Structure of H\textsubscript{2} Diffusion Flames as Revealed by OH Radical Measurements
6.1 Introduction

In Ch. 5, when discussing the structure of the axisymmetric H$_2$/N$_2$ diffusion flames by analyzing the major species and temperature distributions, we observed very good agreement between experiments and numerical simulations. While this observation can serve as a test to justify the use of the computational model for deriving flow field, temperature and major species distributions, correct prediction of phenomena such as pollutant formation is dependent upon being able to predict minor species. Thus, the accuracy of the computations for these components should be investigated as well. Moreover, as was mentioned in Ch. 4 and 5, the high enthalpy content in the radicals can be one of the reasons for the observation of subequilibrium flame temperatures.

Toward this end we perform quantitative measurements of the OH molecule in the flames discussed in Ch. 4 and 5. This molecule is one of the key flame components sustaining the combustion process through the chain-branching reactions [1]. Besides, the quantitative diagnostics of this molecule in flames is well established, and has been used with success in numerous experiments (see [2] and references therein). The quantification of the OH LIF signals (see Ch. 3) requires applying temperature and composition dependent corrections. For this purpose, we can make use of the major species and temperature data that were discussed in the previous chapters. Therefore, the LIF measurements were performed in the same radial and axial positions in each flame as the Raman and CARS measurements. While the OH LIF intensity is sufficiently large to measure the signal without grouping pixels of the CCD camera, the necessity of correcting for its dependence upon temperature and species concentrations meant matching the spatial resolution of the OH measurements to that of the Raman measurements (~ 0.2 mm, see Ch. 4). The experimental setup and measuring procedures of the Raman, CARS and LIF methods are described in detail in Ch. 3. The measurements were performed in flames of pure H$_2$ and 50%H$_2$/50%N$_2$ mixture at the exit velocities $\vartheta = 18, 27$ and 50 cm/s. As was mentioned previously, the choice of the hydrogen/nitrogen mixture as a fuel is determined by matching the boundary conditions of the numerical simulations. Heat transfer to the fuel tube and uncertainty as to the fuel composition at the exit plane of the burner, which are not included in the computations, can make the comparison with the measurements problematical. When the hydrogen/nitrogen mixture is burned, the flame is moved downstream from the burner exit substantially to reduce these problems (indicated by
the fuel tube being at room temperature) and allowed imposing the unburned fuel at room temperature as an inlet boundary condition.

6.2. OH measurements in H$_2$/N$_2$ flames

This section describes the experimental and computational studies of the formation and consumption of the OH molecule in the 50%H$_2$/50%N$_2$ axisymmetric diffusion flames. The radial profiles of OH mole fraction were measured at $z = 3$, 10, 20 and 30 mm above the burner exit. Below, the radial profiles for OH will be presented only for flames with the average fuel exit velocity of 50 cm/s. At $\vartheta = 18$ and 27 cm/s both measurements and calculations show OH profiles very similar to those at 50 cm/s and omitted here for brevity. The influence of the fuel exit velocity on the OH formation and destruction will be discussed by analyzing the axial profiles.

