MODELING AND PARAMETER ESTIMATION IN A PO3G POLYETHER PROCESS WITH TIME DELAY

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A new model is developed to describe batch polycondensation of bio-based 1,3-propanediol (PO3G) to produce a polyether commercialized by DuPont as Cerenol® (see Figure 1). Cerenol® is valued for its biodegradability and low toxicity, as well as high end-group reactivity, low viscosity, low melting point and superior oxidative stability[1]. The proposed model provides an improved fit to the available data compared to the previous model of Cui et al. [2] The main reason for this improvement is that the revised model equations and parameter estimation methodologies that were used account for time delay and accumulation of evaporated water, monomer and linear oligomers in the overhead condenser system. To handle this time delay, existing parameter ranking, subset selection and estimation methods[3-5] were extended to treat the delay associated with the overhead piping as an additional unknown model parameter. Although, the resulting parameter estimates lead to better predictions on average compared to the model of Cui et al., there is still noticeable mismatch between the data and the model predictions. For example, Figure 2 shows dynamic model predictions and data for linear dimer and tetramer concentrations in the reactor obtained using a super-acid catalyst. Further parameter estimation studies are underway to determine whether current estimates correspond only to a local minimum for the optimization problem. In future, the model will be extended to account for formation and evaporation of cyclic oligomers.

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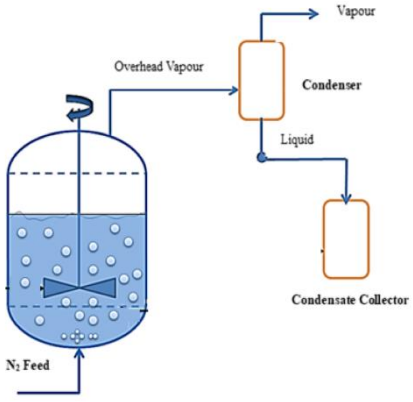

Figure 1 - PO3G reactor and condenser system

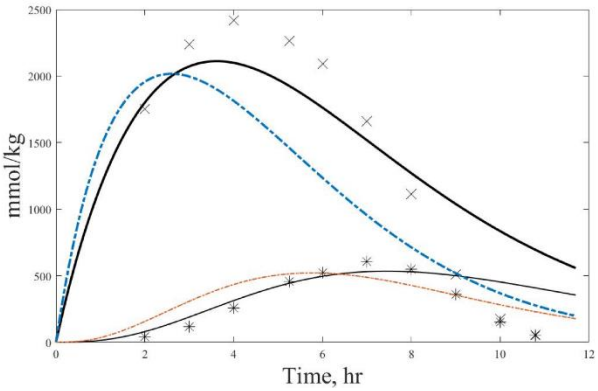

*Figure 2- Concentration of dimer and tetramer in the reactor (dimer: × measured data, -.- prediction without time delay, — prediction with time delay; tetramer: * measured data, -.- prediction without time delay, − prediction with time delay)*