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Discrete Particle Dynamics Simulations of Adhesive Systems with Thermostatting[1] FLINT PIERCE, JEREMY LECHMAN, JOHN HEWSON, Sandia National Laboratories — Aggregation/coagulation/flocculation processes are ubiquitous in modern industry from fields as diverse as waste water treatment, the food industry, algae biofuel production, and materials processing where control of the size and morphology of aggregates is paramount to the application of interest. Population balance models have historically been used with success in predicting aggregation kinetics and size distributions for these processes. However, even the most robust population balance schemes can lack an exact description of the underlying physical processes governing attractive or adhesive particulate matter suspended in a background medium, including finite aggregate strength and yield stress, restructuring length and time scales, and response to hydrodynamic forces. In order to elucidate these phenomena, We develop and use a JKR type model for simulating adhesive particulate matter in a background medium varying from dilute gas to liquid. We evaluate the time and length scales for restructuring/fragmentation that result from this model as a function of aggregate size and fractal dimension. We additionally introduce a method for pairwise thermostatting of the adhesive potential and discuss the applicability of this model to various adhesive systems.

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