

Experimental Investigation of Vinyl Chloride Polymerization at High Conversion—Reactor Dynamics

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SYNOPSIS

A series of suspension polymerizations of vinyl chloride monomer (VCM) was carried out in a 5-L pilot plant reactor over the temperature range, 40–70°C. The reactor pressure and monomer conversion were monitored simultaneously every 7–8 min. The critical conversion X_f , at which the liquid monomer phase is consumed, was considered to occur when the reactor pressure fell to 98% of the vapor pressure of VCM for suspension at the polymerization temperature. The reactor model predictions of pressure are in excellent agreement with the experimental data over the entire conversion and temperature ranges studied. The mechanism of reactor pressure development for VCM suspension polymerization is discussed herein in some detail. For isothermal batch polymerization, the reactor pressure falls in two stages due to the effect of polymer particle morphology on pressure drop. The first stage is due to the volume increase of the vapor phase as a result of volume shrinkage due to conversion of monomer to polymer. The monomer phase is not yet consumed at this stage, but it is trapped in the interstices between primary particles creating a mass transfer resistance; therefore, the reactor pressure drops slowly. The second stage is due to both the volume increase of the vapor phase and to the monomer in the vapor phase diffusing into the polymer phase because of the subsaturation condition with respect to monomer in the polymer phase. The reactor pressure drops dramatically with an increase in monomer conversion at this stage. The present model can be used to predict reactor dynamics during suspension polymerization under varying temperature and pressure conditions.

INTRODUCTION

It is a well known phenomenon that the reactor pressure for isothermal VCM bulk, suspension, and emulsion polymerization remains constant until a critical monomer conversion, where it drops gradually with further increase in conversion. Therefore, VCM polymerization under commercially employed temperatures experiences isobaric and nonisobaric conditions. The transition from the isobaric to the nonisobaric state is attributed to the complete consumption of the liquid monomer-rich phase (essentially pure monomer). Hence, the reactor pressure starts to drop when the monomer phase is essentially consumed; these phenomena are generally assumed to occur simultaneously and are a unique feature of

VCM polymerization. The monomer conversion at which the reactor pressure starts to drop or the monomer phase is consumed is defined as a critical conversion X_f in kinetic modeling. In commercial reactor operation, the polymerization is usually taken beyond the critical conversion X_f and the terminal conversion is estimated using the measured reactor pressure drop (the difference between VCM vapor pressure and the actual reactor pressure). Therefore, the reactor pressure is an important parameter which is used to determine the terminal conversion where the polymerization is terminated to control the quality (porosity, thermal stability, and other processing properties) of poly(vinyl chloride) (PVC).

The monomer conversion, the polymerization rate, and the reactor pressure as a function of reaction time have been studied experimentally by several investigators.^{1–3} However, a model which re-

lates the monomer conversion and the reactor pressure under given reactor operating conditions was developed for the first time based on the assumption of equilibrium partition among phases in our previous publication.⁴ The critical conversion X_f as a function of reactor operating conditions and physical properties of the components in the reactor can be expressed as follows:

$$X_f = M_0 - [D_{g0}(1.0 - W_i)V_r + KW_w] \\ \times \{M_0[1.0 + D_{g0}(1/D_m - 1/D_p)]/(1.0 - D_{g0}/D_m) \\ + D_m(1.0 - \Phi_p)/(\Phi_p D_p)\}^{-1} \quad (1)$$

where D_{g0} , D_m , and D_p are the densities of vapor, monomer, and polymer, respectively. M_0 is the mass of the monomer charged to the reactor at time zero (initially), W_w is the mass of the water charged initially, V_r is the reactor volume, W_i is the reactor initial charge fraction, K is the solubility constant of VCM in water, and Φ_p is the volume fraction of polymer in the polymer phase.

When monomer conversion is greater than the critical conversion X_f , the conversion and reactor pressure relationship is given by

$$X = \left\{ M_0 - \frac{P_m M_m}{RT} \left[(1.0 - W_i)V_r + X_f M_0 \right. \right. \\ \left. \left. \times \left(\frac{1}{D_m} - \frac{1}{D_p} \right) \frac{D_{g0}}{(D_m - D_{g0})} \right] + \frac{KW_w P_m}{P_{m0}} \right\} \\ \times \{ M_0[1.0 + D_m(1.0 - \Phi_p)/(\Phi_p D_p)] \\ + P_m M_m (1/D_m - 1/D_p)/(RT) \}^{-1} \quad (2)$$

where P_m and P_{m0} are the partial and vapor pressures of VCM, respectively. M_m is the molecular weight of monomer. R is the gas constant, and T is the absolute temperature of polymerization.

The reactor initial charge fraction can be expressed as⁴

$$W_i = (W_w/D_w + M_0/D_m \\ - D_{g0}V_r/D_m)/[V_r(1 - D_{g0}/D_m)] \quad (3)$$

where D_w is the density of water.

