An Interactive Chemical Equilibrium Solver for the Personal Computer

By

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The Virginia Tech Equilibrium Chemistry (VTEC) code is a keyboard interactive, user friendly, chemical equilibrium solver for use on a personal computer. The code is particularly suitable for a teaching / learning environment. For a set of reactants at a defined thermodynamic state given by a user, the program will select all species in the JANAF thermochemical database which could exist in the products. The program will then calculate equilibrium composition, flame temperature, and other thermodynamic properties for many common cases. Examples in this thesis show VTEC's ability to predict chemical equilibrium compositions and flame temperature for selected reactions, and demonstrate how VTEC can substitute for and aid in the design of lab experiments, and identify trends in parametric studies.

The 1976 NASA Lewis Chemical Equilibrium Code (CEC76) from which VTEC has been adapted uses Lagrangian multipliers to minimize free energy. CEC76 was written for mainframe computer use. Later versions of CEC76, adapted for personal computer use are available for a fee and have a very minimal user interface.