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Analysis of surface segregation in polymer mixtures: A combination of mean field and statistical associated fluid theories JAROSLAW KRAWCZYK[1], SALVATORE CROCE, BUDDHAPRIYA CHAKRABARTI, Department of Mathematical Sciences, Durham University, South Road, Durham DH1 3LE, United Kingdom., JOS TASCHE, Department of Chemistry, Durham University, South Road, Durham DH1 3LE, United Kingdom. — The surface segregation in polymer mixtures remains a challenging problem for both academic exploration as well as industrial applications. Despite its ubiquity and several theoretical attempts a good agreement between computed and experimentally observed profiles has not yet been achieved. A simple theoretical model proposed in this context by Schmidt and Binder combines Flory-Huggins free energy of mixing with the square gradient theory of wetting of a wall by fluid. While the theory gives us a qualitative understanding of the surface induced segregation and the surface enrichment it lacks the quantitative comparison with the experiment. The statistical associating fluid theory (SAFT) allows us to calculate accurate free energy for a real polymeric materials. In an earlier work we had shown that increasing the bulk modulus of a polymer matrix through which small molecules migrate to the free surface causes reduction in the surface migrant fraction using Schmidt-Binder and self-consistent field theories. In this work we validate this idea by combining mean field theories and SAFT to identify parameter ranges where such an effect should be observable.

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