ON THE DEVELOPMENT OF THERMODYNAMIC MODELING TOOLS FOR COMPLEX HIGH-TEMPERATURE SYSTEMS

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The calculations of the parameters of the equilibrium state of multicomponent heterogeneous systems are widely used in the practice of investigation of high-temperature processes with chemical reactions. Probably the first universal method of calculating equilibrium was prsented in 1951 in the work of NASA employees "General Method and Thermodynamic Tables for Computation of Equilibrium Composition and Temperature of Chemical Reactions". In the USSR, a method for calculating the equilibrium composition and properties of the combustion products of rocket fuels was also developed, a computer program and a database on the thermodynamic properties of substances were created, and in 1971 a reference book was prepared "Thermodynamic and thermophysical properties of combustion products". Later in Baumsn Moscow Higher Technical School a method and a universal algorithm of thermodynamic calculation of multicomponent heterogeneous systems were developed and the program ASTRA was created. The program was used to solve a wide class of problems, in particular, metallurgical and plasma chemical problems. Based on the ASTRA algorithm, a program REAL has been developed for calculating the equilibrium composition and properties of complex thermodynamic systems using the nonideal gas model. Unfortunately, in real processes, thermodynamic equilibrium is not always achieved. For example, when the combustion products in a rocket engine nozzle expand, they are cooled, as a result the chemical reaction rates decrease, the composition is partially "frozen". To analyze these and similar processes, it is necessary to use methods combining the capabilities of thermodynamics and kinetics. Such an approach has been used, in particular, in the creation of software systems CHEMKIN and Chemical Workbench.