6.2.1. Radial OH distributions

The measured and calculated radial OH profiles in the nitrogen-diluted flame at a height of 3 mm above the burner exit are presented in Fig. 6.1. To facilitate the analysis, Fig. 6.1 (and all other figures presenting the radial OH profiles), also includes the horizontal H$_2$O (Fig. 6.1a) and temperature (Fig. 6.1b) profiles. In Fig. 6.1a, we see that the experimental OH data show two sharp peaks (FWHM $\sim$1.5 mm) with maximum of $\sim 6000$ ppm at $r = 6.5$ mm. It should be pointed out that the spatial resolution of $\sim 0.2$ mm is sufficient to resolve these narrow peaks and without missing the position of the maximum. Moreover, the measured OH profile is almost perfectly symmetrical about the centerline. Considering strong dependence of the OH LIF signal upon the temperature and compositions, the symmetrical shape of the OH profile further supports the adequacy of the experimental procedure for deriving the Raman profiles (described in Ch. 4) and the symmetry of the flame using this burner design [3]. The peak of the OH distribution occurs in the region in which the concentrations of H$_2$ and O$_2$ are very low (see Fig. 5.3), and lies slightly farther from the centerline than the maxima of temperature and water mole fraction, i.e., on the lean side of the flame. Similar behavior of the OH mole fraction was predicted numerically [4] and observed experimentally [5-7] in counterflow diffusion flames,
Figure 6.1 Radial profiles of H$_2$O, OH (Fig. 6.1a) and temperature (Fig. 6.1b) at $z = 3$ mm in a flame with $\vartheta = 50$ cm/s. Symbols denote measured OH (circles), H$_2$O (diamonds) and temperature (rectangles). Solid and dashed lines denote calculations without and with thermal diffusion, respectively.

and was also predicted in the computation of an axisymmetric diffusion flame [8]. The similarity in the flame zone with counterflow flames is not surprising at small distances above the burner exit, where diffusion overwhelms convective transfer and a “flame sheet” is a reasonable assumption.

As was already mentioned in Ch. 5, the calculations were performed both incorporating and neglecting thermal diffusion effects. Following Ch. 5, to illustrate differences in the predictions of these two numerical approaches, the computed
profiles are shown per half plane: the results neglecting thermal diffusion are plotted for $r \leq 0$ (solid lines), while the results including thermal diffusion are shown for $r \geq 0$ (dashed lines). Similar to the temperature profiles discussed in Ch. 5, the experimental OH data are in very good agreement with the OH calculations neglecting thermal diffusion, while the profile including thermal diffusion is displaced radially outward. The thermal diffusion calculations also overpredict (by ~1000 ppm) the peak OH mole fractions. While the differences between calculations with and without thermal diffusion are not extremely large, it is quite surprising that the calculations based on a “better” physical model have poorer agreement with the experiment. This intriguing result was already discussed in Ch. 5. Possible reasons for this discrepancy can be uncertainties in the transport properties of the binary mixtures at high temperatures [9], the multicomponent transport model itself [10,11], and differences in the boundary conditions between the experiments performed in the laboratory and the model. In the previous chapter, it was suggested that the boundary conditions were perhaps the largest contributor; but, given the complexity of the problem, a more thorough investigation of all these possibilities seems warranted.

No significant changes are observed in the measured OH profiles when progressing downstream to $z = 10$ mm and 20 mm (Fig. 6.2 and 6.3, respectively). While the differences in the profiles at $z = 3$ mm and 10 mm are modest, the OH profiles at $z = 20$ mm are broader, and the maximum OH mole fraction decreases slightly, to ~5500 ppm. The differences between calculations with and without
Figure 6.2 Radial profiles of H$_2$O, OH (Fig. 6.2a) and temperature (Fig. 6.2b) at $z = 10$ mm in a flame with $\dot{\vartheta} = 50$ cm/s. Symbols denote measured OH (circles), H$_2$O (diamonds) and temperature (rectangles). Solid and dashed lines denote calculations without and with thermal diffusion, respectively.

thermal diffusion have nearly disappeared as result of the softening of the temperature gradients at axial distances above 20 mm. As can be seen from Fig. 6.4, at $z = 30$ mm
the peak OH concentration has further decreased to ~3500 ppm, arising from the depletion of the fuel and slow decrease in the temperature at the position of maximum OH. It is interesting to note the complete absence of the OH molecule at the flame center while the water concentration in this point is > 0.1 mole fraction. Clearly,
Figure 6.4 Radial profiles of H$_2$O, OH (Fig. 6.4a) and temperature (Fig. 6.4b) at $z = 30$ mm in a flame with $\bar{v} = 50$ cm/s. Symbols denote measured OH (circles), H$_2$O (diamonds) and temperature (rectangles). Solid and dashed lines denote calculations without and with thermal diffusion, respectively.

