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BATCH VINYL ACETATE / BUTYL ACRYLATE EMULSION HOMO- AND CO-POLYMERIZATIOS. EFFECT OF TEMPERATURE AND COMPOSITION

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Copolymerization reactions are very important as they allow the production of copolymers with specific properties based on the individual characteristics of each homopolymer. Vinyl acetate / butyl acrylate copolymer latex has significant industrial importance due to its application as water-based paints, adhesives and paper and textile coatings [1, 2, 3, 4].

This work studies the kinetics of batch vinyl acetate (VA) and butyl acrylate (BuA) emulsion homo- and co-polymerization reactions and the effect of reaction temperature. The formulations are presented in Table 1. Conversion was determined by gravimetry, particle sizes were measured by photon correlation spectroscopy and copolymer composition was calculated based on the unreacted monomer contents measured by gas chromatography. Experimental results were compared with simulation results using a detailed mathematical model [5]. This mathematical model includes micelar and homogeneous particle nucleation mechanisms as well as particle coalescence.

Table 1 - Formulations of VA/BuA reactions.

Reactant	VA	BuA	VA/BuA 85/15	VA/BuA 15/85
VA (g)	105.168	-	89.393	15.775
BuA (g)	-	105.168	15.775	89.393
Water (g)	454.832	454.832	454.832	454.832
SLS (g)	1.344	1.344	1.344	1.344
$Na_2S_2O_8$ (g)	1.624	1.624	1.624	1.624
Na_2CO_3 (g)	0.392	0.392	0.392	0.392

In Figure 1 it might be observed that VA and BuA homopolymerize at very similar rates, the VA reactions being slightly faster, and show similar dependencies with reaction temperature (Figure 1a and 1b). The copolymerization reactions (Figure 1c), on the other hand, present much slower reaction rates due to the significant difference in the reactivity ratios of these comonomers ($r_{VA} <<< r_{BuA}$). BuA polymerizes first leading to a significant composition drift during the reaction. The higher the VA fraction in the formulation, the slower is the reaction rate (Figure 1d). Comparison between experimental and simulation results showed an excellent agreement, not only for conversion and composition, but also for particle size evolution. The developed mathematical

model, besides of providing a better comprehension of the complex phenomena involved in emulsion copolymerization reactions, may also be a very useful tool for the optimization of the operational conditions of these reactions.

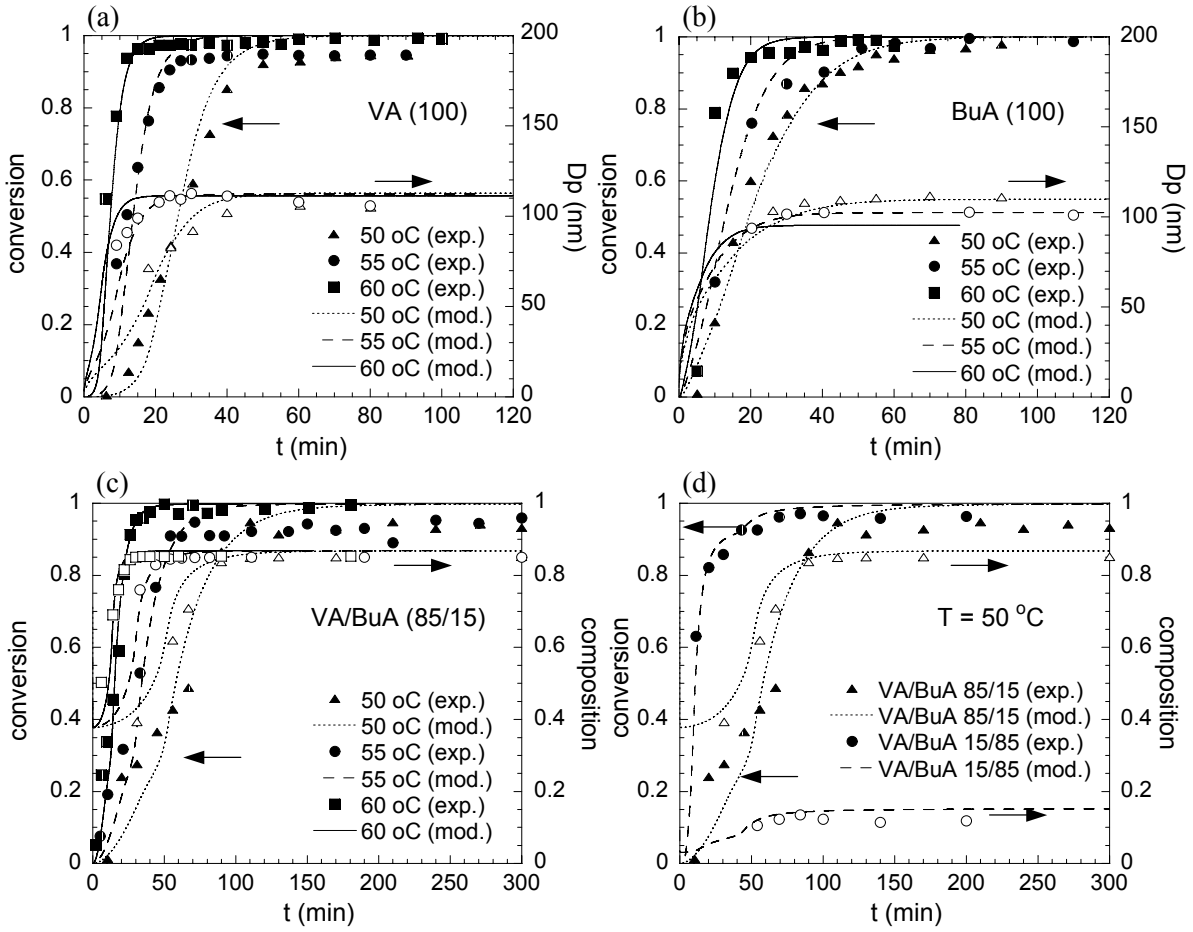

Figure 1 - Effect of reaction temperature on conversion, average particle diameter and copolymer composition during vinyl acetate / butyl acrylate emulsion homo- and co-polymerization reactions.

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References

[1] Waters, J.A., "Latex Paint Formulations" in NATO Advanced Institute on Recent Advances in Polymeric Dispersions, vol. 2, 1996.
[2] Lee, D.I., "Latex Applications in Paper Coating" in NATO Advanced Institute on Recent Advances in Polymeric Dispersions, vol. 2, 1996.
[3] Kong, X.Z., Pichot, C. & Guillot, J., Eur. *Polym. J.*, **24**, No 5, 485-492, 1988.
[4] Saldívar, E., Araujo, O., Giudici, R. & Guerrero-Sánchez, C., **84**, 1320-1338, 2002.
[5] Sayer, C., Internal Report to FAPESP, June 2001.