The polymer volume fraction Φ_p in eqs. (1) and (2) is governed by the Flory-Huggins equation⁵ as follows:

$$\ln(1.0 - \Phi_p) + (1.0 - 1/\bar{n})\Phi_p + \chi\Phi_p^2 = 0 \\ (X = X_f) \quad (4)$$

$$\ln(1.0 - \Phi_p) + (1.0 - 1/\bar{n})\Phi_p + \chi\Phi_p^2 \\ = \ln(P_m/P_{m0}) \quad (X > X_f) \quad (5)$$

where \bar{n} is the number-average chain length of polymer and χ is the monomer-polymer interaction parameter (it was estimated in a previous publication⁴).

This model was examined using equilibrium conversion/pressure data obtained for a nonreacting system (H₂O/PVC/VCM mixture) and the limited literature data in a previous publication.⁴ It remains to be seen whether equilibrium partition of VCM between existing phases is actually closely achieved during polymerization. Comprehensive experimental data of conversion/pressure covering commercial polymerization temperatures have not been published in the literature to date. Therefore, the objectives of the present work are to determine conversion/pressure relationships for VCM suspension polymerization in a pilot plant reactor, and to further compare model predictions of pressure versus monomer conversion with experimental data obtained under various polymerization conditions including batch, semibatch, and temperature programming operation at high conversions.

EXPERIMENTAL

The equipment used for the experiments included an agitated 5-L stainless steel reactor with a calibrated vacuum-pressure gauge and a thermocouple. The reactor temperature was maintained by a steam/water mixture that circulated in the reactor jacket, and controlled with a proportional-integral-derivative controller.

The reactor was filled with a weighed amount of distilled, deionized water with dissolved suspending agent and an aqueous buffer and a weighed amount of initiator at around 5–10°C. A weighed amount of *n*-butane as a tracer and a weighed amount of VCM were injected into the reactor after the reactor was evacuated. Then the reactor temperature was raised to the desired polymerization temperature. The reactor pressure was recorded every 7–8 min and the monomer conversions were measured simultaneously using the online *n*-butane tracer method.⁶

Vinyl chloride monomer was provided by the B. F. Goodrich Company (Niagara Falls, Ontario, Canada).

Suspending agent, polyvinylalcohol (KP-08) (degree of hydrolysis is 71–75 mol %) and initiator, bis(4-*tert*-butylcyclohexyl) peroxydicarbonate

(Perkadox 16-W40) (40 wt % initiator in liquid suspension) were provided by AKZO Chemicals (The Netherlands). Azobis(isobutyronitrile) (AIBN) recrystallized was used as an initiator for polymerization at higher temperatures. Na_2HPO_4 and $\text{NaH}_2\text{PO}_4 \cdot \text{H}_2\text{O}$ were used as an aqueous buffer to control pH of the polymerization system.

The basic conditions and the chemical recipe for the polymerizations are as follows:

Reactor	5.0 L
Temperatures	40, 45, 50, 55, 60, 65, 70°C
Monomer	1116 g
Water	2232 g
Suspending agent	0.08 wt % (based on water)
Buffer	0.08 wt % (based on water)
Initiator	varying amounts

The experimental procedures for temperature programming and for semibatch operation are given in our previous publications.^{7,8}

RESULTS AND DISCUSSION

The comparison between the experimental data and the model predictions is discussed in the following. The parameters involved in the model are as follows:

$$D_m = 947.1 - 1.746t - 3.24 \times 10^{-3}t^2 \text{ (}^\circ\text{C)} \quad (\text{g/L})^{9,10} \quad (6)$$

$$D_p = [\exp(0.4296 - 3.274 \times 10^{-4}T \text{ (K)})] \times 10^3 \quad (\text{g/L})^{11-13} \quad (7)$$

$$D_w = 1011.0 - 0.4484t \text{ (}^\circ\text{C)} \quad (\text{g/L}) \quad (8)$$

$$P_{m0} = 1.27 \times 10^4 \exp[-2.41 \times 10^3/T \text{ (K)}] \quad (\text{atm})^{14} \quad (9)$$

$$K = 0.0472 - 11.6/T \text{ (K)} \quad (10)$$

$$\chi = 1286.4/T \text{ (K)} - 3.02 \quad (11)$$

Combining the thermal expansion factor for PVC¹¹ with the density data^{12,13} yields eq. (7). Equation (9) was obtained from Johnston's data.¹⁴ Equations (10) and (11) were estimated previously.⁴ The other parameters involved in the kinetic model are given in our previous publication.¹⁵

The Critical Conversion X_f

The critical conversion X_f is usually defined as the point where the reactor pressure starts to fall when the liquid monomer as a separate phase is consumed.

This definition is based on the assumption that the reactor pressure starts to drop when the liquid monomer is consumed. However, it is difficult to measure the critical point for liquid VCM phase disappearance in the interstices of the PVC primary particles directly under the high pressures involved during polymerization. The critical conversion data reported in the literature were based on solubility and kinetic data estimation.^{4,16} This is the first investigation to determine the critical conversion by measuring the reactor pressure and the monomer conversion simultaneously during suspension polymerization of VCM. The present experimental results and the model prediction are shown in Figure 1. One can see (Fig. 1) that monomer conversions determined when the reactor pressure starts to drop are much lower than the model predictions. However, the conversions determined at around 98% of the vapor pressure of VCM are in excellent agreement with the model predictions. These results indicate that the reactor pressure drop and the monomer phase depletion do not occur at the same conversion level for suspension polymerization of VCM. In other words, the reactor pressure starts to drop before the monomer phase is completely consumed. The critical conversions determined at around 98% vapor pressure are in agreement with literature data¹⁷⁻²⁰ estimated using solubility and kinetic studies, as shown in Table I, together with the model predictions. Therefore, for suspension polymerization system, the critical conversion X_f cannot be defined as occurring when the reactor pressure starts to drop. It should be defined as the conversion at which the liquid monomer phase is consumed. Based on the present experimental data, the liquid mono-

