jiansheng Pan

CRC Press
Taylor & Francis Group
Boca Raton London New York

CRC Press is an imprint of the
Taylor & Francis Group, an **informa** business

IFHTSE
INTERNATIONAL FEDERATION
FOR HEAT TREATMENT AND
SURFACE ENGINEERING

CRC Press
Taylor & Francis Group
6000 Broken Sound Parkway NW, Suite 300
Boca Raton, FL 33487-2742

Printed in the United States of America on acid-free paper
10 9 8 7 6 5 4 3 2 1

International Standard Book Number-13: 978-0-8493-5019-1 (Hardcover)

Visit the Taylor & Francis Web site at
http://www.taylorandfrancis.com

and the CRC Press Web site at
http://www.crcpress.com

Handbook of

Thermal Process Modeling of Steels

Preface

The whole range of steel thermal processing technology, from casting and plastic forming to welding and heat treatment, not only produces workpieces of the required shape but also optimizes the end-product microstructure. Thermal processing thus plays a central role in quality control, service life, and the ultimate reliability of engineering components, and now represents a fundamental element of any company's competitive capability.

Substantial advances in research, toward increasingly accurate prediction of the microstructure and properties of workpieces produced by thermal processing, were based on solutions of partial differential equations (PDEs) for temperature, concentration, electromagnetic properties, and stress and strain phenomena. Until the widespread use of high-performance computers, analytical solution of PDEs was the only approach to describe these parameters, and this placed severe limitations in terms of prediction for engineering applications so that thermal process developments themselves relied on empiricism and traditional practice. The level of inaccuracy inherent in computational predictions hindered both materials performance improvements and process cost reduction.

Since the 1970s, the pace of development of computer technology has made possible effective solution of PDEs in complicated calculations for boundary and initial conditions, as well as nonlinear and multiple variables. Mathematical models and computer simulation technology have developed rapidly; currently well-established mathematical models integrate fundamental theories of materials science and engineering including heat transfer, thermoelastoplastic mechanics, fluid mechanics, and chemistry to describe physical phenomena occurring during thermal processing. Further, evolution of transient temperature, stress–strain, concentration, microstructure, and flow can now be vividly displayed through the latest visual technology, which can show the effects of individual process parameters. Computation/simulation thus provides an additional decision-making tool for both the process optimization and the design of plant and equipment; it accelerates thermal processing technology development on a scientifically sound computational basis.

The basic mathematical models for thermal processing simulation gradually introduced to date have yielded enormous advantages for some engineering applications. Continued research in this direction attracts increasing attention now that the cutting-edge potential of future developments is evident. Increasingly profound investigations are now in train globally. The number of important research papers in the field has risen sharply over the last three decades. Even so, the existing models are regarded as highly simplified by comparison with real commercial thermal processes. This has meant that the application of computer simulation has thus far been relatively limited precisely because of these simplifying assumptions, and their consequent limited computational accuracy. Extensive and continuing research is still needed.

This book is now offered as both a contribution to work on the limitations described above and as an encouragement to increase the understanding and use of thermal process models and simulation techniques.

The main objectives of this book are, therefore, to provide a useful resource for thermal processing of steels by drawing together

- An approach to a fundamental understanding of thermal process modeling
- A guide to process optimization
- An aid to understand real-time process control
- Some insights into the physical origin of some aspects of materials behavior
- What is involved in predicting material response under real industrial conditions not easily reproduced in the laboratory

Linked objectives are to provide

- A summary of the current state of the art by introducing mathematical modeling methodology actually used in thermal processing
- A practical reference (industrial examples and necessary precautionary measures are included)

It is hoped that this book will

- Increase the potential use of computer simulation by engineers and technicians engaged in thermal processing currently and in the future
- Highlight problems requiring further research and be helpful in promoting thermal process research and applications

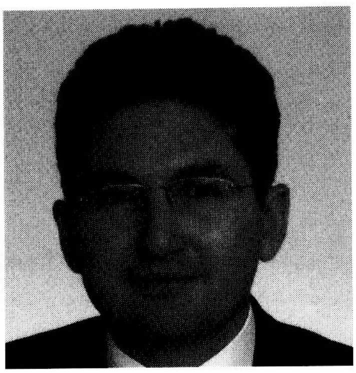
This project was realized due to the hard work of many people. We express our warm appreciation to the authors of the respective chapters for their diligence and contribution. The editors are truly indebted to everyone for their contribution, assistance, encouragement, and constructive criticism throughout the preparation of this book.

