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Absolute Concentration Measurements Using DFWM and Modeling of OH and S_2 in a Fuel-Rich H_2/Air/SO_2 Flame

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Concentration profiles of OH and S_2 in a sulfur-containing premixed H_2/air flame were obtained and compared to numerical calculations. The measurements utilized degenerate four-wave mixing and absorption spectroscopy in parallel (MULTIPLEX spectroscopy) and were numerically simulated for a one-dimensional flat flame. An established reaction mechanism for hydrogen oxidation was extended by reactions for the sulfur chemistry drawn from the literature. The experimental results for the OH and S_2 concentration profiles are in good qualitative agreement with the simulations. However, the model calculations underestimate the S_2 concentrations by two orders of magnitude, indicating that important intermediates and reactions could have been omitted. © 1999 by The Combustion Institute

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INTRODUCTION

In recent years, the details of fuel oxidation have been extensively investigated and this has shed much light on the chemistry of combustion processes, including the formation of pollutants such as nitric oxides, polycyclic aromatic hydrocarbons (PAH), and particulates. However, few studies have focused on the presence of sulfur in flames, in spite of its environmental and technical significance. Consequently, more experimental and theoretical studies are needed, since sulfur-containing fuels are used in large quantities with sulfur concentrations of up to 10% by wt [1].

Sulfur compounds play an important role during combustion and an understanding of sulfur chemistry is crucial. This is especially so for the design of stationary combustion systems employing diffusion flames which favor the formation of reduced sulfur species, like S_2, in areas where fuel-rich conditions prevail. In addition, the design of the staged combustion process, operating in the first stage at fuel equivalence ratios, ϕ, of between 1.6 and 1.8 [2] promotes interest in the sulfur chemistry for fuel-rich flame conditions. In this environment, the presence of sulfur strongly affects such flame characteristics as temperature, burning velocity, and flame radical concentrations, which also influence sooting limits [3–5] and NO_x emissions. For example, in certain fuel-rich flames, the prompt NO formation increases by up to 300% upon the addition of sulfur species [6–8].

An important contribution to the study of sulfur chemistry is that of Zachariah and Smith [9]. They used molecular beam mass spectrometry to investigate rich $H_2/O_2/Ar$ flames doped with SO_2 at low pressure (100–150 Torr). More recently, time-resolved photon emission from sulfur-doped hydrogen air flames at atmospheric pressure has been measured by Cheskis [10], using a pulsed flame photometer detector. Photons emitted from electronically excited sulfur dimers were observed and could be rationalized by a model of explosion at constant pressure.

The purpose of the present work is the experimental and numerical characterization of sulfur-containing H_2/air flames. Profile measurements of combustion components above a flat-flame burner are combined with a mathematical model of sulfur-doped flames. More specifically, OH and S_2 profiles are obtained by a spectroscopic method that utilizes absorption and degenerate four-wave mixing (DFWM) techniques in parallel (MULTIPLEX spectroscopy). The measurements are compared with numerical calculations and discussed in terms of the applied sulfur chemistry model.

The experimental methods are briefly outlined and only details relevant to the presented investigation are given. A complete description of the apparatus and the theoretical background can be found in [11].

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APPARATUS AND EVALUATION PROCEDURE

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The laser light for OH and S_2 excitation was provided by a Nd: YAG (Continuum NY81, Santa Clara, CA) pumped frequency-doubled dye laser system (Continuum ND60 with a KDP crystal that was angle tuned by an autotracking unit). This had a bandwidth of approximately 0.09 cm^{-1}, which was tuned over a wavelength domain of 303 to 315 nm. Pulse energies were 0.5–2.0 mJ with a pulse duration of ≈10 ns. Spatial shaping of the output beam was performed with a telescope (−50 mm, +200 mm). The slightly converging laser beam had a diameter of ≈1 mm at the interaction region. All input beams had identical linear polarization perpendicular to the burner surface. The DFWM experiment was configured in the three-dimensional phase matching or Forward Boxcars geometry. The pump beams are tipped out of the horizontal plane by a small angle (≈1°). Each of the two pump beams accounts for 45% of the total laser power and the probe beam for 10%. The coherent signal beam passed through a mask blocking the input beams, and its divergence was corrected by a 900-mm lens. To reduce stray light, detection occurred about 6 m from the interaction region. Furthermore, the signal was spatially filtered by combining a 30-mm lens and a 50-μm pinhole mounted in front of the photomultiplier tube (PMT/Hamamatsu H3/177 4W). The PMT was spectrally narrowed by two Schott filters (UG 11 and WG 295). Signal processing was by a Boxcar averager (Stanford Research Systems SR 250) and an acquisition system based on a PC.

