

Two-Phase Model for Continuous Final-Stage Melt Polycondensation of Poly(ethylene terephthalate). III. Modeling of Multiple Reactors with Multiple Reaction Zones

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ABSTRACT: A steady-state two-phase model has been developed for a continuous finishing stage of the melt polycondensation process that consists of two rotating-disk reactors in series. Each reactor has multiple reaction zones with different types of rotating disks to establish plug flow profiles and to facilitate the removal of volatile reaction byproducts. The effect on reactor performance of varying the mass transfer parameter was found to be small for the reaction conditions used. The simulation results show that the use of two reactors offers increased flexibility in reactor

operations to obtain the desired polymer properties. Although the proposed model has not been fully validated with experimental or plant data, it has illustrated that the complex multizone reactor system can be easily modeled by the two-phase modeling technique and that added physical insights can be made through numerical model simulations. © 2003 Wiley Periodicals, Inc. *J Appl Polym Sci* 90: 1088–1095, 2003

Key words: polymerization; poly(ethylene terephthalate); reactor modeling

INTRODUCTION

Poly(ethylene terephthalate) (PET) is manufactured commercially by melt polycondensation polymerization processes using dimethyl terephthalate or terephthalic acid as a starting monomer with ethylene glycol. With growing competition with other thermoplastic polymers for many new and existing applications, improving PET quality and the efficiency of PET polymerization technology is a very important issue to PET manufacturers.

A finishing-stage PET reactor is typically a large horizontal cylindrical reactor equipped with such internals as cages, screws, or disks to generate large vapor–liquid interfacial areas for mass transfer and to provide a certain desired fluid flow pattern. Wiped film reactors also are used to make PET polymer. The prepolymer feed to the finishing reactor is generally a low-molecular-weight polymer produced in the

upstream transesterification and prepolymerization stages using stirred tank-type reactors. The finishing reactors are designed and operated for a highly viscous polymer melt to flow without forming any stagnant zones. A high-molecular-weight polymer should also be obtained in a short reaction time, with minimal production of side products such as diethylene glycol and acetaldehyde. In a rotating-disk reactor a fraction of the polymer melt is dragged upward as the shaft rotates, forming a thin layer of polymer melt on the disk surface. Ethylene glycol, a major condensation byproduct, is mostly removed by diffusion from the polymer layers on the disk surface to the vapor phase. The polymer layer, after being exposed to a vapor phase for a short time, is mixed again with the bulk polymer melt.

As polymer melt flows toward the outlet of the reactor, the polymer molecular weight increases and hence does the melt viscosity. In the relatively low-viscosity zones near the inlet of the reactor, maintaining the plug flow profile is important for minimizing the back-mixing that lowers the conversion of functional end groups and hence the polymer molecular weight. On the other hand, in the high-viscosity zones near the outlet of the reactor, minimizing flow resistance becomes more important. Therefore, in many industrial PET processes, different types of disks are used in a reactor. For example, some disks may have holes of different shapes and sizes, and most designs of such disks are proprietary. It is also not uncommon

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to employ two finishing reactors in series operating at different temperatures and/or pressures to effectively increase the polymer molecular weight and to control the concentrations of end groups or side products.

There have been a large number of reports on modeling the finishing stage of PET polymerization.¹⁻¹¹ Many of these articles modeled either a semibatch polycondensation reactor or a single continuous-finishing-stage PET reactor. In our earlier works,^{2,10} we proposed a two-phase model for the finishing-stage melt polycondensation of PET. In the two-phase model plug flow is assumed for the bulk melt phase. No distinction is made between the bulk phase and the polymer layers on the disk surface. Therefore, the polymer phase in the reactor is viewed simply as a mixture of both the bulk and the polymer film phases. The rate of mass transfer of the condensation byproducts from the melt phase to the vapor phase is described through a single mass transfer parameter, and hence the two-phase model is independent of the type of reactor being used. For a given reactor configuration, the mass transfer parameter is determined by fitting the model simulation results with actual polymerization data. The two-phase model developed for a horizontal rotating-disk reactor can also be applied to an industrial wiped film reactor.^{11,12}

In this article we present a mathematical model of a continuous industrial PET process that consists of two reactors equipped with different types of rotating disks. Through modeling and simulation, we investigated the performance of the multizone reactor, and we show here that the two-phase model can easily be extended to a multizone and multireactor polycondensation process model.

