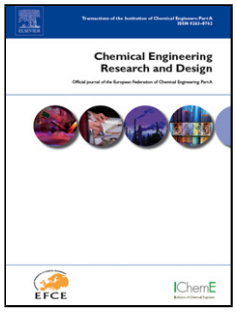

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Adjoint method for parameter identification problems in models of stirred tank chemical reactors

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Abstract

In this paper an adjoint-based algorithm for parameter identification problems in systems of ordinary differential equations (ODEs) is presented. This is done by solving a minimization problem in which the cost function is defined in order to quantify the mismatch between the observed data and the numerical solution of the ODEs. Most of existing local minimizers need the derivatives of both the cost function and the constraints that are usually calculated by finite-difference formulas. In this paper we show how they can be computed much more efficiently and accurately by the so-called adjoint method. We apply this method to the problem of estimating a set of unknown parameters appearing in chemical reaction models. Numerical results showing the efficiency of the adjoint method are included.

Keywords: Chemical kinetics, adjoint method, inverse problem, ODE-constrained optimization

1. Introduction

Mathematical modelling and numerical simulation are fundamental tools in most areas of applied science and engineering. A few examples are biological systems, chemical reactions, fluid mechanics, etc. In general, the models involve unknown parameters which must be identified to define completely the system. Usually, these parameters are estimated by solving an inverse problem which consists in a minimization problem where the cost function depends on the solution of the parameterized model. Depending on the nature of the problem the models can be different mathematical objects as systems of numerical equations, ordinary differential equations or partial differential equations. In this paper we focus on systems of (usually nonlinear) ordinary differential equations.

In order to solve the above mentioned minimization problem numerical algorithms have to be used. Most of local minimizers are gradient-based iterative algorithms requiring, at each iteration, the computation of the derivatives of the objective function, and possibly of the constraints, with respect to the parameters to be identified. In practice, several classical difficulties have to be faced: first, the number of variables and parameters of the model can be large, second the objective function can have several local minima and third the governing equations usually involve nonlinear functions of variables and parameters so their solution have to be computed by numerical discretization methods. Consequently, the original minimization problem is first approximated by a family of minimization problems associated with a discretization parameter involved in the approximation procedure (typically, the time-step of the numerical scheme used to solve numerically the ODEs). Thus, a fully discrete minimization problem is finally solved instead of the original continuous one: both the cost function and the constraints depend on the numerical solution of the parameterized model.

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Abbreviations: ODE, ordinary differential equation; PDE, partial differential equation; STR, stirred-tank reactors; CSTR, continuous stirred tank reactors