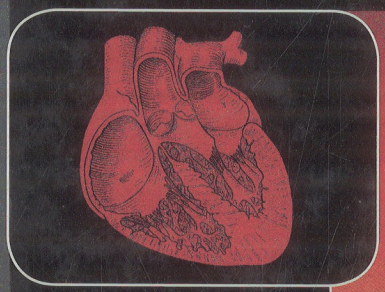
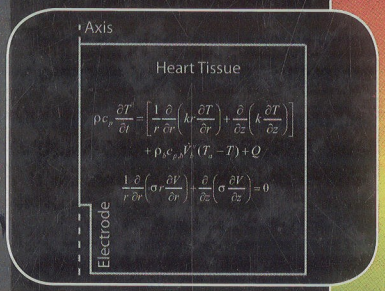
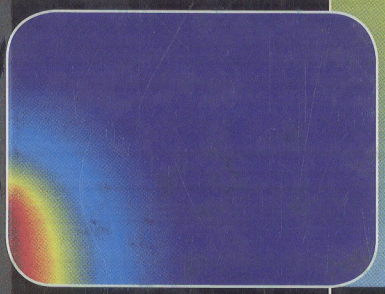
CAMBRIDGE TEXTS IN BIOMEDICAL ENGINEERING

An Introduction to **Modeling of Transport Processes**

Applications to Biomedical Systems







Ashim Datta and Vineet Rakesh

Contents

Preface xiii
Acknowledgments xvii
Introduction and overview xix
List of symbols xxv

I Essential steps **1**

1 Problem formulation **3**
1.1 Context: biomedical transport processes 3
1.2 What is problem formulation? 5
1.3 Steps in problem formulation 7
1.4 Defining goals for problem formulation 9
1.5 Simplify, simplify, simplify 11
1.6 Geometry: setting the computational domain 11
1.7 Governing equations 21
1.8 Boundary and initial conditions 27
1.9 Material properties 32
1.10 Other input parameters 35
1.11 Summary 35
1.12 Problems 37

2 Software implementation 1 **50**
2.1 Choosing a software 50
2.2 Software is not to be used as a blackbox 51
2.3 Organization of a typical CAE software: preprocessing, processing and postprocessing 51
2.4 Some general guidelines to preprocessing 54
2.5 Introduction to preprocessing in a computational software (COMSOL) 55
2.6 Geometry and analysis type 56
2.7 Geometry creation 60

2.7 Geometry creation 60
2.8 Governing equations 65
2.9 Boundary conditions 72
2.10 Initial conditions 77
2.11 Material properties 77
2.12 Miscellaneous implementation aspects 82
2.13 Problems 85

3 Software implementation 2 87
3.1 Which numerical method to use 87
3.2 Items needed in specifying the solution methodology 88
3.3 How to discretize the domain: mesh 88
3.4 How to choose a time step 98
3.5 How to choose a solver to solve the system of linear equations 103
3.6 Problems 106

4 Software implementation 3 108
4.1 Useful information in a biomedical context 109
4.2 Obtaining data at a particular location 111
4.3 Plotting transient data at one or more points, line or surface as a function of time 113
4.4 Obtaining surface/contour plots (in 2D problems) for observing variation within a region 117
4.5 Obtaining a surface plot in a 3D problem 121
4.6 Obtaining average values at a particular time or as a function of time 125
4.7 Obtaining arbitrary functions of computed variables 129
4.8 Creating animations 129
4.9 Dedicated plotting and postprocessing software 131
4.10 Relating to the goals of the simulation: guidelines for postprocessing 131
4.11 Analysis of data obtained from postprocessing 133
4.12 Presenting the simulation results to others 133
4.13 Problems 134
4.14 Appendix 136

5 Validation, sensitivity analysis, optimization and debugging 139
5.1 Types of errors and error reduction 140
5.2 Estimating error: validation of the model 144
5.3 Reducing discretization error: mesh convergence 146

5.4 Estimating uncertainty and relating to design: performing sensitivity analysis 151
5.5 Objective functions: simple optimization 155
5.6 When things don't work: debugging 157
5.7 Problems 161