Here, we also extend our sincere gratitude to Dr. George E. Totten (Totten Associates and a former president of the International Federation for Heat Treatment and Surface Engineering [IFHTSE]) and Robert Wood (secretary general, IFHTSE), whose initial encouragement made this book possible, and to the staff of CRC Press and Taylor & Francis for their patience and assistance throughout the production process.

C. Hakan Gür
Middle East Technical University

Jiansheng Pan
Shanghai, Jiao Tong University

Editors



C. Hakan Gür is a professor in the Department of Metallurgical and Materials Engineering at Middle East Technical University, Ankara, Turkey. He is also the director of the Welding Technology and Nondestructive Testing Research and Application Center at the same university. Professor Gür has published numerous papers on a wide range of topics in materials science and engineering and serves on the editorial boards of national and international journals. His current research includes simulation of tempering and severe plastic deformation processes, nondestructive evaluation of residual stresses, and microstructures obtained by various manufacturing processes.

Jiansheng Pan is a professor in the School of Materials Science and Engineering at Shanghai Jiao Tong University, Shanghai, China. He was an elected member of the Chinese Academy of Engineering in 2001. Professor Pan's expertise is in chemical and thermal processing of steels (including nitriding, carburizing, and quenching) and their computer modeling and simulation. He has established mathematical models of these processes integrating heat and mass transfer, continuum mechanics, fluid mechanics, numerical analysis, and software engineering. These models have been used for computational simulation to design and optimize thermal processes for parts with complicated shape. Pan and his coworkers have published extensively in these areas and have been awarded over 40 Chinese patents. In addition to a number of awards for scientific and technological achievements, Professor Pan was the president of the Chinese Heat Treatment Society (2003–2007) and is the chairman of the Mathematical Modeling and Computer Simulation Activity Group of the International Federation for Heat Treatment and Surface Engineering.

Contributors

María Victoria Bongiovanni
Facultad de Ingeniería
Universidad Austral
Buenos Aires, Argentina

and

Facultad de Ciencias Exactas y Naturales
Universidad de Buenos Aires
Buenos Aires, Argentina

Chris H.J. Davies
Department of Materials Engineering
Monash University
Melbourne, Victoria, Australia

Janez Grum
Faculty of Mechanical Engineering
University of Ljubljana
Ljubljana, Slovenia

Jianfeng Gu
School of Materials Science and Engineering
Shanghai Jiao Tong University
Shanghai, China

C. Hakan Gür
Department of Metallurgical and Materials Engineering
Middle East Technical University
Ankara, Turkey

Sivaraman Guruswamy
Department of Metallurgical Engineering
University of Utah
Salt Lake City, Utah

Bernardo Hernandez-Morales
Departamento de Ingeniería Metalúrgica
Universidad Nacional Autónoma de México
Mexico

Peter Hodgson
Centre for Material and Fibre Innovation
Institute for Technology Research and Innovation
Deakin University
Geelong, Victoria, Australia

John J. Jonas
Department of Materials Engineering
McGill University
Montreal, Quebec, Canada

Valentin Nemkov
Fluxtrol, Inc.
Auburn Hills, Michigan

and

Centre for Induction Technology
Auburn Hills, Michigan

Jiansheng Pan
School of Materials Science and Engineering
Shanghai Jiao Tong University
Shanghai, China

Mario Rosso
R&D Materials and Technologies
Politecnico di Torino
Dipartimento di Scienza dei Materiali e Ingegneria Chimica
Torino, Italy

and

Politecnico di Torino
Sede di Alessandria
Alessandria, Italy

Satyam Suraj Sahay
Tata Research Development and Design Centre
Tata Consultancy Services Limited
Pune, Maharashtra, India