Conversion of the OH molecules to water is sufficiently fast to prevent them from diffusing to the axis from the flame zone where they are produced.

6.2.2. Equilibrium analysis

Numerical simulation, solving the full systems of governing equations with complete chemistry is the preferred approach for predicting combustion processes. Unfortunately, modern computing facilities are still not able to simulate the properties
of 3-dimensional laminar and turbulent flames; the highly nonlinear temperature-dependent chemical source terms in the governing equations require enormous computational power. To circumvent this problem, simplified, “reduced-chemistry”, approaches such as full equilibrium, partial equilibrium, one-step chemistry etc. are frequently used [1,12]. These approaches can be tested by their comparison with full-chemistry calculations in model flames of simplified geometry. If these approximations are valid for the model flames it is reasonable to expect them also to be valid in 3-dimensional flames under similar conditions (such as similar magnitudes of spatial gradients). In addition, the “reduced-chemistry” approximation is very useful for analyses of the experimental data in flames with simplified geometry where the full numerical solution is unavailable. We shall use this approach below in the analysis of the OH measurements in pure hydrogen flames.

The equilibrium OH concentrations are determined using the same approach that was used for the temperature calculations in Ch. 4. The H, O an N element mole fractions, calculated from the measured main species concentrations and flame temperature are used as input parameters in the equilibrium code. Thermodynamic properties of individual species are taken from JANAF tables [13,14]. The full equilibrium approximation is valid when a number of chemical reactions have rates much larger then the rates of convection and diffusion. The total number of “fast” chemical reactions satisfying this criterion should be at least equal to the total number of species minus the total number of elements. The H/O/N system includes 7 species: H, O, OH, H$_2$O, H$_2$, O$_2$ and N$_2$. Therefore, for complete equilibrium this system should have 4 “fast” reactions. At high temperature ($T > 1700$ K) and $P = 1$ atm the rates of only these 3 chemical reactions

\[
\begin{align*}
H + O_2 &= OH + O \quad (6.1) \\
O + H_2 &= OH + H \quad (6.2) \\
OH + H_2 &= H_2O + H. \quad (6.3)
\end{align*}
\]

can be expected to be sufficiently fast (characteristic times < 1 ms) [15] and one can expect that they will be equilibrated in slow flows without sharp temperature and concentrations gradients. An insufficient number of “fast” chemical reactions implies that it is highly unlikely that full chemical equilibrium will be reached in the system under study. This observation is supported by the measurement of OH concentrations in axisymmetric laminar CH$_4$/air [16] and turbulent H$_2$/air [17] flames. On the other hand, at high pressures the rate of the recombination reaction
\[ \text{OH} + \text{H} + \text{M} = \text{H}_2\text{O} + \text{M} \]  

(6.4)

can be sufficiently high to establish full equilibrium on a relatively short time scale in high-temperature flames [18,19].

The partial equilibrium approach utilizing the equilibrium of reactions (6.1 – 6.3) will simplify the chemical kinetic scheme, substantially decreasing computational burden; therefore, this approach deserves examination. When the forward and backward rates of reactions (6.1) – (6.3) are the same, one can write:

\[ k_1 = \frac{[\text{OH}][\text{O}]}{[\text{H}][\text{O}_2]} , \]  

(6.5)

\[ k_2 = \frac{[\text{OH}][\text{H}]}{[\text{O}][\text{H}_2]} , \]  

(6.6)

\[ k_3 = \frac{[\text{H}_2\text{O}][\text{H}]}{[\text{OH}][\text{H}_2]} , \]  

(6.7)

where \( k_1, k_2 \) to \( k_3 \) are the equilibrium constants. Solving the equations (6.4)-(6.6), the mole fractions of intermediates O, H and OH can be expressed as functions of the major species \( \text{O}_2, \text{H}_2 \) and \( \text{H}_2\text{O} \):

\[ [\text{H}] = \left( k_1 k_3 k_2 \right)^{\frac{1}{2}} \left( \frac{[\text{O}_2][\text{H}_2]}{[\text{H}_2\text{O}]} \right)^{\frac{1}{2}} , \]  

