Equilibria in Fuel Cell Gases
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Fuel cells have been increasingly accepted as environmentally compatible, efficient energy conversion systems. In particular, SOFCs may be regarded as the most flexible fuel cells in respect to their flexibility in selecting the types of fuels able to be supplied directly to the fuel electrodes.

Fuel gases including hydrocarbons and alcohols are either directly supplied or reformed in a reformer before supplying to fuel cells. In order to apply such fuel gases, it is in particular essential to know the gas compositions in thermodynamic equilibrium under given operational conditions for any types of fuel cells. In the case that reforming and/or decomposition kinetics are sufficiently fast, the compositions of the fuel gases are identical to those in thermodynamic equilibrium. Thermochemical calculations will give such information for any kinds of fuel gases if their thermochemical data are available. As possible fuels, following species have been taken into account: natural gas (consisting mainly of CH\(_4\)), coal gas (consisting mainly of CO and H\(_2\)), liquefied petroleum gas (LPG, consisting mainly of CH\(_4\) with C\(_3\)H\(_8\)), naphtha (consisting mainly of C\(_5\) and C\(_6\) hydrocarbons), gasoline (consisting mainly of hydrocarbons with carbon numbers around 8), kerosene (consisting mainly of hydrocarbons with carbon numbers around 12), alcohols, biogas, and coke oven gas.

Thermochemical calculations were carried out using a program, HSC chemistry (Version 4.0, Outokumpu Research Oy, Finland) with an extensive thermochemical database. In the present study, the thermochemical data of ca. 300 compounds with carbon numbers of 4 or less and, in addition, possible fuel species such as higher alkanes were taken into account. The calculations were performed by assuming a reactor to which a (mixed) fuel gas was supplied, and the results are shown in Fig. 3. Various other ternary diagrams are reported elsewhere [1].

![Fig. 1: Equilibrium products for (a) methane- and (b) methanol- based fuels with the steam-to-carbon ratio of 1.5.](image)

![Fig. 2: Minimum steam-to-carbon (S/C) ratio needed to prevent carbon deposition in thermodynamic equilibrium for hydrocarbons.](image)

![Fig. 3: Carbon deposition limit lines at various temperatures in the C-H-O diagram.](image)

reliable to operational conditions, including carbon deposition region, gas partial pressures, and electromotive force. As examples, carbon deposition region at temperatures between 100 and 1000°C is shown in Fig. 3. Various other ternary diagrams are reported elsewhere [1].