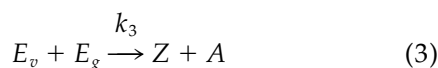
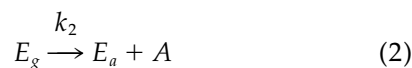
Reaction model

The reactions to be considered in this modeling study include the following reactions, which occur in the melt polycondensation of PET at high temperatures.

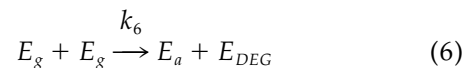
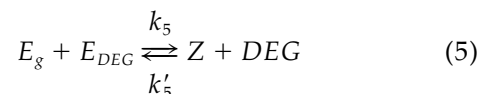
Ester interchange reaction (main polycondensation)



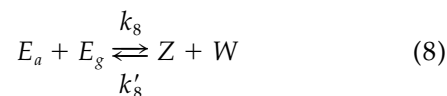
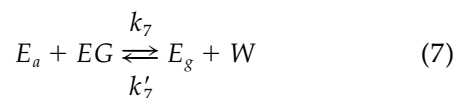
Acetaldehyde formation



Diethylene glycol formation



Water formation



Degradation of diester group



where E_g is the hydroxy ethyl group, EG is ethylene glycol, Z is the diester group, E_a is the carboxylic acid group, A is acetaldehyde, E_v is the vinyl end group, DEG is diethylene glycol, E_{DEG} is the diethylene glycol incorporated in the polymer, and W is water. For quality control purposes, minimizing the concentrations of vinyl end groups and diethylene glycol is of great industrial importance. The acid end group makes the polymer susceptible to hydrolysis during the processing of PET into fibers or filaments, and the vinyl end group causes coloration of the polymer. In the above, it is assumed that acetaldehyde is removed perfectly from the reaction mixture.

To model polymerization kinetics, we used a functional group model in which the rate constants were defined for the reactions between the functional end groups involved in each reaction. Also, note that the effect of catalyst (e.g., Sb_2O_3) is implicitly incorporated into the rate constant values. For the reversible reactions, we assumed that both forward and reverse reactions were equally catalyzed. The reactions leading to the formation of cyclic polymers were assumed to be negligible in our model.

For the nine reactions shown in the above, the following reaction rate equation was derived:

$$\begin{aligned}
 R_1 &= k_1[E_g]^2 - 4k'_1[Z][EG] \\
 R_2 &= k_2[E_g] \\
 R_3 &= k_3[E_v][E_g] \\
 R_4 &= 2k_4[E_g][EG] \\
 R_5 &= k_5[E_g][E_{DEG}] - 4k'_5[Z][DEG] \\
 R_6 &= k_6[E_g]^2 \\
 R_7 &= 2k_7[E_a][EG] - k'_7[E_g][W] \\
 R_8 &= k_8[E_g][E_a] - 2k'_8[Z][W] \\
 R_9 &= k_9[Z]
 \end{aligned}
 \tag{9}$$

The rate constant values are shown in Table I. It should be noted that the rate constant values reported in the literature often have been those obtained for a concentration of a given catalyst (e.g., Sb_2O_3). If a different catalyst concentration were to be used, it is possible the rate constant values would have to be adjusted accordingly. Or kinetic experiments could be performed to determine the rate constant values for the catalyst selected.

Disk types in a rotating-disk reactor

A major function of the disks in a finishing PET reactor is to keep the plug flow profile of the polymer melt in the reactor. Another important function of the disks is to create as large a surface area as possible for the removal of volatile compounds such as ethylene glycol, diethylene glycol, and water. There are many different types of disk designs in the patent literature. Unfortunately, very little is known about the effect of disk geometry on the formation of polymer layers in final-stage PET reactors. In practice, it is nearly impossible to derive a mathematical model to describe the hydrodynamics of the polymer melt in the reactor

TABLE I
Rate Constants^a

Parameter	Value	Units
k_1	$1.36 \times 10^6 \exp(-18,500/RT)$	$\text{L mol}^{-1} \text{min}^{-1}$
k_2	$8.32 \times 10^7 \exp(-29,800/RT)$	l/min
$k_3 = k_5 = k_1$	$1.36 \times 10^6 \exp(-18,500/RT)$	$\text{L mol}^{-1} \text{min}^{-1}$
$k_4 = k_6 = k_2$	$8.32 \times 10^7 \exp(-29,800/RT)$	$\text{L mol}^{-1} \text{min}^{-1}$
k_7	$2.08 \times 10^6 \exp(-17,600/RT)$	$\text{L mol}^{-1} \text{min}^{-1}$
$k_8 = k_7$	$2.08 \times 10^6 \exp(-17,600/RT)$	$\text{L mol}^{-1} \text{min}^{-1}$
k_9	$7.20 \times 10^9 \exp(-37,800/RT)$	min^{-1}

Equilibrium constants: $K_1 = k_1/k'_1 = 0.5$, $K_5 = k_5/k'_5 = 1.0$, $K_7 = k_7/k'_7 = 2.5$, $K_8 = k_8/k'_8 = 1.25$

^a Catalyst (Sb_2O_3) concentration = 0.05 wt %.

