A Posteriori Computation of OH* Radiation from Numerical Simulations in Rocket Combustion Chambers

T. Fiala and T. Sattelmayer
Lehrstuhl für Thermodynamik, Technische Universität München

Numerical simulations are constantly gaining influence in the design process of rocket combustion chambers. To predict the combustion accurately, the simulations have to be validated against experimental results. However, exact measurements of flames in rocket motors are scarce because of the high temperature and pressure levels present. Especially the parameters relevant for combustion like the temperature or the species mass fractions are hard to obtain in this hostile environment.

A quantity that is comparably easy to measure is the line-of-sight integrated flame radiation. Particularly the UV radiation of the excited hydroxyl radical (denoted as OH*) is known as a good marker in rocket flames. It was used to visualize the flame several times in literature. Nevertheless, the OH* radiation is not a direct output of common simulations. The use of the measurements of the OH* radiation for the validation of numerical simulations was therefore limited to now.

The cause of the OH* emission are spontaneous transitions of the hydroxyl radical from the electronically excited state $A^2\Sigma$ into the ground state $X^2\Pi$. If self-absorption of the radiation is neglected, then the radiation of a volume element is directly proportional to the molar concentration of OH*, C_{OH^*}. Above 2700 K, OH* is known to be in thermal equilibrium with its ground state. The relation between the molar concentrations of OH* and OH is in this case given by the well known equilibrium equation:

$$\frac{C_{OH^*}}{C_{OH}} = K_p(T) = \exp\left(\frac{-\Delta G_T^0}{R_u\, T}\right)$$

The difference in the free Gibbs enthalpy of formation ΔG_T^0 can be obtained from literature. The thermal equilibrium of OH* is confirmed for rocket combustion flames in literature.

The formula above relates the flame OH* radiation to the concentration of OH and the temperature. The latter two values are often known from flame simulations. Using the relation above, it is therefore possible to compute the flame radiation from such a simulation a posteriori. This output can then be used to compare the simulation with an experiment.

This method is demonstrated for a laminar, atmospheric non-premixed hydrogen-oxygen jet flame. The stationary, axis-symmetric flame is simulated using a commercial 2D CFD software. The chemical reactions are described by the reaction mechanism developed by O'Conaire et al. The mechanism is extended to directly include OH* using the reactions provided by Kathrotia et al. Without using this extension, the OH* field is also computed a posteriori using the formula above.

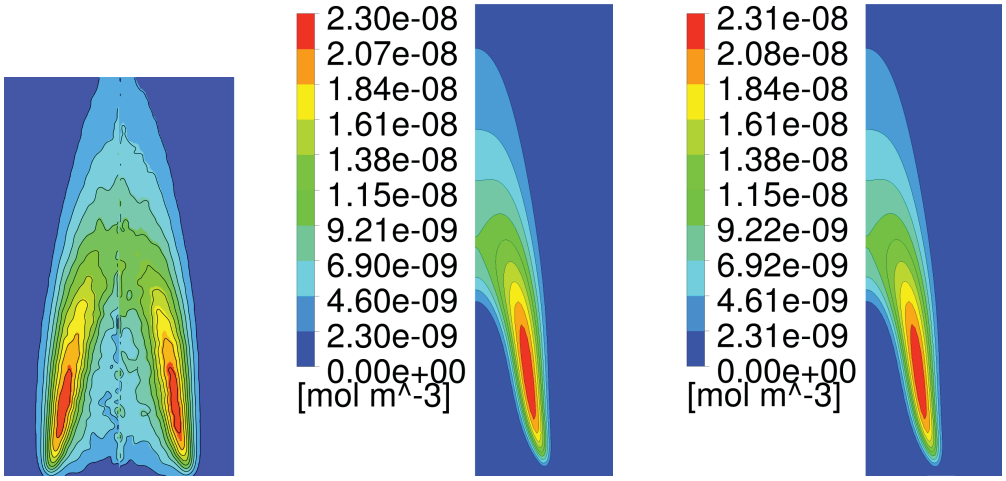

Figure 1: Comparison between the experimentally measured OH* radiation, the molar concentration of OH* computed a posteriori, and the molar concentration of OH* from direct simulation.

The result is compared to the directly simulated OH* field and data from a corresponding experiment. In the experiment, the band-passed radiation of OH* was measured. The radial field shown in figure is obtained by performing an inverse Abel transform. The comparison in Figure 1 shows very good agreement between the data computed a posteriori and the experiment. Comparing the a posteriori output with the detailed mechanism, almost identical profiles and values are observed. This is because of the closeness to equilibrium and the identical Gibbs enthalpies in the reaction mechanism and the method described above.

The laminar test case demonstrates well the ability of the proposed method. Since the temperatures in rocket combustion chambers are commonly higher than in the investigated flame, the assumption of thermal equilibrium between OH* and OH is surely even more justified. For the use in practical applications, the influences of pressure and turbulence still have to be investigated. At the current state, the described method is promising to provide a simple tool to validate rocket combustion simulations.