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THE RELAY RACE METHOD: APPLICATION OF DEM EXTRAPOLATION TO PHARMACEUTICAL PROCESSES

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Despite the expected advances in computing technologies, simulating pharmaceutical processes remains challenging. The reason is the size of the particles and the wide range of particle size distributions found in pharmaceutical powders. Although the number of particles in a DEM simulation can be reduced significantly via coarse-graining coupled with bulk calibration of the contact parameters, the coarse-grained DEM simulations remain computationally expensive in most cases. A full characterization of the residence time distribution (RTD) for a unit operation with a typical hold-up mass in the kilogram range requires simulating several minutes of the unit operation, which could take months of computation time.

The Relay Race method is a DEM extrapolation algorithm based on position mapping that could speed up computationally expensive DEM simulations [1]. The inputs to the Relay Race method are two steady-state DEM states at time points t_0 and t_1. The trajectories of particles are followed from t_0 to t_1. The Relay Race method maps the particles' positions at t_1 back in time to t_0. While there is not a particle located at the same position in general, there are particles at very close positions in dense flows. The Relay Race method is based on the assumption that the continued trajectory of the original particle will be similar to the trajectory of the mapped particle. By iteratively applying this mapping, the full trajectory of every particle is extrapolated using the DEM data at t_0 and t_1.

The Relay Race method has been applied to three unit operations commonly found in a typical continuous direct compression line: a feeder, a continuous mixer, and a tablet press. The RTDs predicted using the Relay Race method are in excellent agreement with the RTDs obtained from full DEM simulations. The agreement persists even in processes with dilute particle flows where higher mapping errors occur in the Relay Race.

Disclaimer: This abstract reflects the views of the authors and should not be constructed to represent FDA's views or policies.

REFERENCES

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