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Heterogeneous Catalysis

The research is mainly dedicated to the extension and refinement of the unsteady state experimentation with the main interest focused on *in situ* measurement of adsorbed intermediates and the mathematical modelling of catalytic reactors for application to catalyst modification [1][2]. An experimental set-up has been developed to investigate simultaneously the surface and gas-phase concentrations (*Fig. 1*). The heart of the installation is a fixed-bed reactor which is directly coupled to a diffuse reflectance (DRIFTS) cell *via* an external recycle loop. The effluent from the reactor is continuously analysed by a mass spectrometer. As only a small amount of catalyst is present in the DRIFTS cell,

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temperature gradients can effectively be avoided. The main reaction takes place in the fixed-bed and allows kinetic studies at high conversion. Arranged in this way, the infrared cell can be considered as a window in the reactor, providing a view on the catalyst at normal reaction conditions.

The identification of the nature of the surface species and active sites involved in catalytic reactions should give *a priori* information on the effect of selective doping of the catalysts. The model reactions that are adapted for investigation are of environmental interest, such as the catalytic reduction of NO [3], or important for the fine chemistry, such as the methylation of benzene derivatives [4]. Besides studies on reaction kinetics, the catalysts are characterized by different physical methods, such as ESCA, X-ray, electronic microscopy.

Polymer Reaction Engineering

The better understanding of the degree of mixing in high viscous media is of crucial interest regarding the product quality during polymerization reactions. For homo-polymerization, the degree of micromixing affects the molecular-mass distribution, whereas for copolymerization, the quality of mixing will in addition strongly influence the product characteristics in term of the product composition and the sequence of monomer units [5][6].

A special reactor composed of a recycle tubular reactor followed by a tubular part, all being completely filled with motionless mixers, was developed in collaboration with industrial partners (*Fig. 2*). The reactors are characterized by their macroscopic and microscopic mixing efficiency. Static mixers show a nearly plug-flow behaviour over a wide range of viscosities (10^{-3}–10^{3} Pa·s). The micromixing as function of power dissipation can be characterized by a chemical method. The results allow the proper design of copolymerisation processes. The high heat transfer capacity of the reactor was studied with load up to 1 MW/m^3 in two pilot plants of different sizes. The concept of the reactor was proved to be efficient for bulk and solution polymerization processes up to industrial scale.

Furthermore, the use of continuous kneaders is studied in collaboration with European partners from industry and academy [7].

The proper design of polymerization reactors is only possible with the knowledge of the intrinsic kinetics. In this respect new calorimetric [8] and microgravimetric [9] methods are developed.

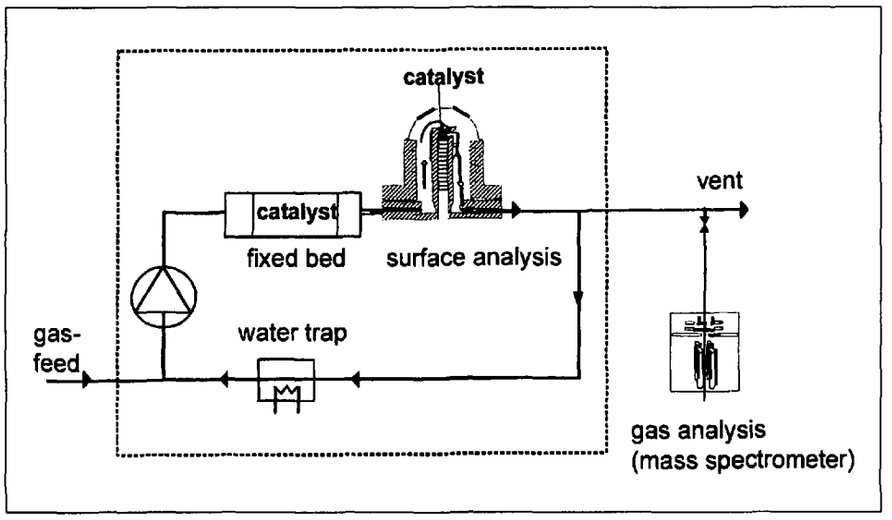

Fig. 1. *DRIFTS-recycle reactor experimental set-up for unsteady-state kinetic investigations with simultaneous* in situ *surface intermediates measurement*

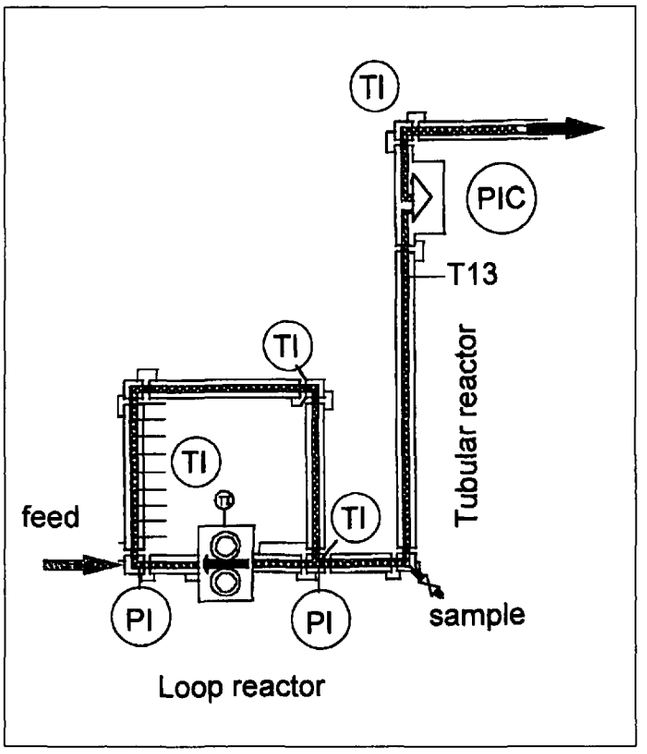

Fig. 2. *Pilot reactor for solution polymerisation*

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