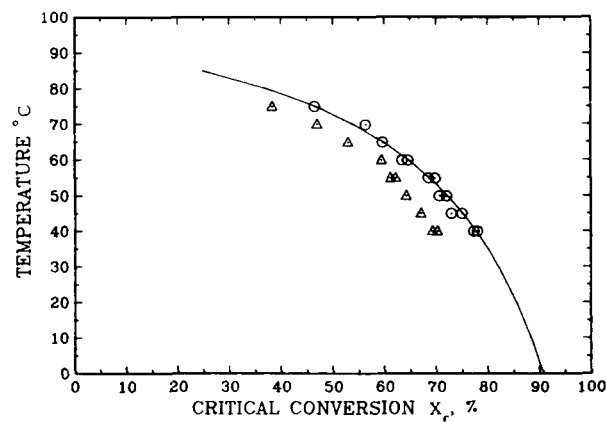


Figure 1 Temperature dependence of the critical conversion for suspension polymerization of VCM: (Δ) at pressure starting to drop; (\odot) at 98–99% P_{m0} ; (—) model prediction.

Table I Comparison of the Critical Conversion X_f Estimated by Different Methods Using Suspension and Emulsion Polymerization Systems

Temperature (°C)	Present Data at 98–99% P_{m0}	X_f (Literature Data)	Model Prediction
40	0.77, 0.78	—	0.78
45	0.73, 0.75	—	0.75
50	0.71, 0.72	0.71 (solubility ¹⁷)	0.72
55	0.69, 0.70	0.70 (kinetics ¹⁸)	0.69
60	0.64, 0.65	0.63–0.64 (kinetics ¹⁹)	0.65
65	0.60	0.687 (solubility ²⁰)	0.60
70	0.56	—	0.54

mer phase is consumed when the reactor pressure reaches 98% of the vapor pressure of monomer at the polymerization temperature. The reason why the pressure drops before the liquid monomer phase is consumed is further discussed in the next section.

The behavior of the critical conversion shown in Figure 1 is significant for both commercial production and for kinetic modeling of the polymerization. To the left side of the curve is the region of two-phase polymerization and to the right side of the curve is the region of single phase polymerization. Therefore, the critical conversion X_f is an important parameter for the kinetics and reactor modeling of VCM polymerization.¹⁵ The thermal stability and porosity of the PVC product decreases significantly with conversion beyond the critical conversion X_f .⁸ Therefore, the critical conversion X_f is the basis for quality control of PVC production. Figure 1 also

shows that the critical conversion increases significantly with a decrease in polymerization temperature. This shows that the conversion when the liquid phase is consumed is quite different for different polymerization temperatures. Pinto,²¹ recently, estimated the critical conversion only using eq. (4) and concluded that the critical conversion is almost constant within the temperature range, 30–60°C. This is in contradiction to the present experimental observations and to the literature data shown in Table I.

Reactor Pressure Development

From the discussion above, it is clear that the kinetics of VCM polymerization can be divided into two distinct stages—two-phase polymerization before X_f and single phase polymerization after X_f . Figures 2 and 3 further show batch reactor pressure profiles for different temperatures over the monomer conversion range of interest commercially. One can see that the model predictions are in excellent agreement with the experimental data. The experimental data show that monomer conversion where the pressure drop occurs depends on the polymerization temperature as shown earlier. At higher temperatures, the reactor pressure starts to fall at lower conversion because the polymer can swell more monomer at higher temperatures.⁴ The experimental data shown in Figures 2 and 3 indicate that the reactor pressure starts to fall gradually at lower conversion than that predicted by the model. The same

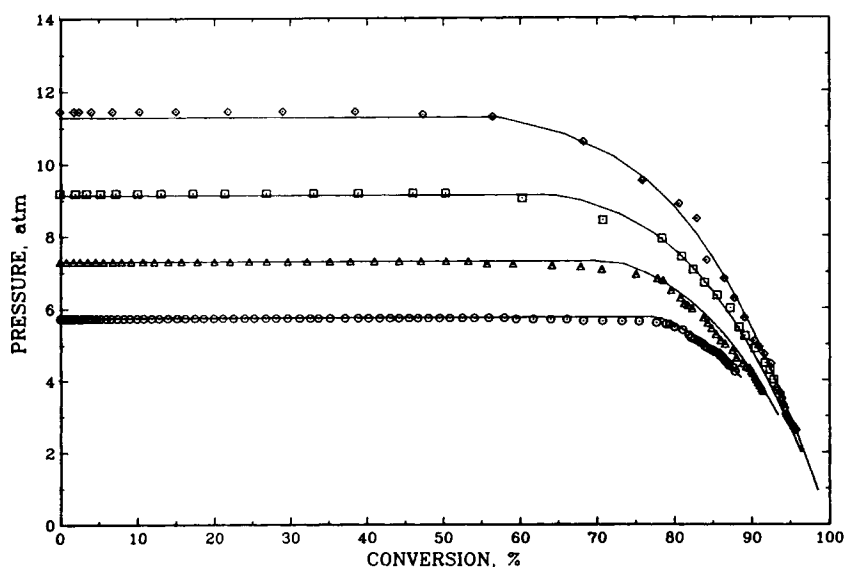


Figure 2 Conversion and temperature dependence of the reactor pressure for suspension polymerization of VCM: (○) 40°C; (△) 50°C; (□) 60°C; (◇) 70°C; (—) model prediction.

