CONTINUUM THERMODYNAMICS OF CHEMICALLY REACTING MULTICOMPONENT FLUID SYSTEMS

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Abstract

Multicomponent diffusion in fluid systems is commonly modeled via the Maxwell-Stefan equations. This approach is also employed for chemically reacting systems, but the standard derivation does not cover this case. This contribution provides a rigorous deduction of the Maxwell-Stefan equations together with an extension to chemically reactive mixtures. The derivation is based on partial balances in particular of the species momenta, where the entropy principle is exploited to obtain information on the interspecies momentum transfer. This yields a closed system of partial mass and momentum balances, from which the system of (extended) Maxwell-Stefan equations follows in the diffusional approximation. The latter is derived from entropy considerations, since the usual scale-separation argument is not feasible in the chemically reactive case.