



Kinetic research on heterogeneously catalysed processes: A questionnaire on the state-of-the-art in industry

A.N.R. Bos^{a)}, L. Lefferts^{b)}, G.B. Marin^{c)}, M.H.G.M. Steijns^{d)}

^{a)} Shell Nederland Chemie. P.O. Box 3005, 3190 GB Hoogvliet, The Netherlands

^{b)} DSM, P.O. Box 18, 6160 MD Geleen. The Netherlands

^{c)} University of Gent. Laboratorium voor Petrochemische Techniek, Krijgslaan 218. B-9000 Gent. Belgium

^{d)} Dow Benelux. P.O. Box 48, 4530 AA Terneuzen. The Netherlands

Abstract

On the initiative of the Working Party 'Chemical Engineering in the Applications of Catalysis' of the European Federation of Chemical Engineering an assessment of the issues in the determination and application of kinetic data within the European industry was performed. The basis of the analysis consisted of a questionnaire put together by researchers from Dow, DSM, Shell and Eindhoven University of Technology. The 24 companies, which have responded to the questionnaire, can be classified into four groups: chemical, oil, engineering contractors and catalyst manufacturers. From the overall input it appears that there are three, equally important, utilisation areas for kinetic data: process development, process optimisation and catalyst development. There is a wide variety of kinetic data sources. Most of the respondents make use of test units which were primarily designed for development and optimisation. Avoiding transport limitations is, certainly in the case of short range projects or for complex feedstocks, not always taken care of. With respect to the modelling approaches, a common philosophy is 'as simple as possible'. Most of the respondents state that "in principle" one should strive for intrinsic kinetics, but the majority nevertheless does for various reasons not separate all transport phenomena from reaction kinetics. Kinetic models are mostly simple first or nth order or Langmuir-Hinshelwood type expressions. More complex kinetic models are scarcely used. Three areas were frequently identified to offer opportunities for improvement. Gathering of kinetic data is too costly and time consuming. There is no systematic approach at all for determination and application of kinetics in case of unstable catalytic performance. Furthermore, the software available for the regression of kinetic data to rate equations based on mechanistic schemes as well as software to model reactors are insufficiently user friendly. The majority of the respondents state that the problems indicated should be solved by cooperation, e.g., between companies, between industry and academia and between the catalysis and the chemical engineering community. A workshop on the above topics was held in December 1996 with 15 companies and 6 academics attending. More information can be obtained from the secretariat of the Working Party.