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A statistical description of small-scale thermochemistry in reactive flows through granular assemblies

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As part of our commitment to sustainability, reliable computational methods for the analysis and redesign of industrial processes and the rational reduction of their resource requirements and carbon footprints are urgently needed. Here, we focus on the combination of the discrete element method (DEM) with unresolved computational fluid dynamics (CFD) to model high-temperature industrial processes in which a granular assembly of centimeter-sized particles is thermochemically treated with a hot gas. Such processes include, for example, the gasification of plastics, the calcination of limestone and the reduction of iron ore. In the unresolved DEM-CFD method, the particles are described in terms of a finite number of degrees of freedom, while the interstitial gas flow and the reactive scalars characterizing the gas' thermochemical state are spatially filtered on a length scale that exceeds the particles' sizes. Since chemical reactions are often nonlinear in the reactive scalars, this approach requires an assumption about the variations of the scalars' values both throughout the void space and along the particle surfaces inside the filter volume. Frequently, the small-scale heterogeneity induced by unsteady particle wakes, chemical reactions, particle heating or surface mass transfer is omitted and the scalars' values on the smallest scales are assumed to coincide with their filtered counterparts.

In order to lift the limitations associated with the assumption of small-scale homogeneity, we enrich the physical description of the gas' thermochemical state by considering the reactive scalars inside a filter volume as random variables and formulating a transport equation for the corresponding density-weighted probability density function (PDF). This approach is gleaned from the field of PDF methods for turbulent reacting single phase flows and permits the incorporation of gas phase chemical reactions without intervening closure assumptions. On the minus side, correlations for small-scale transport remain unclosed and a hypothesis on the relation between the scalars' distributions along the particle surfaces and the joint scalar PDF is needed.

By particularizing the PDF evolution equation to the case of large-scale homogeneity, we are led to the concept of a partially stirred reactor (PaSR) which is coupled, through mass and heat exchanges, to dispersed DEM particles. If the surface distributions associated with the reactive scalars are approximated in terms of the volume-based joint scalar PDF, then the rates at which a DEM particle is heated or acquires mass by heterogeneous surface reactions can be computed as statistics of the joint scalar PDF. Upon incorporation of a micromixing model, the PDF evolution equation for the PaSR is recast in terms of a statistically equivalent jump-drift process whose realizations are integrated in time concomitant with the DEM particles' governing equations. Finally, the combined DEM-PaSR formulation is applied to the thermal treatment of a particle bed by interstitial methane combustion. Here, we investigate the influence of the residence and mixing times on large-scale observables, particularly the average heating rate and pollutant emissions.