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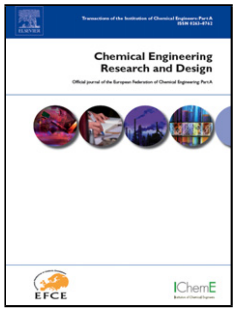

Title: Fractional Monte Carlo time steps for the simulation of coagulation for parallelized flowsheet simulations

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PII: S0263-8762(18)30230-2
DOI: https://doi.org/10.1016/j.cherd.2018.04.046
Reference: CHERD 3163

To appear in:

Received date: 29-1-2018
Revised date: 25-4-2018
Accepted date: 29-4-2018

Please cite this article as: Kotalczyk, G., Kruis, F.E., Fractional Monte Carlo time steps for the simulation of coagulation for parallelized flowsheet simulations.Chemical Engineering Research and Design https://doi.org/10.1016/j.cherd.2018.04.046

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ACCEPTED MANUSCRIPT

Fractional Monte Carlo Time Steps for the Simulation of Coagulation for parallelized Flowsheet Simulations

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Highlights

- Theory for combination of event driven coagulation with mechanisms having different time steps
- Combination of stochastic population balances with flowsheet modeling of multiple compartments
- Validation of novel technique with discrete sectional method shows good accordance
- Low levels of additional noise due to application of artificial synchronizations
- Parallelization of heterogeneous simulation conditions leads to palpable speed up

Abstract

The event-driven Acceptance Rejection (AR) method is a computationally very advantageous Monte Carlo (MC) simulation technique for the solution of population balance equations (PBE) of coagulating systems. In the scope of the event-driven simulation approach, the simulation time is stepwise increased by a simulation time step τ, which is given be the simulated particle properties. Within this time step τ, exactly one coagulation event takes place. The method is therefore not applicable in situations,

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