

# Fluid Dynamics of the Phase Inversion Process in the Bulk Polymerization of High Impact Polystyrene

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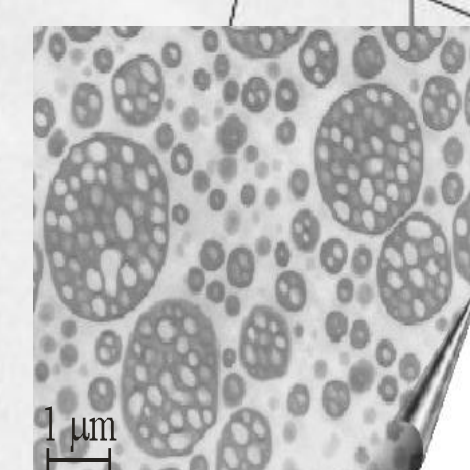
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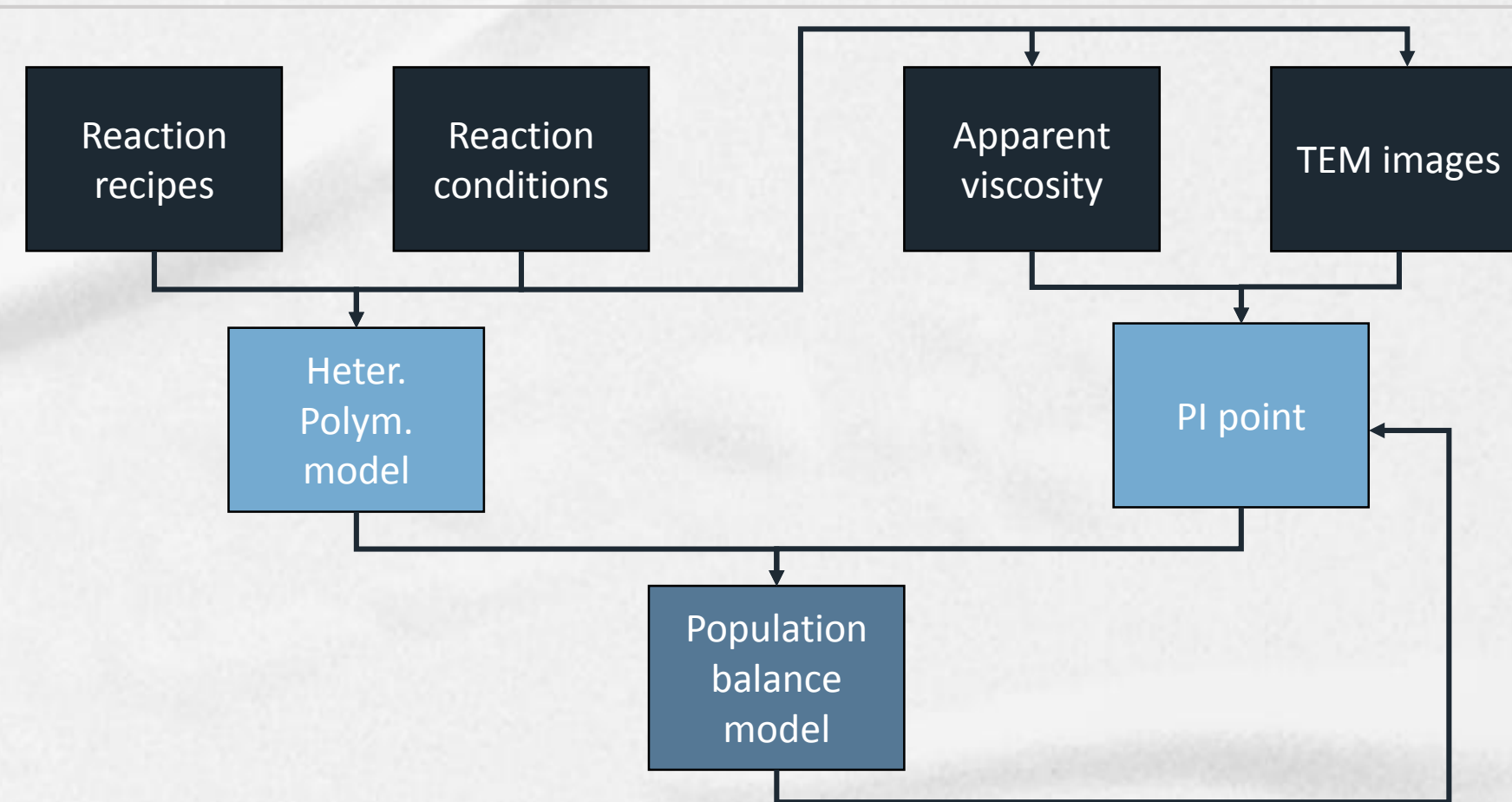
## INTRODUCTION

In the synthesis of HIPS, *phase inversion* (PI) is the critical point at which a dispersed PS-rich phase becomes a continuous matrix, leaving behind a PB-rich phase as dispersed particles that may contain occluded PS-rich droplets inside (occlusions). The size and shape of these particles essentially determine the mechanical properties of the material, which makes PI a critical point during the reaction. In this work, the most popular mechanism for PI – an imbalance between coalescence and break-up of dispersed particles – is assessed through a population balance model, coupled with a heterogeneous polymerization model. Results are adjusted and discussed with experimental evidence gathered from TEM images.



