Calculations of Complex Chemical Reaction Equilibria using Free Energy Minimization and Arc-Length Continuation

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Abstract

In the present paper, we determine the chemical equilibrium compositions for two combustion reactions involving either hydrazine or propane at fixed high pressure and temperature values using several computational approaches. Then, we compute the chemical equilibria for reacting systems under a multitude of temperature and pressure conditions and various initial system compositions. These sensitivity analyses are based on a combination of the method of Lagrangian multipliers and the arc-length continuation technique. Indeed, three industrially relevant case studies are elucidated: (1) the synthesis of ammonia using the Haber process, (2) the gasification of a typical biomass surrogate: glucose using steam and (3) the gasification of cellulose using steam. For all the above reacting systems, our results are benchmarked against their counterparts obtained either from the ubiquitous process simulator: ASPEN-Plus® or from data available in the open literature.

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