II Case studies 177

6 Case studies 179
6.1 Introduction 179
6.2 How to use the case studies 182
6.3 Additional case studies from the work of students at Cornell University 183
Case Study I: Thermal ablation of hepatic tumors 186
Case Study II: Cryosurgery of a wart 201
Case Study III: Drug delivery from a patch 221
Case Study IV: Drug delivery in therapeutic contact lenses 243
Case Study V: Elimination of nitrogen from the blood stream during deep sea diving 251
Case Study VI: Flow in human carotid artery bifurcation 258
Case Study VII: Radioimmunotherapy of metastatic melanoma 270
Case Study VIII: Burn injury in blood-perfused skin 280
Case Study IX: Radiofrequency cardiac ablation 288
Case Study X: Laser irradiation of human breast tumor 303
6.4 Problems 321

III Background theory 333

7 Governing equations and boundary conditions 335
7.1 Conservation of mass: the continuity equation 336
7.2 Conservation of momentum: governing equation for fluid flow 338
7.3 Conservation of thermal energy: governing equation for heat transfer 342
7.4 Governing equation for heat conduction with change of phase 346
7.5 The bioheat transfer equation for mammalian tissue 349
7.6 Conservation of a mass species: governing equation for mass transfer 353
7.7 Non-dimensionalization of the governing equations 357
7.8 Coupling of governing equations 360
7.9 Summary: governing equations 362

7.10 Boundary conditions: general comments 362
7.11 Boundary conditions: fluid mechanics 362
7.12 Boundary conditions for heat transfer 364
7.13 Boundary conditions for mass transfer 367
7.14 Governing equations in various coordinate systems 373
7.15 Problems 378

8 Source terms 379
8.1 Heat source terms due to metabolism and blood flow 380
8.2 A generic form for the heat source term 380
8.3 Heat source term for electromagnetic heating 382
8.4 Microwave heating and its heat source term 384
8.5 Radiofrequency heating and its heat source term 389
8.6 Ferromagnetic heating and its heat source term 392
8.7 Infrared heating and its heat source term 393
8.8 Laser heating and its heat source term 395
8.9 Ultrasonic heating 401
8.10 Mass source terms 405
8.11 Summary 408
8.12 Problems 411

9 Material properties and other input parameters 414
9.1 What material property data and input parameters do we need? 414
9.2 Where do we get data? 415
9.3 How accurate should the data be? 416
9.4 What to do when accurate data is not available 416
9.5 Anatomical and physiological parameters 417
9.6 Rheological properties 424
9.7 Thermal conductivity 427
9.8 Specific heat 429
9.9 Density 433
9.10 Thermal diffusivity 433
9.11 Thermal properties of related materials 434
9.12 Latent heat of fusion and evaporation 434
9.13 Radiative properties 434
9.14 Equilibrium vapor pressure 435
9.15 Properties of an air–water vapor mixture 436
9.16 Mass diffusivity 436
9.17 Partition coefficient 439
9.18 Diffusive permeability and transmissibility 439
9.19 Reaction rate constants 443

9.20 Other parameters 444
9.21 Summary 450
9.22 Problems (short questions) 453

10 Solving the equations: numerical methods 455
10.1 Flexibility of numerical methods 456
10.2 Finite difference method (FDM) 458
10.3 FDM: converting the 1D heat equation to algebraic equations 460
10.4 FDM: stability (limitations in choosing step sizes) 464
10.5 FDM: summary 464
10.6 Finite element method (FEM) 465
10.7 FEM: converting the 1D heat equation to algebraic equations 465
10.8 FEM: solving the linear system of algebraic equations 478
10.9 FEM: choice between linear solvers 483
10.10 FEM: linearization of non-linear equations 483
10.11 FEM: error in the finite element method and its reduction 485
10.12 FEM: convergence of the numerical solution as the mesh is refined 487
10.13 FEM: stability of the numerical solution 488
10.14 FEM: generalization of methodology to more complex situations 488
10.15 FEM: summary 490
10.16 Problems 491

Index 497