DFWM signals versus laser power were measured to ascertain the saturation of the observed transitions ($I/I_{SAT} \gtrsim 1$). At these intensities the influence of the DFWM signal level on the relative rates of dephasing and population transfer collisions is minimized [12]. The collisional independence of saturated DFWM has been verified experimentally for many species, including NO [13] and OH [14–17]. Furthermore at $I/I_{SAT} \approx 1$ the DFWM signal has a decreased dependence on laser intensity [18, 19]. Thus, the signals are assumed to be proportional to the square of the population difference ΔN as well as the line strength B_{ij} of the molecular transition. Replacing ΔN with the ground state population N [since $N(v'',J'') \gg N(v',J')$ at typical flame conditions] yields an expression which enables the DFWM signal to give accurate relative concentration profiles above the flat-flame burner

$$I_{DFWM} \propto [B_{ij} N(v'', J'')]^2 \qquad (1)$$

Compared to laser-induced fluorescence (LIF), the reduction of DFWM signals to concentration for $I/I_{SAT} \approx 1$ (Eq. 1) is advantageous for molecules for which data on the collisional deactivation of the laser-excited state are lacking. For the sulfur dimer, S_2, no quenching, vibrational and rotational energy transfer rates (VET and RET) for the laser-excited $B^3\ \Sigma_u^-$ state are available. Thus, from considerations of the high selectivity of the spectroscopic method and the sensitivity approaching the detection limit of LIF, it was decided to use DFWM for OH and S_2 concentration measurements.

In order to measure the absolute integrated absorption coefficient K, the transmitted probe beam from DFWM was reflected back through the flame to provide an increased absorption length. Its intensity was compared to a reflection off a prism surface in front of the flame that provided the reference signal. Both beams were directed into separate dye cuvettes, containing an optically thin solution of Rhodamin 101B in methanol, and the resulting fluorescence was detected with fast photodiodes. OH was measured by absorption at positions in the flame where there were high concentrations of hydroxyl radical. Absorption signals were processed with a transient digitizer (Tektronix, RTD 720). The absolute number densities were subsequently used to calibrate the relative OH and S_2 DFWM signals. Despite the double pass through the flame, the S_2 absorption was insufficient to yield absolute concentrations.

The laminar hydrogen/air flame was stabilized on a commercially available water-cooled flat flame burner (McKenna Products, Pittsburgh, PA). The diameter of the central section of the burner was 60 mm and mass flow controllers maintained constant flows of air and fuel. Small amounts of SO_2 were added to the flame through a calibrated rotameter. Parts of a

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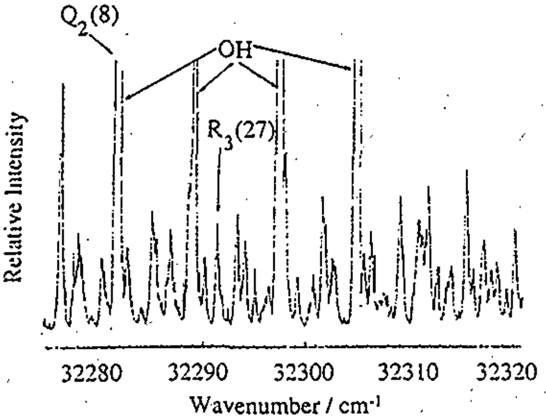

Fig. 1. Typical DFWM spectra obtained in sulfur-doped H_2/air flame. MULTIPLEX measurements performed using the $Q_2(8)$ and $R_3(27)$ transition of OH and S_2, respectively.

F1 typical DFWM spectra in a hydrogen/air flame doped with SO_2 are shown in Fig. 1.

The OH radicals were monitored via the $Q_2(8)$ transitions of the (0,0) band of the electronic $A^2\Sigma^- - X^2\Pi$ system [20–22]. Recent molecular parameters [23] for the $B^3\Sigma_u^- - X^3\Sigma_g^-$ transition of S_2 were used to compute a synthetic spectrum of the molecule within the accuracy of the laser system (≈0.15 cm^{-1}) that overlaps favorably with major features in the experimental spectra. Relative S_2 profile measurements obtained by DFWM on the R_3 (27) transition of the (5,2) band were put on an absolute scale by quantitative comparison with the OH signal intensities. The required Einstein B coefficients for the B-X transition of S_2 were obtained from a calculation of the Hönl-London factors, taking into account the Franck-Condon factors and the electronic transition moment from the literature [24]. The evaluation procedure is described in more detail in [11] and is briefly summarized below.

