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Acquisition of nonlinear kinetics from linear relations: application on homogeneous transesterification reactions

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Abstract

This paper proposes a fast method to determine kinetic parameters in systems with nonlinear concentration dependencies in equilibrium reactions. Without the use of complicated software, the corresponding parameters can be obtained from linear relations, with a minimum number of experimental data, acquired by semi-batch operation. The underlying theory is given for a general equilibrium reaction $A + B \leftrightarrow C + D$ and it is successfully applied for the real case of typical transesterification reactions.

The proposed procedure opens the door for easy, i.e., linear, parameter estimation procedures using commercial software as Excel[®] without the tedious and nerve-racking nonlinear parameter estimation procedures.

The presented methodology gives an easy access to forward as well as backward transesterification rate coefficients, which can be used for simulation purpose for non-steady reactor operation and corresponding optimization.

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