

# COMPUTER-AIDED MODEL BASED ANALYSIS FOR DESIGN AND OPERATION OF A COPOLYMERIZATION PROCESS

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The advances in computer science and computational algorithms for process modelling, process simulation, numerical methods and design/synthesis algorithms, makes it advantageous and helpful to employ computer-aided modelling systems and tools for integrated process analysis. This is illustrated through the study of a copolymerization process, where operational problems due to their complex nonlinear behaviour are usually encountered, indicating thereby, the need for the development of an appropriate process model that can describe the dynamic behaviour over the complete range of conversion. This will allow analysis of the process behaviour, contribute to a better understanding of the polymerization process, help to avoid unsafe conditions of operation, and to develop operational and optimizing control strategies. In this work, through a computer-aided modelling system ICAS-MoT, two first-principles models have been investigated with respect to design and operational issues for solution copolymerization reactors in general, and for the methyl methacrylate/vinyl acetate system in particular. The Model 1 is taken from literature and is commonly used for low conversion region, while the Model 2 has been derived in this work and covers the complete range of conversion. The performances of the two models are compared with respect to the steady state and dynamic behaviour of the polymerization process. The model analyses highlight the influence of the reaction mechanism, the transport phenomena, the process design and conditions of operation on the polymer grade and the production rate.

*Keywords:* polymerization; modelling; computer-aided systems; nonlinear dynamics; numerical analysis; design; simulation.

## INTRODUCTION

Most computer-aided design, analysis and control of chemical processes are model-based and therefore, there is an increasing trend to use computer-aided modelling (CAM) systems and tools for integrated process analysis, design and control. An efficient and flexible CAM system should be able to generate or create the appropriate model for the process under study to allow subsequent model-based investigations of design and/or operational alternatives. Through fast, reliable and efficient modelling steps of a CAM system, it should be possible to generate and investigate numerous alternatives, leading to solutions that otherwise would not be possible to obtain, and thereby, give the opportunity to reduce the time to market and

investment costs through integrated product and process design. To achieve this, a CAM system will need to ensure the integration of existing models into a software environment that supports model (equation) generation, model analysis, model solution, and model validation. Additionally, the CAM system should facilitate the reuse of modelling knowledge during the process life-cycle, so that the information incorporated in the models can be easily translated for different target applications such as steady-state simulation, dynamic simulation, process optimization and experimental design.

The objective of this paper is to highlight the modelling tools available within a CAM system called ICAS-MoT (Sales-Cruz and Gani, 2003) that has been further developed to satisfy the needs for process design, analysis and control through a detailed analysis of the operations of a polymerization process. This process is chosen to illustrate the advantages of using a CAM system because the production of synthetic polymers (i.e., commodity plastics, engineering plastics and speciality polymers) is one of the most important worldwide industries. Each year more than 100 million tons of synthetic polymers are produced worldwide (Ray and Villa, 2000). Many synthetic polymers

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