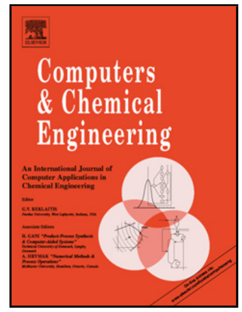
Accepted Manuscript



Title: Identification problem in plug-flow chemical reactors using the adjoint method

Author: A. Bermúdez N. Esteban J.L. Ferrín J.F. Rodríguez-Calo M.R. Sillero-Denamiel

PII: S0098-1354(16)30377-5
DOI: http://dx.doi.org/doi:10.1016/j.compchemeng.2016.11.029
Reference: CACE 5618

To appear in: *Computers and Chemical Engineering*

Received date: 24-5-2016
Revised date: 20-10-2016
Accepted date: 25-11-2016

Identification problem in plug-flow chemical reactors using the adjoint method

A. Bermúdez[a], N. Esteban[b], J.L. Ferrín[a,*], J.F. Rodríguez-Calo[c], M.R. Sillero-Denamiel[d]

[a] *Departamento de Matemática Aplicada. Universidad de Santiago de Compostela. 15782 Santiago de Compostela. Spain*
[b] *Instituto Tecnológico de Matemática Industrial. 15782 Santiago de Compostela. Spain*
[c] *Centro de Tecnología Repsol. 28935 Móstoles (Madrid). Spain*
[d] *IMUS. Universidad de Sevilla. 41012 Sevilla. Spain*

Abstract

The aim of this work is to solve identification problems in plug-flow chemical reactors. For this purpose an adjoint-based algorithm for parameter identification problems in systems of partial differential equations is presented. The adjoint method allows us to calculate the gradient of the objective function and the constraint functions with respect to the unknown parameters significantly reducing the computer time. This leads to solve a minimization problem, in which an objective function is defined in order to quantify the mismatch between the observed data and the numerical solution of the parameterized chemical model. For solving the initial and boundary-value problem we use finite-difference schemes. More precisely, we propose a second-order BDF method initialized with a first-order one. The algorithm proposed was implemented in a computer program and some numerical results are shown. The efficiency of the adjoint method, compared with the classical formula of incremental quotients, is also presented.

Keywords: chemical kinetics, plug-flow reactor, identification, adjoint method, integral method

1. Introduction

Important models from different fields of engineering and applied sciences depend on unknown parameters which must be identified to define completely the system. Examples are common in biological systems, chemical reaction mechanisms, fluid mechanics, etc. Usually, the parameters are estimated by solving a minimization problem, where the objective function depends on the solution of the parameterized model. These models can be systems of numerical, ordinary (ODE) or partial differential equations (PDE). Many optimization algorithms consist of gradient-based iterative methods, which require, at each step, the computation of the derivatives of the objective function and possibly of the constraint functions with respect to the optimization variables. Parameter identification problems present two classical difficulties: first the number of variables and parameters of the model can be large and second the governing equations usually involve nonlinear functions of variables and parameters so, in practice, they have to be solved numerically. Therefore, a discrete minimization problem is considered instead of the continuous one, where the objective function depends on the numerical solution of the parameterized model.

*Corresponding author
Email addresses: alfredo.bermudez@usc.es (A. Bermúdez), noemi.esteban@usc.es (N. Esteban), joseluis.ferrin@usc.es (J.L. Ferrín), jfrodriguezc@repsol.com (J.F. Rodríguez-Calo), mremediossillero-ext@us.es (M.R. Sillero-Denamiel)