(6.8)

\[ [\text{O}] = (k_1 k_3) \left( \frac{[\text{O}_2][\text{H}_2]}{[\text{H}_2\text{O}]} \right) , \]  

(6.9)

\[ [\text{OH}] = (k_1 k_2 [\text{O}_2][\text{H}_2])^{\frac{1}{7}} . \]  

(6.10)

It should be pointed out that using the formulas (6.8) – (6.10) for deriving the intermediates’ concentrations from Raman measurements is not possible in many practical cases. When the H/O/N system is not far away from the equilibrium, concentrations of \( \text{H}_2 \) and \( \text{O}_2 \) are complementary: in the fuel rich zone \( \text{O}_2 \) concentrations are very low, in the fuel-lean zone only trace amounts of \( \text{H}_2 \) are present, and in the stoichiometric region the mole fractions of both species are low. This phenomenon is observed in all flames studied in the present work. Even in turbulent flames, where mixing of fuel and oxidizer occurs at high rates, the Raman measurements show the same trend [17]. Trace concentrations of hydrogen and oxygen in rich and lean zones are far below the detectability limit of the Raman technique and are buried in the background noise, while as seen in Ch. 4, in the
stoichiometric region the mole fractions of both species are detectable, but with an uncertainty of worse than a factor of 2. Fortunately, the numerical calculations are “noise-free”, which gives us the possibility to check the partial equilibrium assumption. Moreover, the very good agreement between the calculated and measured profiles of the temperature, OH and major species provides confidence in this exercise. Towards this end, we calculate the OH profiles expected for partial equilibrium using equation (6.10), with the temperature and major species concentrations taken from the numerical simulations. The results of these calculations for the radial OH profiles at $z = 3, 10, 20$ and $30$ mm are presented in Fig. 6.5. For comparison, the results of the full-equilibrium and full-chemistry calculations are shown in Fig. 6.5 as well. To avoid clutter in the figure, only the calculations based on the numerical simulations without thermal diffusion are presented.

As can be seen in Fig. 6.5, the measured and full-chemistry OH mole fractions are always larger than those calculated using the full-equilibrium approximation. This observation is in striking contrast to that for the major species, whose mole fractions are relatively close to equilibrium in the flames studied (see Ch. 4). Clearly, as was mentioned above, the recombination reaction between OH and H is not sufficiently fast to remove the superequilibrium hydroxyl radicals. Moreover, the strong temperature dependence of the equilibrium OH concentration results in an increase in the degree of nonequilibrium with decreasing flame temperature as illustrated by the OH profile in Fig. 6.5d. This effect was predicted by early laminar flame calculations for pure H$_2$ diffusion flames [8].

Contrary to the equilibrium case, the OH mole fractions derived assuming partial equilibrium are ~ 2 times higher than those from the experiment and full-chemistry calculations. Interestingly, this ratio remains constant when progressing downstream from 3 to 30 mm above the burner exit. According to Eq. 6.10, one possible reason for
Figure 6.5 Radial OH profiles at $z = 3$ (Fig. 6.5a), 10 (Fig. 6.5b), 20 (Fig. 6.5c) and 30 mm (Fig. 6.5d). The symbols denote the experimental data. Solid, dashed and dotted lines denote the calculations performed in full-chemistry, partial equilibrium and full-equilibrium ($x$ 10) approximations.
the difference between full- and partial chemistry approximations is the overprediction of molecular hydrogen and oxygen concentrations. Considering excellent agreement for the OH mole fractions between the measurements and the full-chemistry calculations, it seems very unlikely that the numerical simulations overpredict the trace $\text{H}_2$ and $\text{O}_2$ concentrations. Therefore, we are compelled to conclude that the partial chemistry approximation is not valid in the flames under investigation. This is in contrast to observations in [8]; however, in that study, the partial equilibrium was established at temperatures above 2000 K, while the temperatures here are 1900 K at most. Hydroxyl concentrations below partial equilibrium suggest the two chain-branching reactions (6.1) and (6.2) are individually in equilibrium. We suggest that radicals, produced in these reactions, are removed from the radical pool by fast diffusion, resulting in departure from the partial equilibrium. The steep concentrations gradients and high diffusivity of $\text{H}$ atoms in this flame support this statement. Given the importance of the partial equilibrium assumption, further investigation of the suitability of partial equilibrium for estimating radical concentrations in laminar diffusion flames is recommended.

