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Effect of the good solvent nature in flash nano-precipitation via population balance modelling and computational fluid dynamics coupling approach

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12 October 2024

74th Annual Meeting of the APS Division of Fluid Dynamics

Sunday–Tuesday, November 21–23, 2021; Phoenix Convention Center, Phoenix, Arizona

Session Q08: Particle-laden Flows: Simulations

8:00 AM–9:31 AM, Tuesday, November 23, 2021
Room: North 123

Chair: JESSE CAPECELATRO, University of Michigan

Abstract: Q08.00006 :

Effect of the good solvent nature in flash nano-precipitation via population balance modelling and computational fluid dynamics coupling approach

9:05 AM–9:18 AM

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The effect of the good solvent nature on polymer nano-particles (NP) formation in flash nano-precipitation is here investigated through a combined population balance model-computational fluid dynamics approach (PBM-CFD). Four good solvents are considered: acetone, acetonitrile, tetrahydrofuran and tert-butanol and the different resulting mean NP size is predicted in terms of mean radius of gyration via the Flory law of real polymers. Good solvents effects are here modelled in terms of solute–solvent interactions, using the Flory–Huggins theory and the Hansen solubility parameters. In this way, kinetics and thermodynamics are intertwined in a unique modelling tool. Our results show that the proposed methodology is able to predict the role played by the different good solvents, analysing single factors at the time. More specifically, the dynamics of mixing is decoupled from the dynamics of aggregation achieving a deeper insight into the fundamental fluid properties which affect the final NP size, pointing out the main mechanisms involved and showing a good agreement with experimental data.