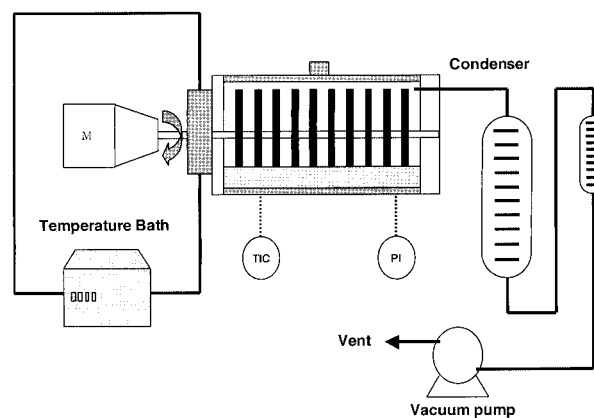


Figure 1 Experimental semibatch rotating-disk polymerization reactor system.

with complex internals—the design of the reactor internals is often regarded as “art” in the PET industry. Even for a simple flat-disk system, estimating the liquid (PET melt) holdup on a rotating disk is not a trivial matter, especially when the disk diameter is large and the melt viscosity is high. Some experimental and modeling efforts have been reported to estimate polymer holdup on a small rotating disk¹; however, the question is whether such a semiempirical model developed for a small laboratory reactor can be applied to a large-scale industrial reactor system. Even with a small flat disk, the liquid holdup on the disk surface is not uniform and is influenced by many factors, such as disk rotating speed and melt viscosity. It is very unfortunate that not much work has been done on the formation of polymer layers on a rotating-disk surface in PET or other similar melt polymerization reactors. But it is also understandable because in practice it is very difficult to make any experimental measurements with a high-viscosity PET melt at high temperatures (e.g., 260°C–300°C) and low pressures (< 10 mmHg).

In this work we carried out semi-batch polymerization experiments using a small-scale rotating-disk reactor with two types of disks (designated Type A and Type B). These disks are the scaled-down versions of large disks used in an industrial PET process. The reactor is made of stainless steel ($D = 14.0$ cm), and the distance between the two neighboring disks can be adjusted by using a spacer. Although the detailed design configurations of these disks are proprietary and not shown here, the Type A disk has many small, circular holes suitable for low-viscosity zones, and the Type B disk has large holes suitable for high-viscosity reaction zones. In each experiment 10 disks of the same type were mounted on a central shaft.

Figure 1 shows the schematic diagram of the experimental semibatch rotating-disk reactor system. Before the experiment prepolymer samples (molecular weight = 5400; obtained from a PET manufacturer)

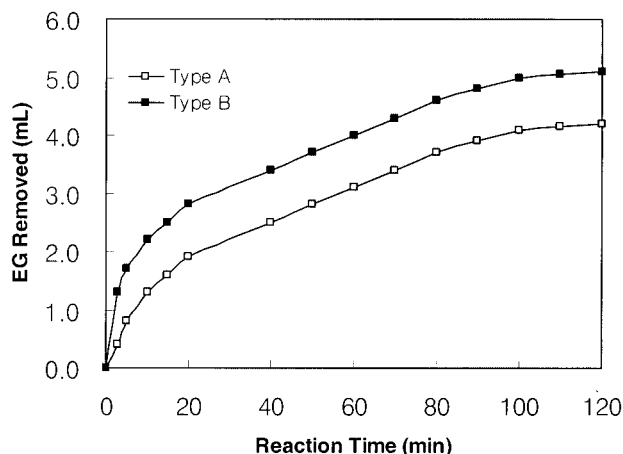


Figure 2 Ethylene glycol removed from the reactor equipped with Type A and Type B disks at 285°C ($P = 5$ mmHg; number of disks = 10; 10 rpm).

were dried in the oven. The reactor was preheated before it was charged with dried prepolymer particles. In the reactor the polymer melt level was maintained at about 40% of the reactor volume. In all experiments the melt level was slightly below the shaft height, and the disk rotating speed was fixed at 10 rpm. No additional catalyst was added to the prepolymer melt. As the reactor temperature was raised to a preset reaction temperature, the reactor pressure was gradually reduced to a desired pressure (5 mmHg). The amount of condensed ethylene glycol removed from the reactor was measured to monitor the progress of polymerization.