6.2.3. Axial OH profiles

OH formation and consumption is illustrated by Fig. 6.6, where the measured and calculated temperature, hydroxyl and water profiles along the centerline in the flame at 50 cm/s are presented. As can be seen, the centerline OH mole fraction is negligibly small throughout first 30 mm above the burner exit, and then grows rapidly to ~450 ppm at $z = 40$ mm. After reaching the maximum, the OH mole fraction decreases to below the detection limit at $z = 80$ mm, where the flame temperature is less than 1300 K. That the maximum OH mole fraction on the centerline is ~ 10 times lower than in the radial profiles reflects the differences in temperature at the axial and radial maxima: ~ 1500 K vs. ~ 1900 K. The numerical simulations with and without thermal diffusion satisfactorily reproduce the rising edge of the OH profile, while overpredicting the post-flame tail. These differences between the experiment and
Figure 6.6 Measured and calculated axial profiles of OH, H$_2$O (Fig. 6.6a) and temperature (Fig. 6.6b) in the flame with $\vartheta = 50$ cm/s.

calculations are similar to those observed in the temperature profiles. Because the numerical simulations predict the fuel-rich and stoichiometric flame zones within the uncertainty of the measurements, where the combustion chemistry is more complicated than on fuel-lean side; we are tempted to ascribe the observed differences to possible differences between the boundary conditions used in the calculations at the outer limits of the computational domain and those existing in the laboratory, as mentioned above. At the exit velocity of the experiment, and at large distances above the burner exit, entrainment of the surrounding air by the coflow cannot be excluded.
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Figure 6.7 Measured and calculated axial profiles of OH, H₂O (Fig. 6.7a) and temperature (Fig. 6.7b) in the flame with $\dot{\vartheta} = 27$ cm/s.

This air entrainment is neglected in the calculations by putting the radial velocity at the outer boundary equal to zero. Air entrainment slows the velocity of combustion products, resulting in an increase in the residence time and thereby an apparently
Figure 6.8 Measured (circles) and calculated OH profiles in $\vartheta = 50$ (Fig. 6.8a) and 27 (Fig. 6.8b) cm/s flames. Solid, dashed and dotted lines denote the calculations performed in full-chemistry, partial equilibrium and full-equilibrium approximations.

faster decrease in the temperature and OH mole fraction. This assumption is supported by comparison of the measurements and calculations at a lower exit velocity. As can be seen from Fig. 6.7, where the temperature, $\text{H}_2\text{O}$ and OH profiles are presented for the flame at $\vartheta = 27$ cm/s, the agreement between the measurements and calculations is
better than for $\vartheta = 50$ cm/s. Following the trend seen in the radial profiles (and in the major species in Ch.5), the calculations without thermal diffusion predict the OH profiles almost quantitatively, while including thermal diffusion shifts the calculated profiles a few millimeters downstream. Whereas the agreement between calculations and measurements is already good, we expect that further improvement can be reached by better matching the boundary conditions. Because matching the boundary conditions of the computation those of the present experiment will lead to an extremely large computational domain [20-23], confining the coflow air in a tube (perhaps at the expense of conveniently being able to perform optical experiments) will guarantee zero mass flux through the boundaries.

As a final point of this section, we present the results of equilibrium analyses for the axial profiles. This analysis was performed by the same procedure that was employed for the radial profiles. The results of these calculations are shown in Fig. 6.8. As expected, the calculations show exactly the same trends as was found in the analysis of the horizontal profiles: the full equilibrium underpredicts and partial equilibrium overpredicts the OH mole fractions obtained from both measurement and full-chemistry calculation.

