Design of a polystyrene plant for differing

Business

Design of a Polystyrene Plant for Differing Single-Pass Conversions

November 25, 2013 Introduction Polystyrene is one of the most widely used plastics, with applications ranging from food packaging to appliances to manufacturing (Maier). On an industrial scale, polystyrene is derived from its monomer, styrene. This is achieved by free-radical polymerization of a solution of monomer, polymer, and initiator. This reaction is a multistep radical reaction that includes initiation, propagation, and termination (Eq.

B.

1 through Eq. B. 5). Figure A. l shows a process that produces 1000 kg/hr of olystyrene in an isothermal plug flow reactor at a styrene conversion of lower than 80%. Azobisisobutyronitrile (AIBN) initiator is fed into the reactor at a concentration of 0.

022 mol/L. The stream exiting the reactor is fed into an evaporator that perfectly separates unreacted styrene from the mixture. Unreacted styrene is recycled back into the reactor feed at a recycle ratio of 1 (in reference to fresh styrene feed).

Costs associated with operating the plant increase with the size of the reactor ($200 per m3), with the rate styrene is fed into the reactor ($70 per kg/hr), and with the power equired to pump the viscous mixture through the length of the reactor ($1 5×10-5 per W). We will determine the optimal single-pass conversion for a polystyrene plant described above. Design Approach Qualitatively, to achieve a larger single-pass monomer conversion, a larger reactor volume is need, necessitating more power to pump the reaction mixture through the length of the reactor.

Both of these factors will contribute an increase in overall cost.

In return, however? less fresh styrene feed is needed, contributing to a decrease in overall cost. There is a single pass conversion that best balances these cost ontributing factors. To determine the single-pass conversion that minimizes plant- operating costs, the following design approach was taken. To summarize the design approach, differential equations relating monomer conversion, initiator conversion, and reactor pressure to reactor volume are solved with a numeric solver.

The solutions to these equations result in reactor volume and pressure drop parameters for any given single-pass conversion.

Pressure drop is then related to power, while styrene feed is expressed as a function of single-pass conversion. Finally, the three esulting parameters – reactor volume, power, and styrene feed – are related to cost to determine the optimal single-pass monomer conversion. First a differential equation relating monomer conversion to reactor volume is written in terms of known quantities (see appendix D, sec. 1 for full derivation). The process begins with a species mass balance for a differential of a plug flow reactor (Eq.

D. l . 1). Rate equations for monomer and initiator consumption are applied to their respective species balances (Eq.

D.

l . 7 and Eq. D. l . 8).

Algebraic manipulation yields a differential quation relating single-pass conversion of monomer to reactor volume (Eq. D. l . 10). Next, a differential equation relating pressure to reactor volume must be expressed in terms of conversions and other known quantities (see appendix D, sec 2 for full derivation).

A number of substitutions are made using equations from Appendix B. (Eq. D. 2. 1 through Eq. D.

2. 10). First, the friction factor equation is rearranged to produce a differential equation relating pressure and volume (Eq. D. 2. 1).

The Blasius relation and the definition of the Reynold’s number are then applied to the equation to remove its dependence friction factor (Eq. D. 2. 2). Finally, an expression relating the viscosity of the reacting mixture to conversions and known quantities is derived (Eq.

D. 2. 9) and substituted into the differential equation (Eq. D. 2.

10). We now have a system of three differential equations that describe reactor behavior. This system of differential equations can be solved numerically for a given single-pass conversion using the Matlab function ODE45 which utilizes a Runga-Kutta algorithm.

Next, an expression relating fresh styrene feed rate to single pass monomer conversion is derived (see appendix D, sec 3 for full derivation). A species mass balance on polystyrene is performed with the entire reactor as the control volume (Eq. D.

3. 1). Following considerable algebra and application of the recycle ratio, an expression is reached relating initial feed of styrene to single-pass monomer conversion (Eq. D. 3.

7). Following, an equation relating the power needed to pump the reaction mixture through the length of the PFR to the pressure drop across the reactor is derived. This results in Eq.

D. 4.

As stated previously, the cost of the reactor is dependent on three factors: reactor volume, initial feed of styrene, and power. Numerical solutions to each of these factors are determined for a range of single pass conversion values based on the equations derived above. These solutions are scaled by corresponding unit costs, then summed to determine the total cost for reactors with each single- pass conversion within the chosen range (Appendix F). The code used to calculate cost as a function of single-pass conversion contains a “ for loop”, iterating over a conversion range of 0. 0001 to 0.

50.

The results are then used to generate a plot of reactor cost versus single-pass monomer conversion (Figure F. 2). The local minimum f this plot corresponds to the optimal single-pass styrene conversion. Numerically, the single-pass conversion requiring the lowest cost is found using the ‘ min’ function in Matlab.

The optimal single-pass conversion corresponds to a specific reactor volume, pressure drop, and initial feed rate, which are all be expressed in the final recommended design. Results Figures E. I, E. 2, and E. 3 show respectively how reactor volume, styrene feed flow-rate, and pressure drop vary with single-pass styrene conversion.

As conversion increases, pressure drop increases. This effect is especially dramatic beyond a conversion of round 35%. Similarly, reactor volume increases with conversion, though the effects are not nearly as pronounced within the set conversion range. Meanwhile, feed flow rate diminishes with increasing conversion. Over the conversion range of 0. 001 to 0.

50, pressure drop ranges from 9. 2 billion Pa to 17 trillion Pa, reactor volume ranges from 26 m3 to 42m3, and feed flow rate ranges from 5 million kg/h to 1000 kg/h. Scaling these design parameters by their respective unit costs produces Figure F. 1.

This plot displays the relative contribution to overall cost by each of the relevant design parameters.

For conversions below . 43, feed is the primary cost, while power becomes the primary cost at high conversions. Plant optimization is determined from the combination of the curves in Figure F. l . Figure F.

2 shows a plot of the overall reactor cost versus single-pass styrene conversion. At conversions lower than 30% and higher than 40%, the cost of the reactor increases dramatically. The local minimum of the curve

corresponds to the optimal single-pass conversion – the conversion at which overall costs are minimized.

Numerically, the minimum cost occurs at a conversion of 37. 4%. Recommended Design The optimal polystyrene plant design is obtained at the conversion that requires the lowest cost to run the plant.

In order to produce 1000 of polystyrene at the lowest cost, we recommend a styrene conversion of 37. 4% and reactor volume of 36. 1 m3. At these values, the pressure drop is approximately 53. 5 billion Pa, the required styrene feed rate is 1338 , and the cost required to run the reactor is $107, 415.

Appendix A: Process Diagram Figure A. : A fresh feed of styrene is combined with a recycle stream of pure styrene and fed into a plug flow reactor to produce polystyrene that is separated from the ecycle with an evaporator. Appendix B’ Styrene Polymerization Balanced Reaction: Styrene monomer, M, polymerizes to polystyrene, Pn (Eq. 8. 1) Polymerization Mechanism: Initiation: The initiator, I, breaks down into radicals, R, at a rate of kd. (Eq.

8. 2) Propagation: Kp is the rate of the propagation reaction.