The amounts of ethylene glycol (EG) removed from the reactor with Type A and Type B disks at 285°C are shown in Figure 2. Notice that the reaction rates were slightly higher with Type B disks than with Type A disks but that the difference was rather small. Although Type A disks are not as effective as Type B disks in obtaining high-molecular-weight polymer, Type A disks might be needed to establish a plug flow profile when used in the upstream portion of the continuous rotating disk, where the melt viscosity is relatively low. Using the data shown in Figure 2 and the method described by Cheong and Choi,¹ we estimated the effective propagation rate constants at 285°C: $\tilde{k}_1 = 0.0244 \text{ L mol}^{-1} \text{ min}^{-1}$ (Type A disks), $\tilde{k}_2 = 0.0562 \text{ L mol}^{-1} \text{ min}^{-1}$ (Type B disks). Because the same prepolymer was used at the same reaction temperature, it is thought that Type B disks with larger holes were more efficient than Type A disks with smaller holes by providing larger mass transfer areas. These rate constant values were smaller than the literature value of the intrinsic propagation rate constant at 285°C ($0.077 \text{ L mol}^{-1} \text{ min}^{-1}$) but not too far from it. It should be noted that these rate constant values are "effective" rate constants because the effects of mass

transfer resistance for ethylene glycol removal are implicitly incorporated in the rate constants. But the mass transfer effect was believed to be small because initial reaction rate data (e.g., initial ethylene glycol generation rates) were used to estimate the propagation rate constant.

Steady-state continuous reactor model

The industrial finishing polymerization reactor system to be modeled in this study is schematically illustrated in Figure 3. The process consists of two equal-size rotating-disk reactors connected in series. Both reactors are operated at 287°C but at different pressures (5 and 1.0 mmHg, respectively). A relatively low-molecular-weight PET prepolymer ($M_n = 5400$) was supplied to the first reactor, which consisted of three "virtual reaction zones" separated by three sections of different types of disks (volume ratio 1:3.4:0.8). Here a "virtual zone" is defined as the reactor segment equipped with the same type of rotating disks. Each reaction compartment consisted of a disk, bulk liquid (melt) pool, and polymer layer on the disk. Because the disks were spaced equally, the number of disks determined the length of each reaction zone. The output from the first reactor was directly fed to the second reactor, which had two reaction zones (volume ratio 1:1.67). The PET molecular weight at the outlet of the second reactor was 22,000 [or X_n (degree of polymerization) = 113].

The geometry of the rotating disk used in each zone was different. Here, the main reason for using different types of disks was to maintain the plug flow profile and to enhance the gas-liquid contact area as the melt viscosity increased with an increase in molecular weight. In the commercial PET process using these reactors, polymer sample is taken only at the outlet of the second reactor. In fact, in any commercial PET processes, it is nearly impossible to take polymer samples along the reactor. Therefore, it is often difficult to validate a process model because there is only one steady state data point (i.e., at reactor outlet) that can be used for model-plant comparison.

To model the two-reactor system, the two-phase model proposed by Laubriet et al.² for a single PET reactor was used. In the original two-phase model, the entire rotating-disk reactor was modeled as a composite of two phases: the melt phase and the vapor phase. In a real finishing polymerization reactor, the melt phase consists of a bulk melt phase and a film phase at

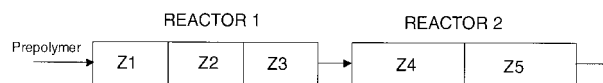


Figure 3 A schematic of two-reactor PET process with multiple reaction zones.

the surface of rotating disks. There are also some ethylene glycol bubbles in the bulk melt phase that contribute to the total gas–liquid interfacial mass transfer area. Therefore, it is quite complicated to determine or estimate the exact vapor–liquid interfacial area. Moreover, the liquid holdup on each disk is strongly dependent on the rotating speed, melt viscosity, disk geometry, and so forth.

