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Flux-Based Modeling of Coupled Momentum, Mass and Heat Transfer and Chemical Reactions in Multicomponent Systems[1] ANTONY BERIS, SOHAM JARIWALA, NORMAN WAGNER, University of Delaware —

Since the pioneering work of Bird, Stewart and Lightfoot, “Transport Phenomena” (1960), momentum, heat and mass transfer have been unified under the same title. However, the unification has never been completed. Whereas an evolution equation in time is provided for the momentum flux, the mass and heat fluxes are determined through a direct assignment by constitutive equations. In the present work we establish the full unification of transport phenomena by developing appropriate evolution equations for all fluxes through the inclusion of inertial effects. This is achieved by using the nonequilibrium thermodynamics single generator bracket formulation developed in Beris & Edwards “Thermodynamics of Flowing Systems” (1994). The derived equations are shown to be fully consistent with the Stefan-Maxwell/Soret-Dufour equations as derived from kinetic theory, which in turn, can be used for dilute gases to obtain all transport coefficients. The evolution equations result to the traditional Fourier and Fick laws in the long time limit. We also show how chemical reactions can be consistently incorporated in a way that can also accommodate flow-induced effects. In addition to inertia, those can include extra stresses when macromolecular components are involved.

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