### 6.3. OH measurements in pure H$_2$ diffusion flames

As mentioned above, concern about the interaction of the flame with the fuel tube, and uncertainty regarding the fuel inlet conditions precluded performing numerical simulations of the pure hydrogen flames. While this undoubtedly handicaps the analysis of the transport-chemistry interactions, choice of these flames as an object for experimental investigation is favored by the practical importance of pure hydrogen as a perspective environmentally friendly fuel. Moreover, the large differences between the fuel and oxidizer densities are expected to result in more pronounced effects due to fast hydrogen diffusivity. In Ch. 4 we have discussed the general properties of pure hydrogen diffusion flames by analyzing the Raman measurements of the temperature and main components. Here we supplement this discussion by comparison of the measured LIF OH profiles with the equilibrium calculations in the hydrogen flame at $\vartheta = 18$ cm/s. While the estimates discussed above show the unlikelihood of reaching full equilibrium in H/O/N system at atmospheric pressure, the equilibrium calculations presented in Ch. 4 reasonably indicate the trends observed in the species mole fractions. We must point out here, however, the fact that, due to
the measurement uncertainty, the $\text{H}_2$ and $\text{O}_2$ mole fractions in the region of substantial \(\text{OH}\) mole fraction are too low to be used reliably in partial equilibrium calculations.

To continue the discussion in Ch. 4 on the physical processes occurring in these flames, the calculated equilibrium \(\text{OH}\) mole fractions are presented in Fig. 6.9 as a function of the equivalence ratio \(\phi\) for three different elemental oxygen/nitrogen ratios in mixture. We recall that for characterizing differential diffusion we introduced in Ch. 4 the coefficient \(R\), which is the elemental oxygen/nitrogen ratio normalized to that of pure air. As we can see from Fig. 6.9, the equilibrium hydroxyl concentration is strongly dependant upon \(R\): changing \(R\) from 1 to 0.8 results in a decrease in the equilibrium \(\text{OH}\) mole fraction at stoichiometric conditions by a more than a factor of two.

6.3.1. \(\text{OH}\) radial distributions

The measured radial profile of \(\text{OH}\), together with the values calculated using the full-equilibrium approximation accounting for differential diffusion, at \(z = 3\) mm are
Figure 6.10 Radial distribution of OH, major species (Fig. 6.10a) and temperature (Fig. 6.10b) at $z = 3$ mm in pure H$_2$ diffusion flame at 18 cm/s exit velocity.

shown in Fig. 6.10. This figure also includes the radial profiles of water (Fig. 6.10a) and temperature (Fig. 6.10b). As can be seen, the measured OH distribution is very similar to that observed in H$_2$/N$_2$ flame with exit velocity of 50 cm/s (Fig. 6.1): the maximum OH mole fractions are similar (~ 6000 ppm for the nitrogen-diluted fuel and ~10000 ppm for the pure hydrogen) and they are located at similar radial position (~
7 mm). This similarity can be explained as follows. The local concentrations of the major species in the two flames do not differ greatly at the location of the OH maxima, which implies similar transport rates. However, since the local temperatures differ by roughly 200 K, we expect the concentration of OH to be somewhat higher in the pure flame than in the hydrogen/nitrogen mixture. It is interesting to point out that in contrast to the measured values, the equilibrium OH mole fractions differ substantially (almost ten times) in these flames. More importantly, we observe that the difference between the measured OH mole fraction and the equilibrium value is ~ 0.8 mole fraction. Comparing this value with the difference shown in Fig. 4.11, we see that this degree of super-equilibrium OH concentration is consistent with a temperature “depression” of several hundred degrees. We thus attribute the “residual” difference between the equilibrium value assuming differential diffusion and the measured maximum temperature in the radial profile to chemical non-equilibrium. Essential in drawing this conclusion is the inclusion of differential diffusion in determining the correct equilibrium OH mole fraction. Looking at Fig. 6.9, the equal diffusivity assumption would give a maximum difference in the maximum OH mole fraction of only ~ 0.3, insufficient to give the required decrease in temperature. We therefore conclude that the differential diffusion is a significant factor determining the properties of the hydrogen/air flames.