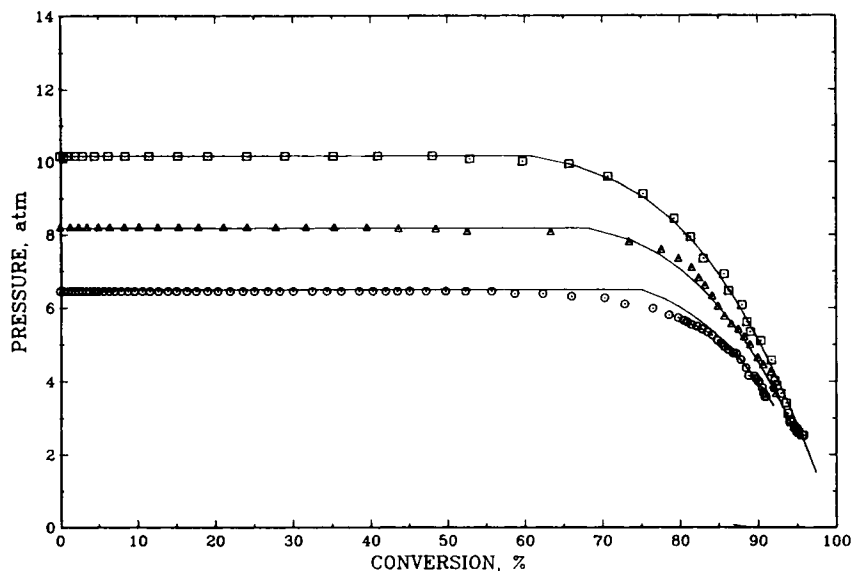


Figure 3 Conversion and temperature dependence of the reactor pressure for suspension polymerization of VCM: (○) 45°C; (△) 55°C; (□) 65°C; (—) model prediction.

phenomenon was observed by Meeks¹ and Nilsson et al.² for suspension polymerization of VCM. However, this phenomenon is not observed during emulsion polymerization of VCM, where the reactor pressure remains constant as long as VCM droplets are present.² Nilsson et al.² explained the early pressure drop which occurs before the liquid monomer is consumed during suspension polymerization as the capillary condensation of monomer in the fine pores of the PVC particles. Therefore, the conversion at the point where the pressure drops for suspension polymerization seems to depend on the morphology of the PVC particles.

For suspension polymerization in a batch reactor, the reactor pressure drop is due to an increase in volume of the vapor phase, a decrease in the number of moles of VCM in the vapor phase or both. Figure 4 shows the quantitative relationship between the reactor pressure development and monomer distribution during suspension polymerization at 50°C. One can see that the reactor pressure starts to drop at around 55–60% conversion under the present conditions. According to the monomer mass balance,⁴ there is about 15–20% monomer in the liquid monomer phase at this conversion range (see Fig. 4). Therefore, the monomer phase is still in equilibrium with the polymer phase when the reactor pressure starts to fall. Thus, before the liquid monomer phase is consumed, VCM in the vapor phase will not diffuse into the polymer phase. In other words, the number of moles of VCM in the vapor phase cannot decrease when the liquid monomer

phase is still available. Hence, the only possible cause for a pressure drop is an increase in the volume of the vapor phase as a result of reaction volume shrinkage due to monomer being converted to polymer. In this conversion stage, the polymerization rate reaches a maximum for a normal polymerization system. The volume shrinking rate is also maximum at this conversion range. Hence, the volume of the vapor phase increases significantly. To maintain the pressure constant, the monomer in the liquid monomer phase must diffuse through the polymer–water interface and the water phase into the vapor phase. PVC particle morphology development experiences several aggregate stages through the entire conversion range.²² In suspension polymerization, a dense skin surrounding PVC particle (PVC–water interface) can be formed.^{23,24} At relatively low conversions, the continuous structure of PVC particle is not complete, the monomer in the monomer phase (in the interstices of the primary particle) is free to diffuse into the vapor phase to maintain the constant pressure as shown in Figures 2 and 3. At a conversion close to X_f , the PVC internal structure and the skin surrounding the particle become rigid enough to give a significant resistance for monomer diffusion. Thus the monomer diffusion rate from the monomer phase in the interstices cannot compensate for the vapor phase volume increase. Consequently, the reactor pressure drops gradually even when the liquid monomer phase exists. When the liquid monomer phase is completely consumed ($X > X_f$), the monomer concentration in the polymer phase decreases