In view of these difficulties in quantifying the model parameters, the most important advantages of the two-phase model are its simplicity and its independence of reactor geometry. There is only one model parameter: the overall mass transfer parameter ($k_L a$). Here, the specific mass transfer area (a) incorporates every possible gas–liquid interfacial area in the system, including the surface areas of ethylene glycol gas bubbles. The mass transfer parameter value can be estimated using the plant data and model simulation results. On the other hand, a drawback of the two-phase model is that some reactor-specific design or operating factors are hard to incorporate directly into the model structure (e.g., disk geometry, disk rotating speed, etc.) because the effects of such factors are lumped into a single mass transfer parameter.

To quantify the mass transfer and reaction rates from the melt phase, the melt holdup on each disk needs to be known. In general, the polymer layer (polymer film) thickness on a rotating disk is dependent on various factors such as disk rotating speed, disk size, disk geometry (e.g., holes), and melt viscosity.³ It is extremely difficult to measure or estimate the melt holdup on a rotating disk in actual PET reactors.

It is assumed that the flow of the bulk melt phase was of plug flow and that the vapor phase was perfectly mixed. The interfacial concentrations of the volatile species such as ethylene glycol were calculated using the Flory–Huggins equation. According to a hydrodynamic study with a model fluid, back-mixing occurs to some extent between the two adjacent disk compartments, but the plug flow assumption gives a reasonable representation of the overall reactor flow or residence time distribution characteristics.²

Following are the modeling equations for the multizone reactor system. Here, the vapor phase conditions are identical for all zones in the same reactor; only the mass transfer parameter value differs in these reaction zones. For the i th reaction zone, the steady-state model equations take the following form:

For nonvolatile species:

$$\frac{1}{\theta_i} \frac{d[E_g]_i}{dz} = -2R_{1i} - R_{2i} - R_{3i} - R_{4i} - R_{5i} - 2R_{6i} + R_{7i} - R_{8i} \quad (10)$$

$$\frac{1}{\theta_i} \frac{d[E_{ad}]_i}{dz} = R_{2i} + R_{4i} + R_{6i} - R_{7i} - R_{8i} + R_{9i} \quad (11)$$

$$\frac{1}{\theta_i} \frac{d[Z]_i}{dz} = R_{1i} + R_{3i} + R_{5i} + R_{8i} - R_{9i} \quad (12)$$

$$\frac{1}{\theta_i} \frac{d[E_v]_i}{dz} = -R_{3i} + R_{9i} \quad (13)$$

$$\frac{1}{\theta_i} \frac{d[E_{DEG}]_i}{dz} = -R_{5i} + R_{6i} \quad (14)$$

For volatile species:

$$\frac{1}{\theta_i} \frac{d[EG]_i}{dz} = R_{1i} - R_{4i} - R_{7i} - (k_L a)_{EG,i} ([EG]_i - [EG^*]_i) \quad (15)$$

$$\frac{1}{\theta_i} \frac{d[W]_i}{dz} = R_{7i} + R_{8i} - (k_L a)_{W,i} ([W]_i - [W^*]_i) \quad (16)$$

$$\frac{1}{\theta_i} \frac{d[DEG]_i}{dz} = R_{4i} + R_{5i} - (k_L a)_{DEG,i} ([DEG]_i - [DEG^*]_i) \quad (17)$$

where R_{ki} is the k th reaction in the i th reaction zone ($i = 1-5$) and $[EG^*]$ is the equilibrium concentration of ethylene glycol at the gas–liquid interface. Note that in the three-zone model, the mean residence time, θ_i , is not necessarily the same for the three zones because the length or volume of each zone depends on either the number of disks or on the total length or volume in which different types of disks are installed. In eqs. (15) and (16) separate mass transfer parameters for ethylene glycol, water, and diethylene glycol are used; however, in our model simulations we assumed that a single overall mass transfer parameter represented the mass transfer effect for these volatile species. In practice, estimating the individual mass transfer parameter values is very difficult, and the overall mass transfer parameter is used as an adjustable model parameter.² The standard simulation conditions are shown in Table II. The composition in the vapor phase was calculated using the method described in a previous article.²

Model simulation results

The major reactor model outputs are: polymer molecular weight, amount of ethylene glycol generated, concentrations of functional end groups in the bulk melt phase, and concentrations of volatile species in the vapor phase. Because there are many functional end groups and volatile groups, it would be more appro-

