

Feedback controllability assessment and control of particle size distribution in emulsion polymerisation

Charles D. Immanuel*, Ying Wang, Nicola Bianco

Department of Chemical Engineering, Centre for Process Systems Engineering, Imperial College, London SW7 2AZ, UK

Available online 28 July 2007

Abstract

In this article, the importance of particle size distribution (PSD) control as a means for the inferential control of the rheology of emulsion polymers is illustrated. A controllability assessment is presented to illustrate the attainability or otherwise of bimodal PSD using feedback control through a consideration of the process mechanisms—measurement limitations and process constraints that prevent the implementation of feedback corrections. The suitability of a batch-to-batch iterative feedback PSD control is demonstrated, which could act in addition to any in-batch feedback control, the latter being less feasible in certain cases, as argued in this article. A detailed population balance model is used for the batch-to-batch control, which simplifies model update and feedback correction.

© 2007 Elsevier Ltd. All rights reserved.

Keywords: PSD control; Emulsion polymerisation; Population balances; Batch-to-batch feedback; Feedback controllability

1. Introduction

1.1. Importance of PSD

In emulsion polymerisation, the polymer is produced within particles that span the sub-micron size range. The particle size distribution (PSD) is determined by three major particle-level phenomena, namely, nucleation, growth and coagulation, which are influenced by process manipulations (surfactants, monomers, initiators, etc.) in complex ways [see Fig. 1]. The particle-level phenomena interact with each other, and are regulated through an integrated feedback from the PSD, resulting in a highly non-linear process. The PSD plays a strong role in determining the rheology of the emulsion polymers. In particular, it is seen that the rheology is determined by three factors, *viz.* the polymer content (solids content) of the latex, the maximum packing factor, and the particle–particle interaction

parameter (Schneider et al., 2002). Of these three factors, the maximum packing factor is directly related to the PSD of the latex. In addition, there is an interrelationship between the PSD and solids content. Overall, the mechanism relating the rheology with the process inputs is highly interactive and non-linear.

Arevalillo et al. (2006) have recently reported the relation between PSD and rheology, in the framework of previous models (Krieger and Dougherty, 1959; Mooney, 1951; Sudduth, 1993; Luckham and Ukeje, 1999). In this model, the maximum packing factor is calculated as shown in Eq. (1), where $F(r)$ denotes the particle density, \bar{r} is the average particle radius, and β is a parameter in the model. This is then used to compute the relative viscosity η_r using Eq. (2), where ϕ is the polymer (solids) content of the latex, $[\eta]$ is the intrinsic viscosity (a parameter) and σ is the particle–particle interaction parameter given by $\sigma = k_1 \exp[-k_2(\phi_n - \phi)^{1/3} \gamma^{k_3}]$. The interaction parameter depends on the shear stress γ :

$$\phi_n = \frac{\int_0^\infty r^3 F(r) dr}{\int_0^\infty \max(0, (r - \bar{r})^3) F(r) dr + \frac{1}{\beta} \int_0^\infty [(r + \bar{r})^3 - \max(0, (r - \bar{r})^3)] F(r) dr}, \quad (1)$$

$$\ln(\eta_r) = \left(\frac{[\eta]\phi_n}{\sigma - 1} \right) \left(\left(\frac{\phi_n - \phi}{\phi_n} \right)^{1-\sigma} - 1 \right). \quad (2)$$

* Corresponding author. fax: +44 20 7594 6606.

E-mail address: c.immanuel@imperial.ac.uk (C.D. Immanuel).

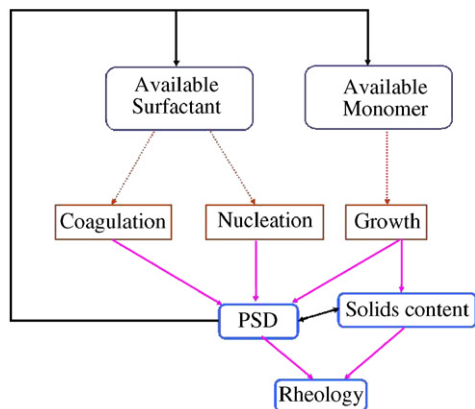


Fig. 1. An integrated systems representation of the emulsion polymerisation process and the evolution of the rheology of the emulsion polymer.

The model is employed in the present study to illustrate the effect of PSD on rheology. The effect of PSD on the maximum packing factor can be broken into the effects of the number of modes in the PSD, the size of the modes, and the amount of particles in each mode. Fig. 2a shows the effect of the polymer solids content ϕ on the rheology, for the PSD shown in Fig. 2b. The value of the maximum packing factor $\phi_n = 0.65$ for this PSD. It is seen that as the value of ϕ approaches ϕ_n , the viscosity increases exponentially, thereby illustrating the effect of the polymer solids content on rheology. It has to be mentioned here that this model is said to have a reduced validity at lower solids content due to differences in the mechanisms that influence rheology of dilute emulsions.