Continuing the flame structure discussion, Fig. 6.11 presents the radial profile of OH mole fraction, together with profiles of water and temperature at the axial position of maximum temperature (z = 20 mm). When deriving the OH mole fractions, the experimental data were smoothed according to the procedure described in Ch. 3. Here again, the measured mole fractions are higher than those calculated in the equilibrium approximation. Interestingly, we observe a local minimum in the OH profile at this axial location, absent in the temperature profile at this position. Given the strong correlation between temperature and OH mole fraction, it is reasonable to expect
higher OH concentrations solely in the higher temperature regions. An example can be found in Fig. 6.4 showing differences between the temperature and OH profiles at $z = 30$ mm in the diluted flame; even though the centerline temperature is growing, the OH is still confined to narrow peaks. Because the Raman measurements show that
hydrogen is completely consumed at $z = 20$ mm (Ch. 4, Fig. 4.10), we ascribe the non-monotonic behavior of the OH profile to transport of the hydroxyl molecules from the reaction zones located upstream of this position, where OH is formed.

Further downstream, at $z = 70$ mm, the OH mole fraction was below the detectable limit at all radial positions.

### 6.3.2. Axial OH profiles

The measured axial profile of OH, together with the values calculated using the full-equilibrium approximation accounting for differential diffusion of OH molecules along the flame centerline are shown in Fig. 6.12. The axial profiles of water (Fig. 6.12a) and temperature (Fig. 6.12b) are also presented in this figure. The centerline OH mole fraction is negligibly small throughout the first 15 mm above the burner exit then rises sharply to roughly 3000 ppm at $z = 25$ mm. After reaching the maximum, the OH concentration decreases to below the detection limit above $z = 50$ mm, where the flame temperatures decrease to below 1500 K. We also observe that maximum OH concentration is located slightly downstream of the position of the maximum temperature and H$_2$O mole fraction, suggesting, together with the results in Fig. 6.11, that hydroxyl is not produced on the centerline but transported from the more peripheral parts of the flame by diffusion and convection. This conclusion is also supported by comparing the measured and calculated OH equilibrium profiles. We observe that the measured OH concentrations exceed the equilibrium values, but to much less a degree than observed for the radial profiles. Hydroxyl, produced in the flame zone at the boundary between fuel and air, has been consumed by recombination reactions during transport to the centerline. It should be pointed out that while showing similar behavior with measurements in the H$_2$/N$_2$ diffusion flames,
the axial OH profiles reach significantly higher maximum OH mole fractions. This higher OH concentration is most certainly due to the higher temperature of the pure H₂ flame (2100 K for the pure fuel vs. 1500 K for the H₂/N₂ fuel).
6.4. Conclusions

We observe good agreement between the measured hydroxyl concentrations and those obtained by numerical solution of the governing equations incorporating full-chemistry and detailed transport in the H₂/N₂ axisymmetric flames. Similar to the results obtained for the temperature and major species mole fractions shown in Ch. 5, the OH mole fractions are predicted better in calculations without thermal diffusion than in calculations incorporating thermal diffusion. Analysis of the reduced-chemistry models performed in H₂/N₂ flames shows that the full equilibrium approach underpredicts the measured OH mole fractions at all locations, while the partial-equilibrium model overpredicts the mole fractions. In the flames of pure hydrogen, a substantial impact of differential transport on the properties of these flames is exposed by comparing the measured OH mole fractions with those calculated in the equilibrium approximation. The results show that both finite-rate chemistry and differential molecular diffusion are responsible for “depressing” the temperature below the value calculated for adiabatic equilibrium assuming equal molecular diffusivity.

References