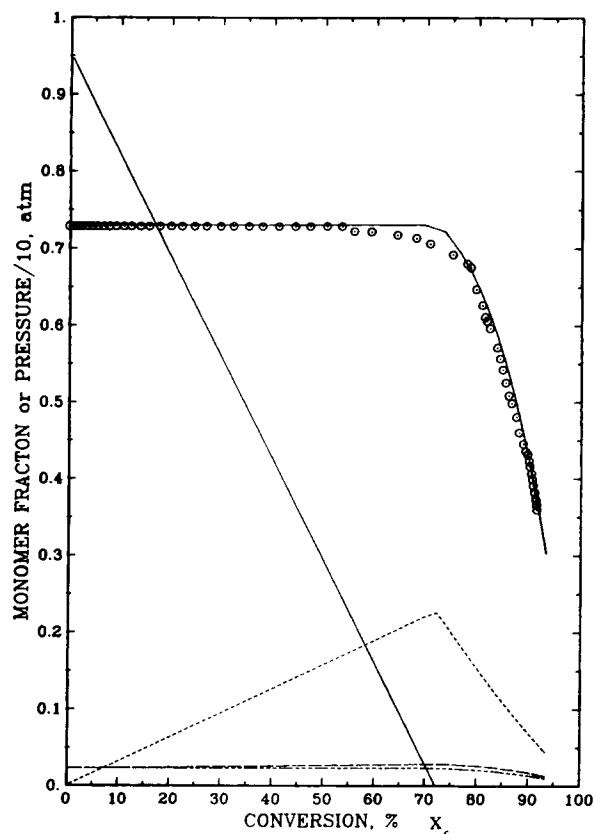


Figure 4 Relation between reactor pressure development and monomer distribution for suspension polymerization of VCM at 50°C. (—) monomer fraction in the monomer phase; (· · ·) monomer fraction in the polymer phase; (---) monomer fraction in the gas phase; (- · -) monomer fraction in the water phase; (○) reactor pressure; (—) model prediction of pressure.

often dramatically, and monomer in the water and vapor phases transfers to the polymer phase where it continues to polymerize. In fact, the monomer in the vapor phase diffuses through the water phase and into the polymer phase and the reactor pressure drops significantly as monomer conversion increases (see Figs. 2 and 3). The mechanism of monomer diffusion among phases before and after X_f is schematically shown in Figure 5. Thus, the reactor pressure drop for suspension polymerization can be divided into two stages: The first stage is due to the decrease in rate of monomer transfer from the liquid monomer phase in the interstices of the porous polymer domain through the water phase and into the vapor phase because of the resistance provided by the fixed PVC particle structure. As a result, the reactor pressure drops slowly before the liquid monomer phase is completely consumed. The start-

ing point for the first stage cannot be strictly defined. The second stage is due to both the increase in the volume of the vapor phase and to the fact that the VCM in the vapor phase diffuses through the water phase and into the polymer phase since the liquid monomer phase no longer exists. Consequently, the reactor pressure can drop dramatically with an increase in monomer conversion in this stage. The second stage starts at about when the pressure equals 98% of the vapor pressure of VCM for suspension polymerization under the present experimental conditions. The relationship between the reactor pressure and PVC particle morphology development is illustrated in Figure 6. Therefore, for suspension polymerization, the instantaneous equilibrium assumption may not be valid during the first stage of the pressure drop.

Emulsion polymerization of VCM is carried out in batch, semibatch, and continuous processes. The reactor dynamics in terms of monomer conversion history and polymerization rate has been studied in some detail.²⁵ However, little work has been done for the reactor pressure development in emulsion polymerization.² For emulsion polymerization, the monomer phase (no initiator or radicals in the liquid monomer phase) is not in the interstices of the polymer particles as they do not exist since the polymer particles are isolated primary particles. The monomer phase (monomer droplets) is not in direct contact with the polymer particles and, hence, monomer can exert its full vapor pressure to maintain the reactor pressure constant up to the very point when the monomer phase is consumed. Therefore, the reactor pressure starts to drop at the critical conversion X_f . This is the reason why the pressure drop occurs at a higher conversion for emulsion than for suspension polymerization at the same reactor operation conditions as demonstrated by Nilsson et al.² experimentally. Hence, the critical conversion X_f for emulsion polymerization occurs when the liquid monomer phase is consumed and the reactor pressure starts to fall simultaneously.

For bulk VCM polymerization, monomer is the continuous phase at low conversions. At higher conversions, the monomer phase is in the interstices of the primary particles. However, PVC particles made by bulk process have no dense skin surrounding the particles as PVC particles made by suspension process often do.^{24,26} Therefore, the resistance for mass transfer of monomer in bulk PVC particle from the liquid monomer phase to the vapor phase should be much smaller than that for suspension PVC particles. The reactor pressure for bulk polymerization may start to drop very near the critical conversion