Gustavo Sánchez Sarmiento
Facultad de Ingeniería
Universidad de Buenos Aires
Buenos Aires, Argentina

and

Facultad de Ingeniería
Universidad Austral
Buenos Aires, Argentina

Wei Shi
Department of Mechanical Engineering
Tsinghua University
Beijing, China

Caner Şimşir
Stiftung Institüt für Werkstofftechnik (IWT)
Bremen, Germany

Božo Smoljan
Department of Materials Science and Engineering
University of Rijeka
Rijeka, Croatia

Weimin Zhang
School of Materials Science and Engineering
Shanghai Jiao Tong University
Shanghai, China

Contents

1 Mathematical Fundamentals of Thermal Process Modeling of Steels

Jiansheng Pan and Jianfeng Gu

CONTENTS

Steels are usually under the action of multiple physical variable fields, such as temperature field, fluid field, electric field, magnetic field, plasm field, and so on during thermal processing. Thus, heat conduction, diffusion, phase transformation, evolution of microstructure, and mechanical deformation are simultaneously taken place inside. This chapter includes the mathematical fundamentals of the most widely used numerical analysis methods for the solution of partial differential equations (PDEs), and the basic knowledge of continuum mechanics, fluid mechanics, phase transformation kinetics, etc. All these are indispensable for the establishment of the coupled mathematical models and realization of numerical simulation of thermal processing.

1.1 THERMAL PROCESS PDEs AND THEIR SOLUTIONS

1.1.1 PDEs for Heat Conduction and Diffusion

The first step of computer simulation of thermal processing is to establish an accurate mathematical model, i.e., the PDEs and boundary conditions that can quantificationally describe the related phenomena.

The PDE describing the temperature field inside a solid is usually expressed as follows:

$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right)+Q=\rho c_p\frac{\partial T}{\partial \tau} \tag{1.1}$$

where

- T is the temperature
- τ is the time
- x, y, z are the coordinates
- λ is the thermal conduction coefficient
- ρ is the density
- c_p is the heat capacity
- Q is the intensity of the internal heat resource

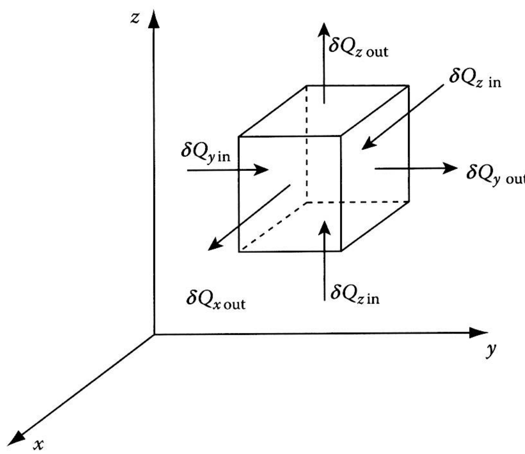


FIGURE 1.1 Heat flux along coordinates subjected to an infinitesimal element.

Equation 1.1 has a very clear physical concept, and can be illustrated as in Figure 1.1. The first item on the left-hand side of the equation is the net heat flux input to the infinitesimally small element along axis x, i.e., the difference between the heat flux entering $\delta Q_{x\text{in}}$ and the heat flux effusing $\delta Q_{x\text{out}}$. The second and third items are the net heat flux along axes y and z, respectively (Figure 1.1). The intensity of the internal heat source Q may be caused by different factors, such as phase transformation, plastic work, electricity current, etc. The right-hand side of the equation stands for the change in heat accumulating in the infinitesimal element per time unit due to the temperature change. Equation 1.1 shows that the sum of the heat input and heat generated by the internal heat source is equal to the change in heat accumulating for an infinitesimal element in each time unit, so it functions in accordance with the energy conservative law. The heat conduction coefficient λ, density ρ, heat capacity c_p, and the intensity of the internal heat source are usually the functions of temperature, making Equation 1.1 a nonlinear PDE.

There are three kinds of boundary conditions for heat exchange in all kinds of thermal processing technologies.

