Uncertainty of the rate parameters of several important elementary reactions of the H_2 and syngas combustion systems

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Databases of elementary combustion reactions characterize the uncertainty limits of the rate coefficients with uncertainty parameter *f* (i.e. [1-2]). Re-evaluation of the temperature-dependent uncertainty parameter $f(T)$ is proposed by considering all available direct measurements and theoretical calculations [3]. A procedure is presented for making function $f(T)$ consistent with the recommended Arrhenius expression. It is shown that the corresponding uncertainty domain of the Arrhenius parameters is convex and centrally symmetric around the recommended parameter set. The determination of the covariance matrix of the Arrhenius parameters from function $f(T)$ is briefly reviewed here [4-5]. It was found that function $f(T)$, after being made consistent, can be stored efficiently using the covariance matrix of the Arrhenius parameters. The calculation of the uncertainty of a reverse rate coefficient from the uncertainty of the forward rate coefficient and the uncertainty of the thermodynamic data is discussed. For the rate coefficients of several hundred elementary reactions, a large number of experimental and theoretical determinations is available, and a normal distribution can be assumed for the uncertainty of ln *k*. If little information is available for the rate coefficient, equal probability of the Arrhenius parameters within their domain of uncertainty can be assumed. Algorithms are provided for sampling the Arrhenius parameters with either normal or uniform distributions. A suite of computer codes is presented that allows the straightforward application of these methods. For 22 important elementary reactions of the H_2 and wet CO combustion systems, the Arrhenius parameters and 3rd body collision efficiencies were collected from experimental, theoretical and review publications. For each elementary reaction, k_{min} and k_{max} limits were determined at several temperatures within a defined range of temperature. These rate coefficient limits are used to obtain a consistent uncertainty function $f(T)$ and to calculate the covariance matrix of the Arrhenius parameters. Uncertainty ranges for the 3rd body collision efficiencies are also recommended.

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