Part III
CTDS Modelling and Simulation

There are several features that distinguish the modelling and simulation activity within the continuous time dynamic system (CTDS) domain. Perhaps one of the most important is the dependence of the project's success upon the selection of the behaviour generation tool that is best suited to the nature of the conceptual model. Because the conceptual model in this domain always includes a set of differential equations, the tools in question relates to the numerical procedures for solving these equations (we restrict our discussions to the case where only ordinary differential equations (ode's) are included in the model).

Many families of approaches for the solution of ode's can be found in the literature, and within each family there generally are numerous specific options. The methods in these families have their characteristic strengths and weaknesses and are often best suited for specific categories of problems. Furthermore, the use of any of these methods usually involves the specification of values for embedded parameters. The range of options is indeed wide and can even become daunting. To embark on a modelling and simulation project in this environment without some appreciation for the issues involved can be foolhardy. Our objective in the third part of this book is to provide a basic foundation for dealing with these issues.

In Chap. 8 we establish a context for the discussion by formulating a range of simple CTDS conceptual models. For the most part, these have their origins in the portions of physical world where behaviour can be readily characterized by familiar laws of physics. This central role of the laws of physics is a typical circumstance in the CTDS domain and should not be interpreted as a biased perspective. However this is not to suggest that CSTD models cannot be formulated in the absence of directly applicable physical laws, and we illustrate this point by providing an example of the formulation of a credible CTDS model based entirely on intuitive arguments. The final topic in Chap. 8 is a brief examination of the problem of transforming a conceptual model that has evolved with higher order differential equations, into an equivalent set of first order differential equations. Such a format is frequently required by numerical software.

In Chap. 9 we provide an overview of some of the basic numerical tools for solving the ode's of the CTDS conceptual model. The presentation is relatively

informal and is at an introductory level. Features that have practical relevance, especially those that can lead to numerical difficulties, are emphasized.

Because of our assumed absence of random affects in the CTDS models which we treat in this book, it is conveniently feasible to include classical optimization requirements in the project goals. This topic is examined in Chap. 10. The typical objective here is to find values for parameters within the conceptual model which yield a minimum value for a prescribed performance (or criterion) function. Such a function could, for example, correspond to the operating cost of some chemical process. We outline several minimization procedures that could be applied in a CTDS context.

As a concluding comment in this synopsis, we encourage the reader to examine Annex 3 where we have provided a brief introduction to MATLAB, a comprehensive software tool for a wide range of numerical problems. Our emphasis in Annex 3 is, however, very much restricted to features that have relevance to simulation experiments with CTDS conceptual models.