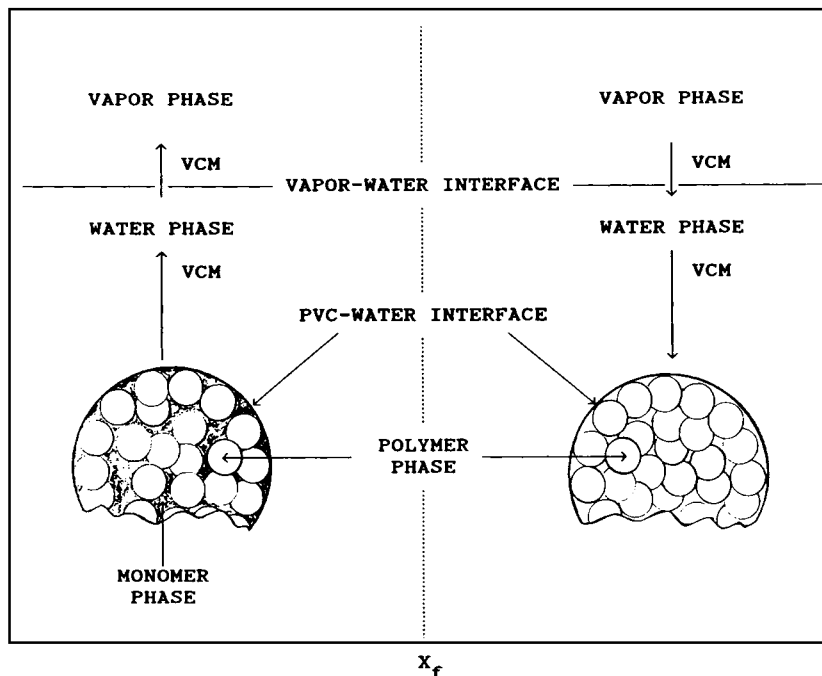


Figure 5 Monomer transfer before and after the critical conversion X_f .

X_f . Detailed experimental data of conversion/pressure for bulk polymerization are not available in the literature to confirm this, however.

From the discussion above, one knows that reactor pressure profile for VCM polymerization depends on the polymerization process. The present model fails to describe the first stage pressure drop for suspension polymerization. However, this will

not significantly affect the model applications because the first stage pressure drop is relatively small ($\sim 2\%$ of the vapor pressure of VCM). Figure 7 shows the effect of temperature on the reactor pressure at high conversions ($X > X_f$). Although the reactor pressure increases with an increase in temperature, the pressure cannot reach the vapor pressure of pure monomer at the temperature because

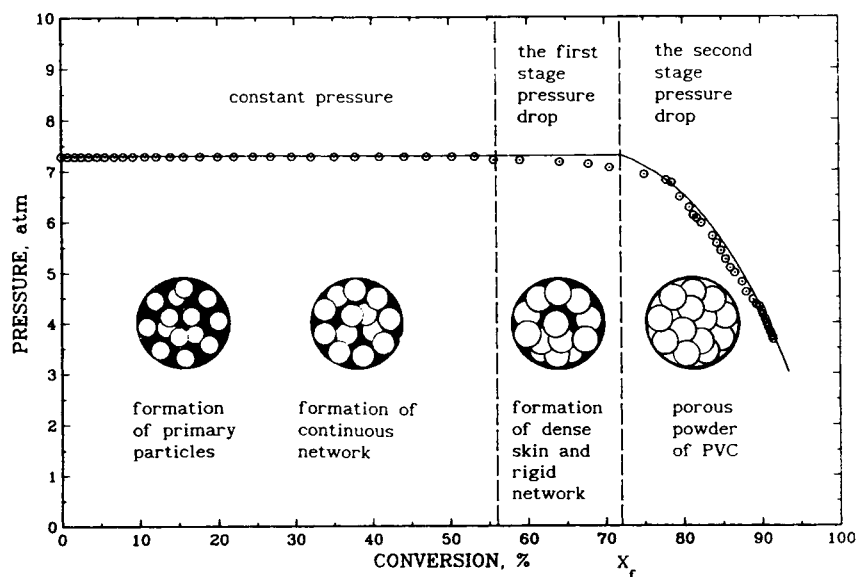


Figure 6 Relationship between the reactor pressure and PVC morphology development.

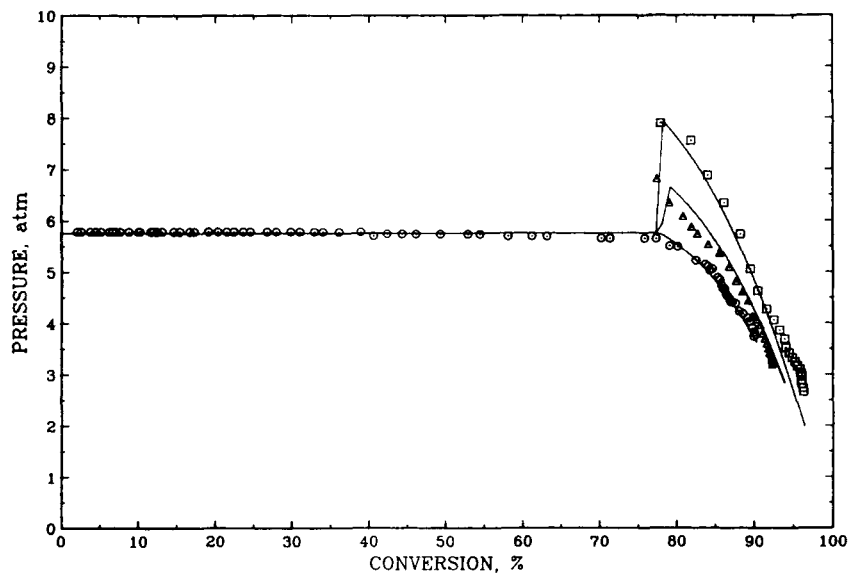


Figure 7 Effect of temperature on the reactor pressure at high conversions: (○) 40°C; (△) 50°C; (□) 60°C; (—) model prediction.

