

ABSTRACT

COMPUTER SIMULATION OF THE KINETICS OF POLYMERISATION OF ACRYLIC MONOMERS IN A SEMI-BATCH EMULSION PROCESS

Emulsion polymerisation processes may conveniently be performed using semi-batch processes in order to reduce rate of heat evolution and maintain thermal control. In selecting the feed rate it is important to understand the kinetics of polymerisation so that starved-feed conditions and feed-rate control of exotherm are maintained.

Commercial kinetic modelling software (REACTION[®] from BatchCAD) is available for simulation of small-molecule kinetics. The software can, however, be adapted for use with polymerising systems if reasonable approximations are made. This procedure is shown for copolymerisation of two monomers of unequal reactivity in a semi-batch process initiated by a persulphate radical source. It is necessary to include terms for mass transfer to latex particles as well as terms for reaction in order to obtain good kinetic fitting. The resulting deterministic model shows how the kinetic terms vary with feed rate only during the early phases of the addition, possibly reflecting a non-integral reaction order. Kinetics for the steady-state phase of the addition were accurately fitted.

The approach used is a practical combination of manual and computer fitting for the kinetics and an abbreviated representation of the terms for the growth phase of the reaction. It avoids unnecessary sophistication but is flexible enough to model the process with the required accuracy. Consumption of monomer is modelled and the resulting rate of heat release may be expressed by including calorimetric terms.

N Medcalf

Smith and Nephew Group Research Centre, York Science Park, Heslington, York, YO1 5DF