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Kinetic-parameters-free determination of thermally safe operation conditions for isoperibolic homogeneous semibatch reactions: A practical procedure

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Abstract

In the fine and pharmaceutical chemical industries, the kinetic parameters of exothermic reactions are often unavailable because this process is time-consuming and money-consuming. Hence, it is essential to develop kinetic-parameters-free procedure to determine thermally safe operating conditions for exothermic semibatch reactions. In this work, a practical procedure without any reaction kinetic parameter information required has been developed and presented. It just needs several isothermal RC1 (reaction calorimetry) tests, which are convenient to conduct in practice. Such a practical procedure, based on two crucial theoretical tools: Ry_{min}-Wt plot and $\nu_A DaR_E\kappa$-X_{ac} plot, allows one not only to keep safe conditions but also to optimize the reactor productivity. In addition, this method is also feasible for the cases of the exothermic reactions with low value of Ex and low mixing heat. Moreover, this method is supposed to be inapplicable when encountering autocatalytic reactions.

Keywords: Safe operating conditions; Semibatch reactors; Thermal runaway; Reaction calorimetry; QFS

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