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The temperature scanning reactor III: Experimental procedures and data processing

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Abstract

The theory of Temperature Scanning Reactors (TSRs), presented in full elsewhere [1–3], is free of virtually all approximations which would limit its utility in kinetic studies. This is not to say that temperature scanning (TS) is free of difficulties when the theory is implemented in practice. Below we discuss the features of an experimental TS reactor in operation in our laboratories and present experimental procedures and data-handling techniques which deal with the real-life difficulties encountered in using temperature scanning. The operation of real temperature scanning reactors is confronted by the practical realities of dealing with hardware limitations, uncertainties in calibration, signal noise and other such difficulties which, in this type of operation, pose very different problems from those encountered in conventional kinetic experiments. In particular, there is much new ground to be broken in learning how best to deal with TS kinetic data, which are more akin to a signal, in the sense used in data transmission for purposes of communication, than to the individual experimental data points we are accustomed to collecting in conventional isothermal kinetics research. We report here on some of our efforts to deal with these problems, for example, through the use of signal filtering, two dimensional splining and other mathematical techniques, some of which are new to the field of kinetics. The temperature scanning method itself is very new, so that it comes as no surprise that the data interpretation and visualisation methods which it entails, and its operational requirements, will pose unfamiliar challenges to both experimentalists and theoreticians for some time to come.

Keywords: Data filtering; Temprature scanning; Kinetics; Experimental methods

1. Introduction

In previous papers [3,4] we have described the theory and operation of various temperature scanning reactors: Batch Reactors (TS-BR), Stream-Swept Reactors (TS-SSR), Continuous Stirred Tank Reactors (TS-CSTR) and Plug-Flow Reactors (TS-PFR). Computer simulations of the operation of these reactors have been presented elsewhere [3] to provide numerical examples and to illustrate the very different and unfamiliar appearance of the data one collects from these "kinetics instruments". Of course, computer simulations provide ideal, perfect data: no set-point uncertainties in reactor control; no noise in the measurement of the parameters being monitored; and no calibration errors.

In real experiments these are all difficulties to be dealt with. This paper describes some of the experimental procedures and data-handling

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