## MATERIALS & METHODS

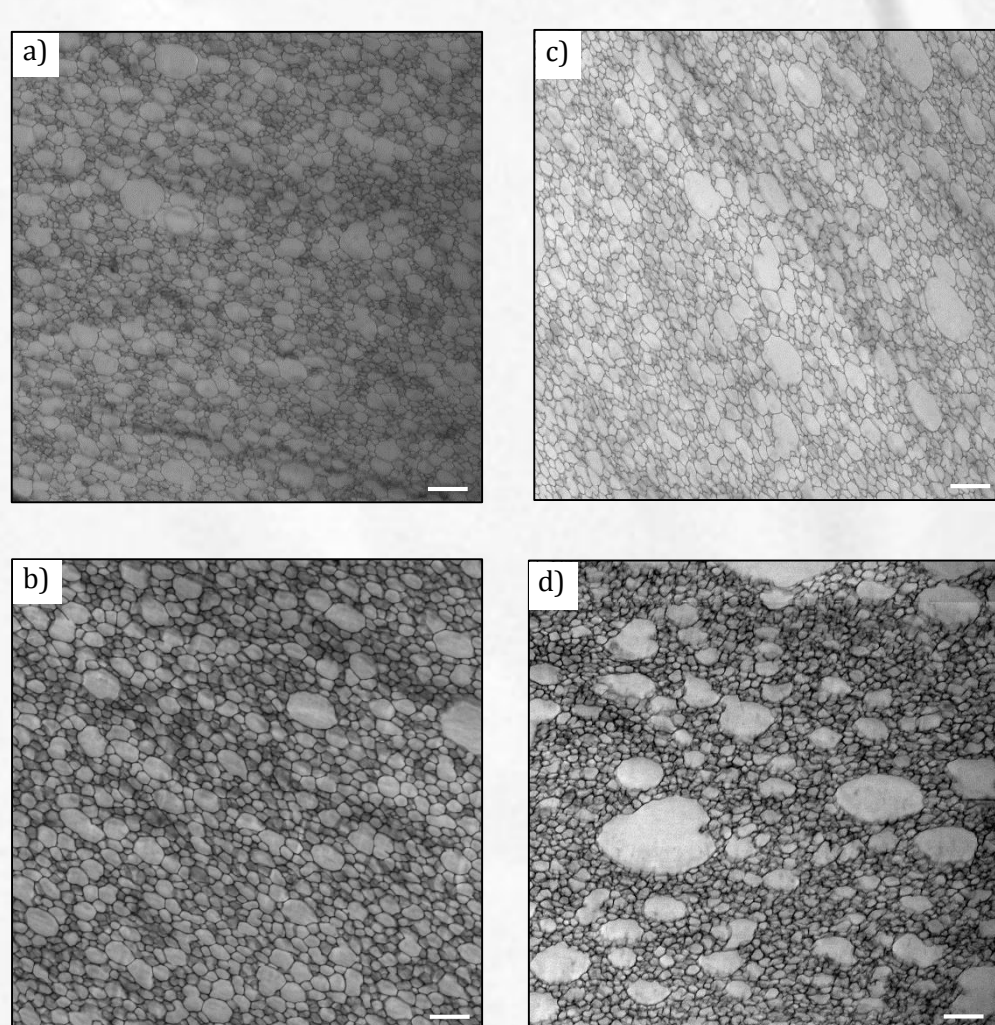
- 8 HIPS polymerizations varying initiator (BPO) concentration, temperature and stirring speed.
- Samples characterized to determine: conversion (gravimetry), molecular weights (SEC), grafting efficiency (solvent extraction), apparent viscosity (Brookfield viscometer) and morphology (TEM).
- Phase inversion periods determined with local drop of apparent viscosity.
- Particle size distributions obtained from TEM images



$$\frac{\partial f(v,t)}{\partial t} + \frac{\partial}{\partial v} (\dot{V}_{v(t)} f(v,t)) = \int_v^\infty \theta_b(v') \omega_b(v') f(v',t) \beta(v|v') dv' - \omega_b(v) f(v,t) + \frac{1}{\theta_c} \int_0^v \omega_c(v-v',v') f(v-v',t) f(v',t) dv' - f(v,t) \int_0^\infty \omega_c(v,v') f(v',t) dv'$$