the monomer phase has been consumed. The reactor pressure drops sharply with an increase in conversion. Therefore, temperature programming at high conversions is considered safe within a reasonable temperature range. Figure 8 shows the reactor pressure dynamics for semibatch operation at high conversions.⁷ One can see that the reactor pressure can

be maintained by properly feeding fresh monomer into the reactor. This proves that the monomer added during semibatch operation rapidly diffuses through the water phase and into the polymer particles to maintain a constant pressure. If diffusion of added monomer were slow, monomer droplets would exist and the reactor pressure would equal

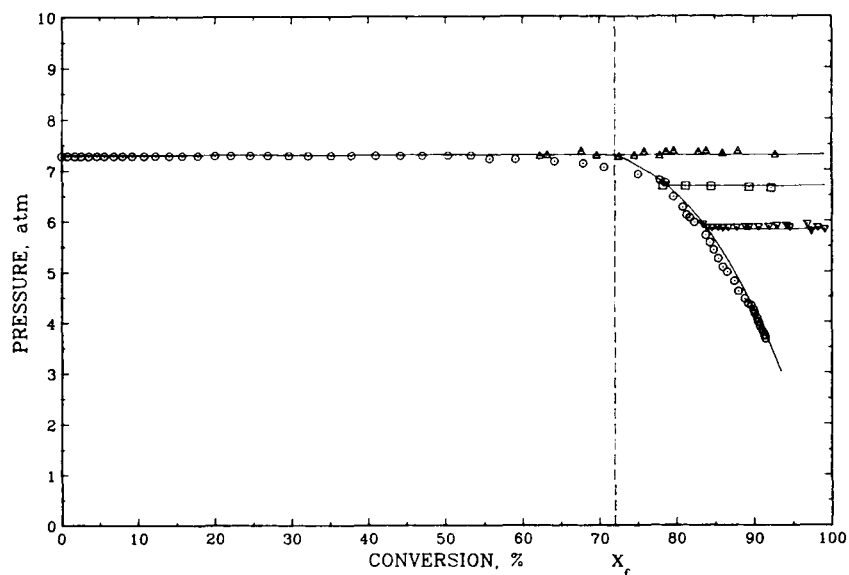


Figure 8 Conversion dependence of the reactor pressure for batch and semibatch suspension polymerization of VCM at 50°C; (○) batch process; (△) semibatch at vapor pressure; (□) semibatch at 90% of the vapor pressure; (▽) semibatch at 78% of the vapor pressure; (—) model prediction.

the VCM vapor pressure. This observation further confirms the pressure development mechanism discussed above. The model predictions are in satisfactory agreement with the temperature programming and semibatch pressure data.

Combining the reactor pressure model with the polymerization rate model,¹⁵ one can calculate the relationship between monomer conversion and reactor pressure development with polymerization time as shown in Figure 9. This figure shows typical dynamic behavior of VCM isothermal polymerization in a batch reactor. One can see that the polymerization proceeds under isobaric condition until around 72% conversion; then the reactor pressure decreases dramatically. In the nonisobaric period, the conversion increases slowly with time. This rapid decrease in polymerization rate indicates that the polymerization rate decreases not only due to the reduction in monomer concentration in the polymer phase but also due to a fall in propagation rate constant, initiator efficiency, and decomposition rate constant for peroxide initiator.¹⁵ For this typical run, when the conversion reaches 85%, the reactor pressure is about 80% of the initial pressure at 300 min (see Fig. 9). From 300 to 600 min, the conversion only increases by about only 7%. The final pressure is about 50% of the initial one. Hence, further polymerization after 85% conversion is very time-consuming if done batchwise and isothermally. Furthermore, the nonisobaric polymerization leading to

low monomer concentration will cause a significant deterioration in the thermal stability of the PVC product.⁸ From the point of view of productivity and quality, commercial polymerizations should be terminated at about 85% conversion at 50°C if done batchwise and isothermally. Figure 10 further shows the pressure and polymerization rate relationship versus conversion. During isobaric polymerization, the reaction rate increases significantly with an increase in conversion. However, the reaction rate decreases dramatically in the nonisobaric period. Note that the polymerization rate is reaching a maximum in the first stage of the reactor pressure drop. Hence, the heat peak of the commercial reactor often occurs just after the reactor pressure starts to fall, especially for initiator systems with long half-life. When the liquid monomer phase is consumed, the polymerization rate decreases immediately. In other words, the heat peak cannot occur after the monomer phase is consumed. Figures 9 and 10 suggest a potential to optimize the batch reactor for VCM polymerization. For conversions less than the critical conversion X_f , the polymerization rate should be linearized to effectively use the heat removal capacity of the reactor. This can be achieved using multi-initiators system. For conversions beyond X_f , an effective way to improve the reactor performance is to increase polymerization rate by increasing monomer concentration. This can be done using a semibatch process as described in our previous publication.⁷

