**Weber, C. F.**

**Convergence of the equilibrium code SOLGASMIX.** (English) Zbl 0911.65049

J. Comput. Phys. 145, No. 2, 655-670 (1998).

The paper presents a mathematical examination of the computer program SOLGASMIX used to compute the equilibrium of a chemical system. The code is based on the Gibbs-energy minimization which can be formulated as a constraints optimization problem. The letter is then restated by means of Lagrange multipliers. An important role in the Lagrangian plays the so-called 'active set', the proper identification of which is the most difficult aspect of the problem. In this regard SOLGASMIX offers effective capability.

The solution of the original problem leads finally to a system of nonlinear equations, which can be treated iteratively using a Newton type method. That is the nonlinear system is linearized and a linear system is solved on each iteration step. Thereby two difficulties may arise: (i) the linear system becomes singular at some iteration step and (ii) the sequence of iterates fails to converge. It is shown on sample practical examples that the first difficulty can be overcome by simple reformulation of the problem, e.g. by adequately determining what chemical species should be present in the input. In the situation where the iteration procedure fails to converge, a linear interpolation scheme, based on oscillation of Gibbs energies, yields a legitimate approximation for the equilibrium.

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**MSC:**

65K05 Numerical mathematical programming methods
65H10 Numerical computation of solutions to systems of equations
80A32 Chemically reacting flows
90C30 Nonlinear programming

**Keywords:**

chemical equilibrium; constrainted optimization; computer program SOLGASMIX; convergence; Gibbs-energy minimization; system of nonlinear equations; Newton type method

**Software:**

ChemSage; MACSYMA; SOLGASMIX

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