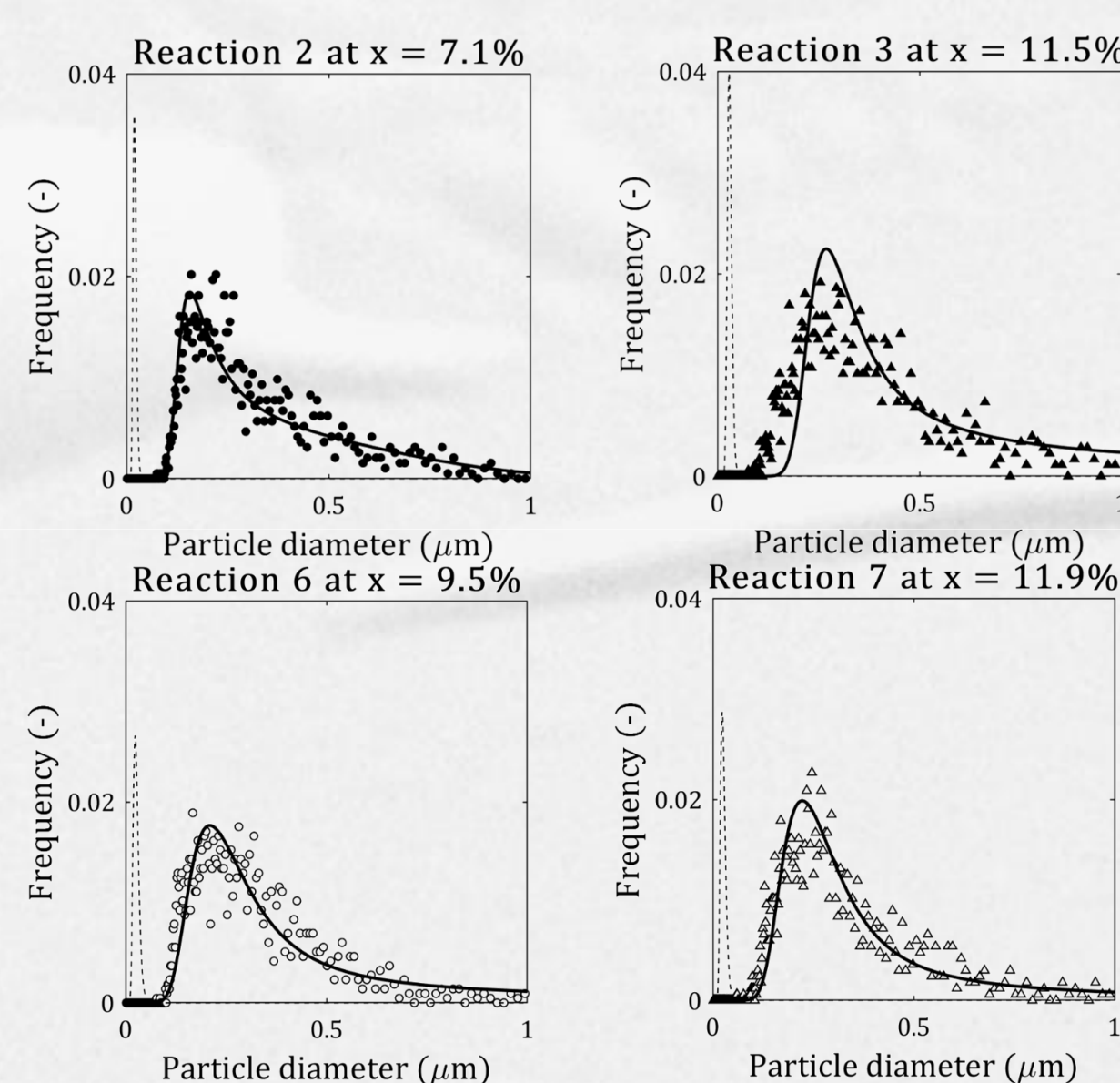
## RESULTS

### MORPHOLOGY

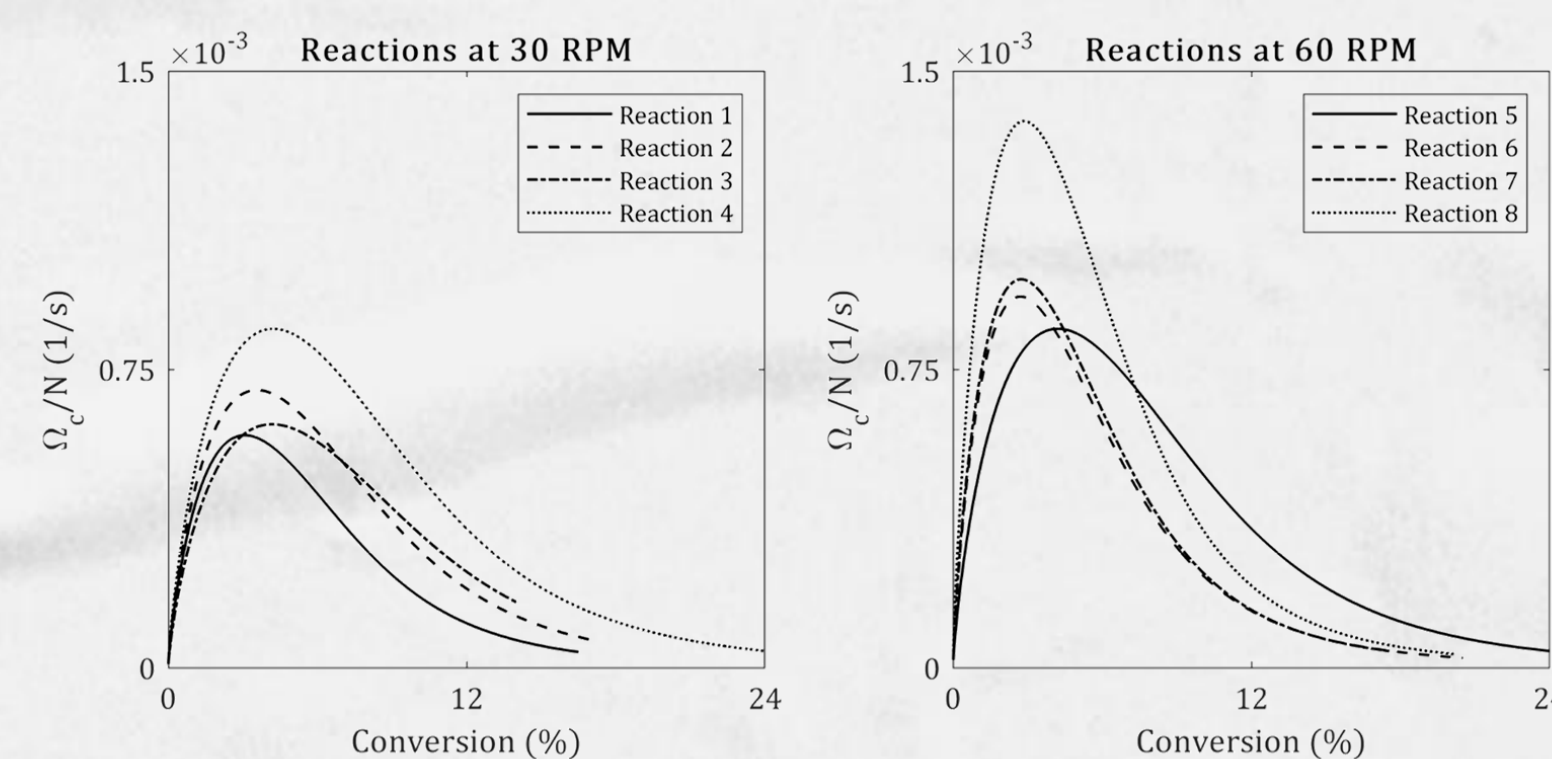


a) Reaction 2, 7.1%, b) Reaction 3, 11.5%  
c) Reaction 6, 9.5%, d) Reaction 7, 11.9%

### MODEL ADJUSTMENT



### PHASE INVERSION ASSESSMENT



No spiking occurs. Coalescence rates naturally decrease along each reaction, due to:

- Increase in phase viscosities
- Increase in dispersed phase density
- Decrease in total particle number
- Increase in interfacial tension attenuated by the presence of graft copolymer

## CONCLUSIONS

Fluid-dynamics of HIPS pre-polymerization process was successfully modeled with a population balance equation coupled with a heterogeneous polymerization model. Predicted PSDs are in very good agreement with observed by TEM. Phase inversion points in all reactions were detected by rheological measurements and verified by microscopy.

Theoretical results seem to indicate that phase inversion does not occur by an exponential increase in particle coalescence, as widely suggested.

Further research is required to confirm that a different criterion for phase inversion is required in this system.

Ongoing work will use a PB equation to predict particle morphology at the inversion point.

## REFERENCES

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3. Maffi, J. M., Casis, N., Acuña, P., Morales, G., Estenoz, D. A., *Pol. Eng. Sci.*, 60(3), pp. 491-502,, 2020.