242p Steady State Modeling of Reactive Distillation Using Homotopy Continuation

Nitin Kaistha and MV Pavan Kumar

Homotopy continuation is applied to the industrially important MTBE and methyl acetate reactive distillation (RD) columns to analyze for steady state multiplicities. Continuation is applied in two distinct ways, with respect to tray catalyst mass and with respect to column inputs. Catalyst mass continuation provides a tool for convergence to a steady state solution of the highly nonlinear governing equations. Also, the solution diagram reveals the occurrence of multiple steady states. For the MTBE column, up to five steady states in the kinetically controlled regime are detected. Of these, only three remain in the limit of reaction equilibrium on the trays. For the methyl acetate column, three steady states in both the kinetically controlled and reaction equilibrium regimes are obtained at fixed reflux rate and reboiler duty. If the column specification is changed to fixed reflux ratio and reboiler duty, only a single steady state solution is observed. The column operating policy thus substantially impacts the existence of multiple steady states. Column input continuation is used to obtain the complex relationships between input variables (reboiler duty, reflux rate etc) and output variables (tray temperatures, conversion etc). Steady state multiplicities are seen in both the MTBE and methyl acetate columns. A thorough understanding of these multiplicities is essential for devising robust control strategies.