Analysing the Thermodynamics of Steam Reforming with Maple

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Abstract

The catalytic steam reforming process converts hydrocarbons into mixtures of hydrogen, carbon monoxide, carbon dioxide, and methane. It is widely used in industry for the production of hydrogen, synthesis gas, ammonia, methanol and other useful chemicals. Important data for the design and optimization of a steam reformer are provided by thermodynamic calculations. For instance, to find the most economic reaction conditions and for predicting the carbon boundaries, it is necessary to study the reaction behavior with respect to the operating parameters. Steam reforming of a general hydrocarbon is based on the following simple system of reaction equations:

1. The methane-steam equality

$$\mathrm{CH_4 + H_2O \rightleftharpoons CO + 3H_2}$$

2. The water-gas shift

$$\mathrm{CO + H_2O \rightleftharpoons CO_2 + H_2}$$

3. The carbon-methanation equality

$$\mathrm{CH_4 \rightleftharpoons C + 2H_2}$$

Using symbolic methods we introduce a flexible computation model for the thermodynamic description of the steam reforming process. The product gas composition at equilibrium is determined by solving a system of multiparameter nonlinear equations for the reaction extents. The applied computation techniques are chosen graduated according to the computation effort needed and range from direct calculations in Maple to the automatic generation of Fortran programs for complete

parameter studies. We analyse the effects of temperature, pressure and the steam to carbon ratio on the equilibrium gas composition and the carbon formation. The theoretical equilibrium compositions are found to be closely matching with those obtained in experiments. The computed data were used to determine the mass and energy balances of a pilot reactor for reforming organic waste (fluids and gases).

This work presents an example of interdisciplinary work done in the field of scientific computing at the institutes for applied mathematics and physical chemistry of the research centre Jülich . It illustrates how the use of modern computing tools such as Maple changes the approach of mathematical modeling in science. The concept of scientific computation has evolved from a field encompassing primarily numerical methods to a much broader field that includes algebraic and analytical methods, numerical methods, and graphics.