TABLE II
Standard Simulation Conditions

Reactor 1: 287°C, 2.5 mmHg, residence time = 60 min, volume = 3500 L
Reactor 2: 287°C, 1.0 mmHg, residence time = 60 min, volume = 3500 L
Reaction zone length in Reactor 1: Zone 1/Zone 2/Zone 3 = 1:3.4:0.8
Reaction zone length in Reactor 2: Zone 4/Zone 5 = 1:1.7
Standard mass transfer parameter ($k_L a$) = 2.7 s ⁻¹
Feed prepolymer molecular weight: 5400
End group concentrations in the feed (mol/L):
$[E_s] = 0.42445$, $[E_a] = 5.54 \times 10^{-3}$, $[Z] = 6.0448$, $[E_v] = 1.35 \times 10^{-3}$
$[E_{DEG}] = 0.0168$, $[EG] = 1.49 \times 10^{-3}$, $[W] = 1.08 \times 10^{-4}$, $[DEG] = 1.02 \times 10^{-4}$
Vapor pressure data:
Ethylene glycol
$\ln P_{EG}^0 = 49.703 - \frac{8576.7}{T} - 4.042 \ln T$ (P in mmHg, T in K)
Water
$\ln P_W^0 = 18.568 - \frac{4047.6}{T - 33.3}$
Diethylene glycol
$\ln P_{DEG}^0 = 17.033 - \frac{4122.5}{T - 122.5}$

priate to look at some key process outputs rather than to show all of them.

Effect of mass transfer parameter

One of the primary interests in our modeling and simulation study was to discover whether the employment of different types of disks would affect the reactor performance, that is, polymer molecular weight (X_n). Because the mass transfer parameter values for three types of disks were not available, the preset value of the mass transfer parameter near the entrance of the first reactor ($k_L a_{\text{initial}}$) was chosen as a standard value, and the mass transfer parameters in five reaction zones in two reactors were assigned as follows:

Reactor 1: Zone 1 (100% of $k_L a_{\text{initial}}$), Zone 2 (80% of $k_L a_{\text{initial}}$), Zone 3 (60% of $k_L a_{\text{initial}}$)

Reactor 2: Zone 4 (40% of $k_L a_{\text{initial}}$), Zone 5 (20% of $k_L a_{\text{initial}}$)

The mass transfer parameter is reduced along the reactor length because as the viscosity of PET melt increases, the melt holdup on the disk surfaces increases and the overall mass transfer parameter value decreases. It is noted that the assignment of $k_L a$ values in five reaction zones was not based on any experimental data or theoretical model.

Figure 4 shows the X_n (number-average degree of polymerization) values with varying mass transfer pa-

rameter values (thin lines) and with fixed mass transfer parameter values for every section of the reactor (heavy lines). Surprisingly, Figure 4 shows that polymer molecular weight was not as strongly affected by the mass transfer parameter values as expected. For the $k_L a$ values larger than 10 min⁻¹, there was practically no difference between the two simulation results. It is interesting to note that X_n values increased more rapidly as the mass transfer parameter value was increased, indicating that the polymerization was strongly mass transfer-controlled for the reaction conditions used in the simulations. Figure 4 also indicates that it was possible to tune the model parameter ($k_L a$) to match the outlet polymer molecular weight. For the outlet X_n value of 113 (plant data), it appears that $k_L a = 2.7$ min⁻¹ gives the best fit. As mentioned earlier, no measurements of molecular weight at other positions in the reactor are available. Therefore, it is not strictly correct to say that simply comparing the model-predicted and experimentally measured single-outlet polymer molecular weight values validates the model.

In our standard model calculations, the first reactor pressure was set at 2.5 mmHg and the second reactor pressure at 1.0 mmHg (industrial reactor conditions). The base mass transfer parameter value at the inlet of the reactor was set at 2.7 min⁻¹, and the $k_L a$ values in five reaction zones were distributed as in the above example. With the first reactor pressure kept at 2.5 mmHg, we varied the second reactor pressure to 2.5, 1.0, and 0.1 mmHg. The simulation results are shown in Figure 5. Notice that reducing the second reactor pressure had a large effect on polymer molecular weight. Figure 6 shows the effect of pressure in the second reactor on the concentrations (mol/L) of various functional end groups and volatile compounds (water and DEG). Notice that with a decrease in the Reactor 2 pressure, vinyl end group concentration ($[E_v]$) tended to increase, but the concentrations of acid groups and all other undesired side products decreased. Figure 6 also shows that diethylene glycol in

