Dynamic Modeling and Experimental Validation of the MMA Cell-Cast Process for Plastic Sheet Production

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The dynamic modeling and experimental validation of the model response of the poly(methyl methacrylate) (PMMA) cell-cast process for plastic sheet production is presented. It is based on the straightforward initiation, propagation, and termination reaction polymerization mechanism. The sheet molding process was modeled by a two-dimensional dynamic mathematical model able to predict conversion, temperature, and molecular weight averages. The mathematical model is cast as a partial differential equations (PDEs) system that is discretized using the numerical method of lines. The resulting set of ordinary differential equations, representing the heat and mass balances for this polymerization system, are then solved by standard ordinary differential equations (ODE) solvers. Comparison of the model prediction capabilities against experimental temperature measurements taken at the extremes of the PMMA sheet being produced are presented.

1. Introduction

Global economy and high commercial pressure demand manufacturing better and cheaper products, reducing capital and operating costs. From a process systems engineering (PSE)[1,2] point of view, there is a wide scope for process improvement by using advanced mathematical modeling techniques. Once a reliable model is available, it can be used for several purposes such as simulation, control, process synthesis, steady-state and dynamic process optimization, etc. Polymerization reaction engineering constitutes a field where process improvements can be achieved trough appropriate process modeling. A common disadvantage of polymerization products relates to product heterogeneous features due to variations in raw material quality, changing process operating conditions, etc. Product heterogeneous characteristics tend to reduce process profit margins. By developing reliable polymerization models, process operating conditions could be determined, leading to homogeneous product quality. Of course, the details embedded in a model will depend on its economical impact and the available process knowledge. Working along the above ideas, in this work, our aim is to derive a first principles distributed dynamic mathematical model of an industrial polymerization system and to validate it by comparing its dynamic response against experimental pilot-plant data. The reported work represents a long-term research effort aiming to improve polymerization reaction operating conditions, hence leading to better product characteristics and increased profit margins, through advanced modeling, optimization, and control techniques. In particular, in this work, we address the poly(methyl methacrylate) (PMMA) industrial manufacturing process.

PMMA is used, for instance, in the rear lights of cars. The spectator protection in ice hockey stadiums is made of PMMA, as are the largest windows and aquariums around the world. The material is also used to produce laser disks, and sometimes for DVDs. PMMA has a good degree of compatibility with human tissue and can be used for replacement of intraocular lenses in the eye when the original lens has been removed in the treatment of cataracts. In orthopedics, PMMA bone cement is used to affix implants and to remodel lost bone. Dentures are often made of this material, too. Commercial production of PMMA sheets can be carried out by processes such as cell casting (either in batch or continuous bulk polymerization), melt calendering, and melt-extrusion. The cell-casting process is becoming more important for PMMA production because of its flexibility in producing PMMA sheets with diverse physical and mechanical properties.[3]

In Figure 1, one of the flowsheets for the industrial manufacture of MMA is shown. In this, process monomer and small amounts of initiators react in a semibatch reaction system where a prepolymerization step takes place. The aim of the prepolymerization step is to mix the reactants, to remove the inhibitors normally contained in commercial MMA, and to heat the reaction mixture until polymerization reaction conditions are reached. Normally, in the prepolymerization step, only modest monomer conversion values (∼15−20%) are obtained. The prepolymer material is introduced into the casting mold in the form of a viscous liquid where polymerization reactions will proceed until most of the remaining monomer is consumed. The polymerization of the material contained between the glass plates is then carried out by heating the molds while the glass plates are clamped together. Initially, when the reaction heat produced at low conversion is small (because of the very low polymerization rate at those conditions), heat is provided to the molds by inserting them inside hot water baths. There, PMMA plastic sheet polymerization takes place. It has been reported[4,5] that this process tends to produce nonuniform (i.e., measured in terms of molecular weight averages) plastic sheets, because polymerization does not take place at the same rate inside the PMMA polymerization mixture. Temperature variation is, perhaps, the main reason to explain polymer nonuniformity. Therefore, tight control of the operating conditions should help to diminish the

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10.1021/ie060206u CCC: $33.50 © 2006 American Chemical Society
Published on Web 09/28/2006