The first boundary condition S_1: The temperature of the boundary (usually certain surfaces) is known; it is a constant or function of time.

$$T_s = C(\tau) \tag{1.2}$$

The second boundary condition S_2: The heat flux of the boundary is known.

$$\lambda \frac{\partial T}{\partial n} = q \tag{1.3}$$

where

$\partial T/\partial n$ is the temperature gradient on the boundary along the external normal direction
q is the heat flux through the boundary surface

The third boundary condition S_3: The heat transfer coefficient between the workpiece and environment is known.

$$-\lambda\left(\frac{\partial T}{\partial n}\right) = h(T_a - T_s) \tag{1.4}$$

where

T_a is the environment temperature

T_s is the surface temperature of the workpiece

h is the overall heat transfer coefficient, representing the heat quantity exchanged between the workpiece surface and the environment per unit area and unit time when their temperature difference is 1°C

It is worth mentioning that only convective heat transfer occurs in some cases; however, radiation heat transfer should also be considered in other complicated ones, such as gas quenching and heating under protective atmosphere. Hence, the overall heat transfer coefficient h should be the sum of the convective heat transfer coefficient h_c and the radiation heat transfer coefficient h_r. Therefore, we have

$$h = h_c + h_r \tag{1.5}$$

The radiation heat transfer coefficient h_r can be obtained as follows:

$$h_r = \varepsilon\sigma(T_a^2 + T_s^2)(T_a + T_s) \tag{1.6}$$

where

ε is the radiation emissivity of the workpiece

σ is the Stefan–Boltzmann constant

The boundary condition can be set according to the specific thermal process, and the temperature field inside the workpiece at different times, the so-called unsteady temperature field, can be obtained by solving Equation 1.1. When the temperature field inside the workpiece does not change with time any more, it arrives at the steady temperature field, and the left-hand side of Equation 1.1 becomes zero.

The unsteady concentration field inside the workpiece subjected to carburizing or nitriding is usually governed by the following PDE.

$$\frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D\frac{\partial C}{\partial z}\right) = \frac{\partial C}{\partial \tau} \tag{1.7}$$

where

C is the concentration of the element being penetrated (carbon or nitrogen)

D is the diffusion coefficient

The boundary conditions can also be classified into the following three kinds.

Boundary s_1: The surface concentration is known.

$$C_s = C \tag{1.8}$$

Boundary s_2: The mass flux through the surface is known.

$$D\left(\frac{\partial C}{\partial n}\right) = q \tag{1.9}$$

Boundary s_3: The mass transfer coefficient between the workpiece surface and environment (ambient media) is known.

$$-D\left(\frac{\partial C}{\partial n}\right) = \beta(C_g - C_s) \quad (1.10)$$

where

D is the diffusion coefficient
β is the mass transfer coefficient
C_g is the atmosphere potential of carbon (or nitrogen)
C_s is the surface concentration of carbon (or nitrogen)

Although the diffusion and heat conduction PDEs describe different physical phenomena, their mathematical expression and solving method are exactly the same.

1.1.2 Solving Methods for PDEs

Usually, there are two methods to solve the PDEs, analytical method and numerical method. The analytical method, taking specific boundary conditions and initial conditions, can obtain the analytical solution by deduction (for example, variables separation method), which is a type of mathematical representation clearly describing certain field variables under space coordinates and time.

The analytical solution has the advantage of concision and accuracy, so it is also called exact solution. Although it plays an important role in fundamental research, it is only applicable to very few cases with relatively simple boundary and initial conditions. Therefore, the analytical solution cannot cope with massive problems under practical manufacture environment, which are featured with complicated boundary conditions and a high degree of nonlinearity.

The numerical solution, also named approximate solution, is applicable for different kinds of boundary conditions and can cope with nonlinear problems. It is the most basic simulation method in engineering. Up to now, the finite-element method (FEM) and finite-difference method (FDM) are the most widely used methods in simulation of the process, and their common characteristic is discretization of continuous functions, thus transforming the PDEs into large systems of simultaneous algebraic equations and solving the large algebraic equation group finally (Figure 1.2).