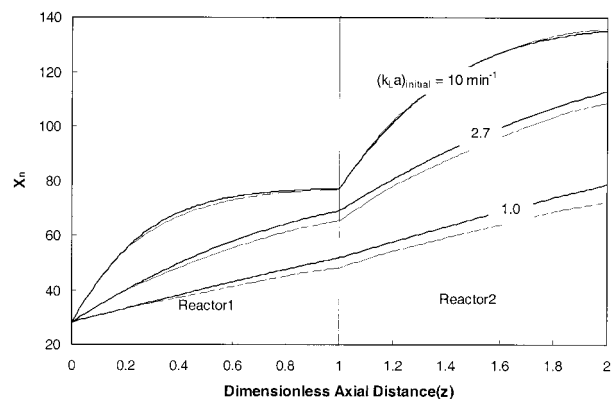


Figure 4 Effect of mass transfer parameter on degree of polymerization at 285°C ($P_1 = 2.5$ mmHg; $P_2 = 1$ mmHg).

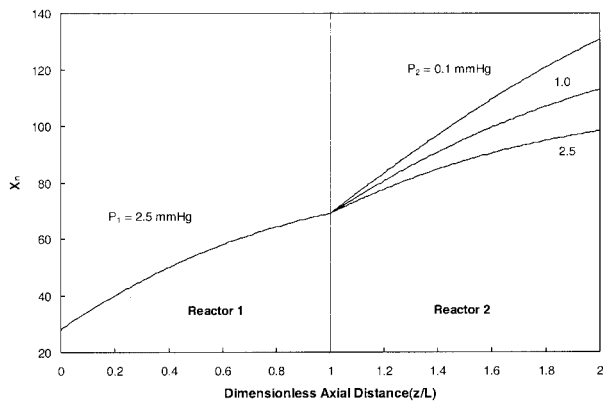


Figure 5 Effect of second reactor pressure on X_n with P_1 fixed at 2.5 mmHg.

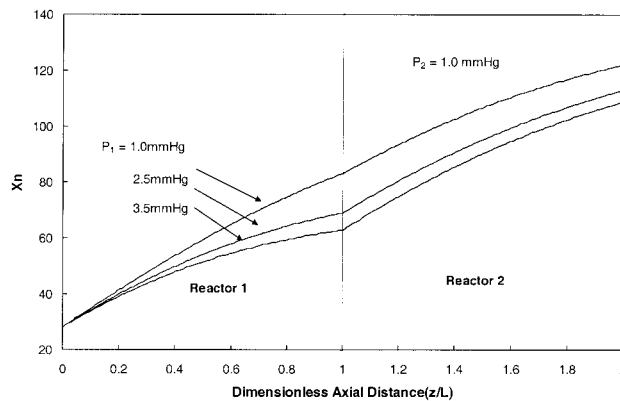


Figure 7 Effect of first reactor pressure with second reactor pressure fixed at 1.0 mmHg.

the polymer (E_{DEG}) was much larger than the free diethylene glycol concentration (DEG). Figure 7 shows the effect of pressure in the first reactor with pressure in the second reactor fixed at 1 mmHg. From Figures 5 and 7 it can be concluded that reducing the pressure in either the first reactor or the second reactor can increase polymer molecular weight.

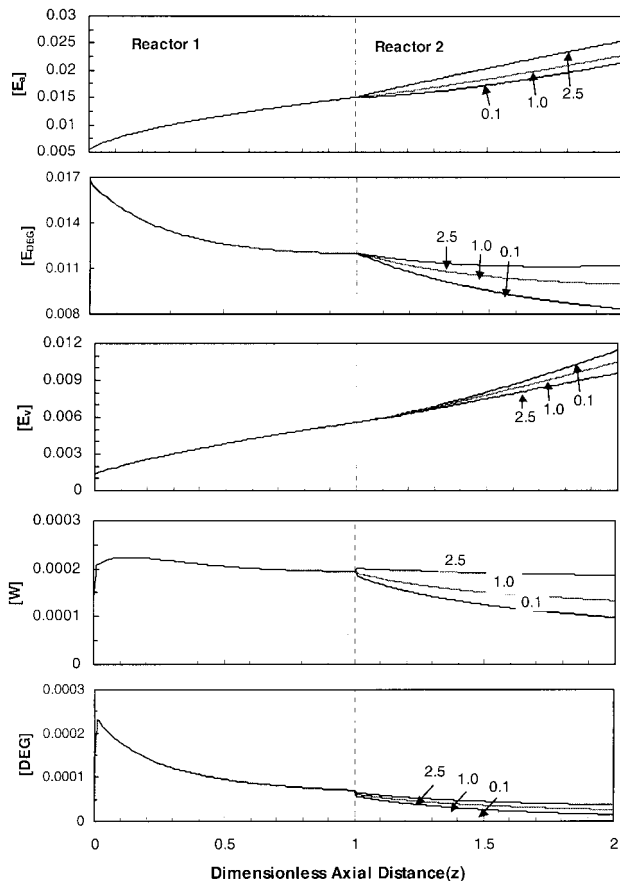


Figure 6 Effect of second reactor pressure on the concentrations of end groups and volatile compounds.

