

Software Functionality Assessment for Kinetic Reaction Model Development, Model Discrimination, Parameter Estimation and Design of Experiments

Rob J. Berger^a, Johan Hoorn^b, Jan Verstraete^c and Jan Willem Verwijs^d
EUROKIN (<http://www.dct.tudelft.nl/eurokin/>)

^a Delft University of Technology, Julianalaan 136, 2628 BL Delft, The Netherlands
(R.J.Berger@tnw.tudelft.nl)

^b DSM Research, P.O. Box 18, 6160 MD Geleen, The Netherlands

^c Institut Français du Pétrole, CEDI "René Navarre", Solaize, P.O. Box 3, 69390 Vernaison, France.

^d Dow Benelux N.V., ES/MD, P.O. Box 48, 4530 AA Terneuzen, The Netherlands.

An inventory was carried out on the capabilities and user-friendliness of commercially available modeling packages aimed at estimation of (kinetic) parameters and capable to describe two or more dimensional reactor models. Four case studies were developed in order to evaluate these packages in more detail. It appeared that all the packages need improvement in order to become really good and user friendly. Especially the quality of the statistics, the number of useful statistical tools and several user-friendliness aspects need significant improvement. However, discussion of these issues with the software vendors already initiated the developers of the packages to improve the software functionality. This paper is a result of co-operation within Eurokin, a consortium of over 10 European companies and 4 universities.