Parameter Estimation Algorithms for kinetic modeling from noisy measurements.

Fabiana Zama*, Dario Frascari†, Davide Pinelli†

Abstract

Aim of this work is to present a comparative study of parameter estimation algorithms for modeling the kinetic and transport terms frequently occurring in chemical process problems, such as fermentation, biodegradation or adsorption.

We consider time dependent diffusion, convection, interfacial transport and reaction models with non-linear reaction or transport terms, and we focus on the estimation of the parameters from noisy measurements.

Such problems are ill-posed in the sense that noise present in the data leads to poor solutions, hence regularization methods are used.

The parameter estimation problem is formalized as constrained optimization problem where the objective function represents the fit to noisy measurements and the constraint is related to the regularity of the solution.

In the present work we define several test problems with characteristic kinetic terms and investigate estimation parameters algorithms using both L_2 and L_1 norms. An adaptive iterative framework for computing the regularization parameter is also proposed.

*Department of Mathematics, University of Bologna, P.zza Porta S. Donato 5 40127 Bologna

†Department of Civil, Chemistry, Environmental and Materials Engineering, University of Bologna, Via Terracini 28, 40131 Bologna