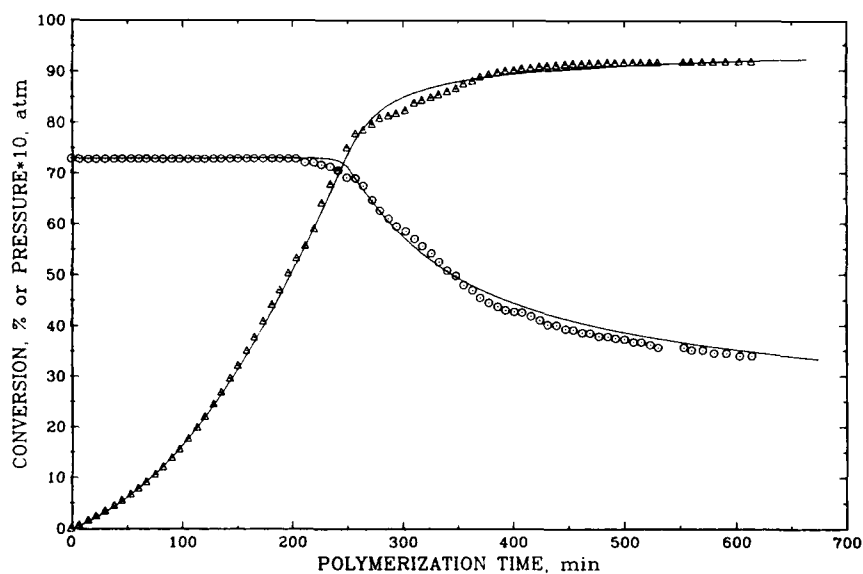


Figure 9 Monomer conversion and reactor pressure development for isothermal suspension polymerization of VCM in batch reactor at 50°C. Initiator Perkadox 16-W40 with $[I] = 0.175$ wt %: (\odot) reactor pressure; (Δ) monomer conversion; (—) model prediction.

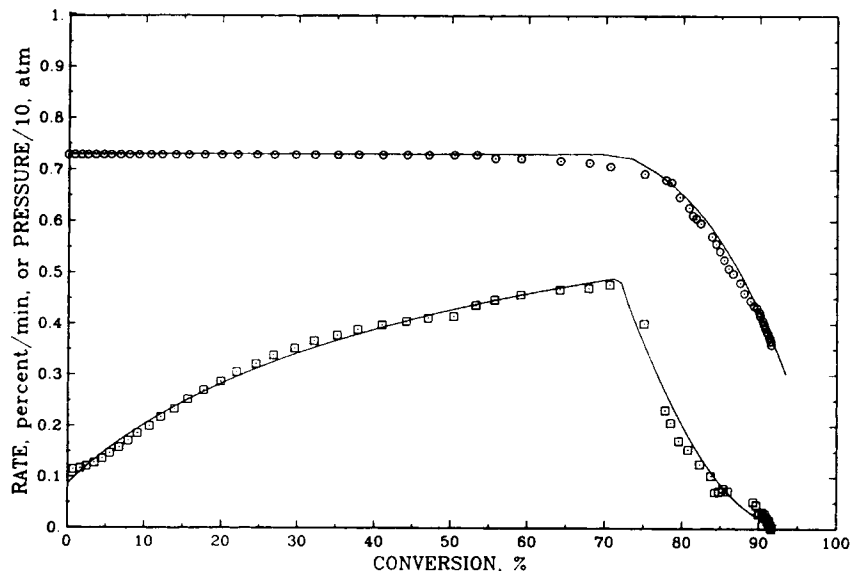


Figure 10 Conversion dependence of polymerization rate and reactor pressure for suspension polymerization of VCM at 50°C. Initiator Perkadox 16-W40 with $[I] = 0.175$ wt %: (\odot) reactor pressure; (\square) reaction rate; (—) model prediction.

CONCLUSIONS

For suspension polymerization of VCM in a batch reactor, the reactor pressure starts to fall before the liquid monomer phase is consumed due to the effect of PVC morphology on trapped liquid monomer. The critical conversion X_f at which the liquid monomer phase is consumed is at about 98% of the vapor pressure of VCM at the polymerization temperature. The reactor pressure drop occurs in two stages: The first stage is due to the volume increase of the vapor phase as a result of volume shrinking of the reacting phases where the reactor pressure drops slowly; the second stage is due to the volume increase of the vapor phase and the monomer in the vapor phase diffusing into the water and polymer phases as a result of the decrease in monomer concentration in the polymer phase where the pressure drops dramatically with an increase in monomer conversion. The model predictions are in excellent agreement with the experimental data over the entire conversion range at different temperatures. The model can be used to predict the reactor pressure development under different operating conditions. Combining the present pressure calculation and kinetic models, one can describe the dynamic behavior of VCM polymerization in batch and semibatch suspension reactors. The present model can be used for reactor simulation and optimization of VCM polymerization

and for the determination of the optimal terminal conversion for a particular PVC product.

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