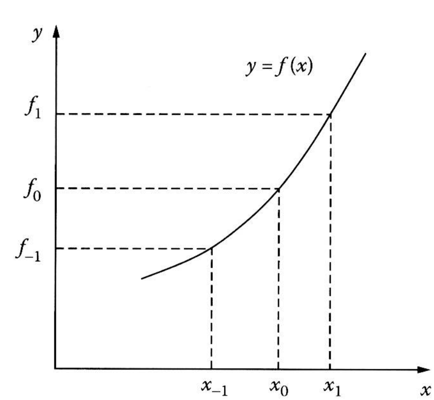


FIGURE 1.2 Discretization of the continuous function.

1.2 FINITE-DIFFERENCE METHOD

1.2.1 Introduction of FDM Principle

First, for a continuous function of x, namely $f(x), f_{-1}, f_0$, and f_1 are retained as the values of f at x_{-1}, x_0, and x_1, respectively (Figure 1.2). When the function has all its derivatives defined at x_0 and f_1, f_{-1} can be expressed by a Taylor series as follows:

$$f_1 = f_0 + \Delta x \cdot f_0' + \frac{(\Delta x)^2}{2!} f_0'' + \frac{(\Delta x)^3}{3!} f_0''' + \frac{(\Delta x)^{iV}}{4!} f_0^{iV} + \cdots \tag{1.11}$$

$$f_{-1} = f_0 - \Delta x \cdot f_0' + \frac{(\Delta x)^2}{2!} f_0'' - \frac{(\Delta x)^3}{3!} f_0''' + \frac{(\Delta x)^{iV}}{4!} f_0^{iV} - \cdots \tag{1.12}$$

Truncating the items after $(\Delta x)^2$, Equation 1.11 can be written as

$$\left.\frac{\partial f}{\partial x}\right|_{x=x_0} = f_0' = \frac{f_1 - f_0}{\Delta x} - \frac{\Delta x}{2} f_0'' \approx \frac{f_1 - f_0}{\Delta x} \tag{1.13}$$

Equation 1.13 is the first-order forward difference with its truncation error of $\Omega(\Delta x)$. Here $\Omega(\Delta x)$ is a formal mathematical notation, which represents terms of order Δx.

In the same way, another difference scheme from Equation 1.12 can be obtained as follows:

$$\left.\frac{\partial f}{\partial x}\right|_{x=x_0} = f_0' = \frac{f_0 - f_{-1}}{\Delta x} + \frac{\Delta x}{2} f_0'' \approx \frac{f_0 - f_{-1}}{\Delta x} \tag{1.14}$$

This is the first-order backward difference with its truncation error of $\Omega(\Delta x)$.

Subtracting Equation 1.12 from Equation 1.11 yields

$$\frac{\partial f}{\partial x} = f_0' = \frac{f_1 - f_{-1}}{2} + 2\frac{(\Delta x)^2}{3!} f_0''' \approx \frac{f_1 - f_{-1}}{2} \tag{1.15}$$

Equation 1.15 is the second-order central difference with its truncation error of $\Omega(\Delta x^2)$.

Summing Equations 1.11 and 1.12, and solving for $\partial^2 f/\partial x^2$, we have

$$\frac{\partial^2 f}{\partial x^2} = f_0'' = \frac{f_1 - 2f_0 + f_{-1}}{(\Delta x)^2} + 2\frac{(\Delta x)^2}{4!} f_0^{iV} \approx \frac{f_1 - 2f_0 + f_{-1}}{(\Delta x)^2} \tag{1.16}$$

Equation 1.16 is the second-order central second difference with its truncation error of $\Omega(\Delta x^2)$.

It can be observed that the truncation error, originating from the replacement of the partial derivatives by finite-difference quotients, makes the FDM solution an approximate one; however, the accuracy can be improved by reducing the step size.

1.2.2 FDM for One-Dimensional Heat Conduction and Diffusion

In this section, two simple cases are taken to elucidate the FDM to solve the PDEs in engineering. The first case is the unsteady, one-dimensional heat conduction PDE without an internal heat resource item, and the second one is the one-dimensional diffusion PDE.

The governing PDE for the unsteady, one-dimensional heat conduction without an internal heat resource item has the following concise form:

$$a\frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial \tau} \tag{1.17}$$