Focussing on a high polymer content latex, the effect of the number of modes in the PSD and the size of the modes on the rheology are presented in Fig. 3. Four cases are considered: case 1 is a bimodal distribution with clearly separated modes, case 2 is a unimodal PSD with only the small size mode from case 1, case 3 is a unimodal PSD with only the large size mode from case 1, and case 4 is a bimodal PSD with the two modes merging into each other (same as Fig. 2b). It is seen that a unimodal PSD comprising the small size mode only (case 2) results in considerably reduced viscosity for the same polymer content, having the largest possible packing factor value of $\phi_n = 0.7654$. The other three cases produce comparable viscosities, with case 4 (merging modes) producing the lowest viscosity among the three and case 3 producing the highest viscosity. A complementary issue is the ability to attain the said solids content (and appreciable conversion of the monomers) with all these PSD cases, particularly cases 2 and 3, in view of the interrelation between PSD and solids content (conversion) as depicted in Fig. 1. Case 1 with a clear bimodal PSD has a larger value of ϕ_n ($\phi_n = 0.6472$) than case 3 ($\phi_n = 0.6439$), as the smaller particles can pack between the larger ones. This effect is even more profound in case 4 ($\phi_n = 0.6504$). Overall, for the particular value of the relative magnitude of particles in the two modes, the change in ϕ_n is small among cases 1, 3 and 4.

Fig. 4 presents results that examine the effect of the relative amounts of particles in the two modes. It is seen that an increase

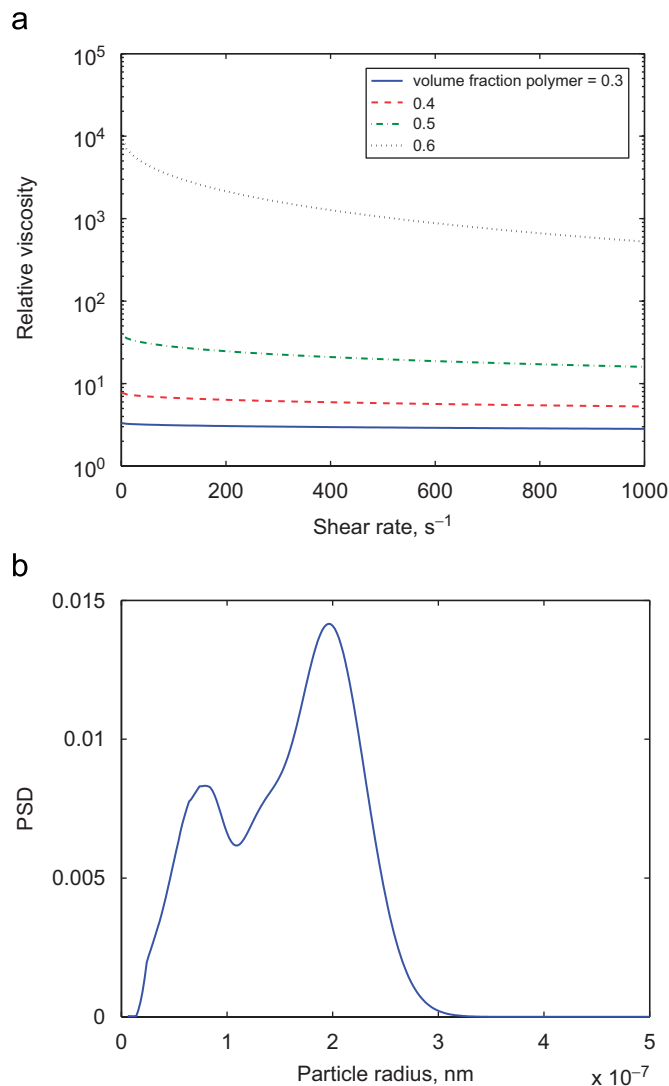


Fig. 2. Variation of rheology with polymer solids content of the emulsion (a) for a fixed PSD (b).

in the relative amount of the larger particles results in a drop in the viscosity by causing an increase in the maximum packing factor from 0.6504 to 0.6678. A similar drop is also evident with an increase in the number of particles in the smaller mode. The drop in this case is much less significant, and the change in the maximum packing factor is also much smaller, from 0.6504 to 0.6512.

The results presented here clearly illustrate that the PSD can considerably influence the rheology. In particular, the number of modes, the sizes of the modes, and the relative amounts of particles in the different modes influence the maximum packing factor directly. The PSD also influences the solids content indirectly via the polymerisation mechanisms, and both PSD and solids content influence the rheology.

It is also evident that there is a non-unique relationship between PSD and rheology, with a considerable range of choices for the PSD that would lead to the desired rheology. Thus, in view of the interrelation between PSD and solids content, and

Download English Version:

<https://daneshyari.com/en/article/159203>

Download Persian Version:

<https://daneshyari.com/article/159203>

[Daneshyari.com](https://daneshyari.com)