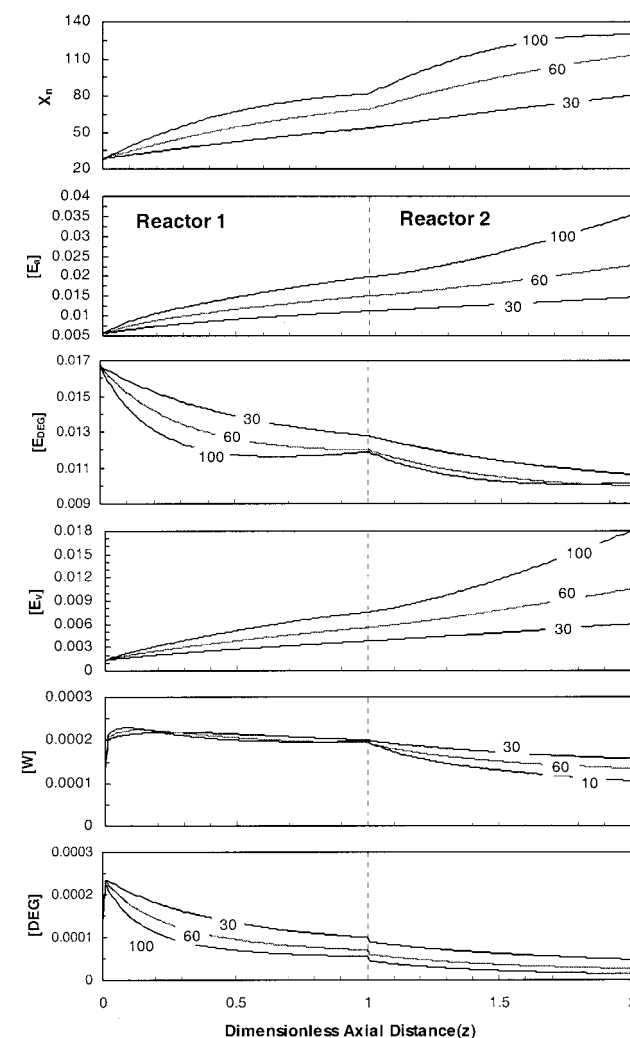


Figure 8 Effect of reactor residence time (in minutes).

size, the residence time in each reactor is also same. Figure 8 shows that the effect of residence time is surprisingly large, especially on acid end group and vinyl end group concentrations. Longer residence time yields higher-molecular-weight polymer, but acid end group and vinyl end group concentrations increase significantly with reaction time. The optimum acid group concentration may vary depending on the specific applications of PET. For example, low-acid end group concentration is desirable for tire cords in order to reduce hydrolytic degradation, but for bottle-grade PET resins, there is an optimum acid end group in the precursor polymer to maximize the reactivity in solid-state polymerization.¹³ Therefore, it is recommended that through a sensitivity analysis study, as presented above, optimal reactor operating conditions be designed to meet specific product specifications.

CONCLUSIONS

In this study we extended the two-phase model developed for a single-zone reactor to a multizone PET finishing reactor. The PET reactor system considered in this work as a simulation example is an industrial two-reactor system with multiple reaction zones with different types of disks. In this model the bulk melt phase of the plug flow was assumed, and the effective mass transfer parameter value in each reaction zone was gradually reduced along the reactor length to simulate the decreasing mass transfer efficiency. Because it was almost impossible to take samples from the reactor other than at the outlet of the second reactor, it is difficult to say that the multizone model presented here is perfectly valid. Nevertheless, the

model developed in this work illustrates that the two-phase model can be easily adapted to either a multi-zone or a multiple-reactor system. Although the extensive simulation results are not shown, some examples presented in this work clearly indicate that various reactor operating conditions may have to be adjusted to optimize the product quality represented by molecular weight, end group, and side product concentrations. The model simulations suggest that the employment of two reactors in series gives an increased degree of freedom to achieve such operational goals.

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