First, by taking advantage of the high sensitivity of the DFWM signals, the relative concentrations of OH and S_2 were mapped by monitoring the DFWM signals as a function of height above the burner surface. In a second step, absorption spectroscopy gave the absolute number density of OH at a position in the flame where a significant level of the radical occurred. Third, these measurements were linked to the relative OH profile to yield the absolute concentration of hydroxyl as a function of height above the burner surface. Finally, the relative S_2 profile obtained by DFWM was located on an absolute scale by quantitative comparison with the OH profile.

The errors involved in the present experiment are itemized as follows. First, absorption measurements of OH at positions of high concentration are accurate to approximately ±10%. This error includes uncertainties in the optical path length, temperature, and the Voigt a parameter, which is involved when the "curve of growth" technique is applied to convert the integrated absorptions to absolute concentrations [25–28]. Second, profiles of OH are detected by accumulating the DFWM peak intensities of 1000 laser shots for a given height above the burner and using the squared dependence of the signal on number density. The typical standard deviation due to the pulse-to-pulse variation is ±10%. Including the uncertainties in the Boltzmann distribution due to the temperature variations through the flame, a total error in the OH concentration profile is about 30%. Third, DFWM profiles are evaluated from Eq. 1. Taking into account the pulse-to-pulse variations of the DFWM signals, the errors for the induced absorption coefficients, especially for S_2 (25%), the concentration profile of S_2 is assumed to be accurate to approximately ±60%. The detection limits for the sulfur dimer were found to be about 200 ppm, an order of magnitude less sensitive as compared to the OH radical. A decreased sensitivity for S_2 is rationalized by considering the small ground-state rotational constant of the molecule resulting in a high number density of states. At typical flame temperatures a substantial number of these states are populated.

The accuracy of the OH concentration measurements were verified in an atmospheric H_2/air flame. Results agree within the error limits with concentration profiles obtained from a numerical simulation of a one-dimensional flat-flame burner (see below).

SIMULATIONS

The numerical simulation was for a one-dimensional flat flame burner model. The governing equations and solution methods are described

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elsewhere [29, 30]. The hydrogen oxidation mechanism proposed by Warnatz [31] was implemented and modified with the most recent AQ: 1 kinetic data of the CEC evaluation group [32]. The sulfur chemistry for the S/H/O system was taken from Zachariah and Smith [9] and applied without any changes to the kinetic data except that more recent transport and thermodynamic data for HSO and HSO_2 were used [33]. Unfortunately, a more complete reaction scheme is not available from the literature. As a consequence, the nitrogen/sulfur chemistry is omitted in the model and this could account for differences between the calculated and measured OH and S_2 concentration profiles (see below).

We confirmed the mathematical modeling by computing the fuel-rich, low pressure $H_2/O_2/Ar$ flame investigated by Zachariah and Smith [9]. Minor discrepancies in the temperature and concentration profiles were found and could be rationalized as follows: (i) as mentioned above, a more recent and detailed O/H reaction scheme was applied; (ii) the latest data for transport and thermodynamic properties for HSO and HSO_2 were implemented; (iii) the energy equations were solved numerically in this work, as opposed to the use of measured temperature data as input for the model [9].

RESULTS AND DISCUSSION

Concentration profiles of OH and S_2 were measured above the flat-flame burner. Data were obtained at different height increments above the burner surface for premixed atmospheric H_2/air flames doped with SO_2 to yield a mole fraction of 0.09. The flow rates for H_2 and air were 4.36 and 9.21 slpm (standard liter per minute), resulting in an equivalence ratio of $\phi = 1.13$. Selected profile measurements are F2-T1 shown in Fig. 2 and listed in Table 1 and are compared with the flame simulation. In addition, a sulfur-doped C_3H_8/air flame was investigated experimentally and results are presented for comparison. For this flame the flow of C_3H_8 and air were 0.632 and 10.3 slpm, respectively. SO_2 was added to the fuel flow to produce a mole fraction of 0.003.

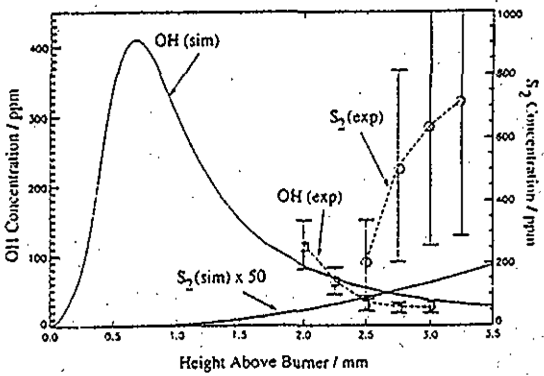

Fig. 2. Concentration profiles for OH and S_2 for $H_2/air/SO_2$ flame above flat-flame burner. □ and ○ indicate experimental concentrations for OH and S_2, respectively. Lines represent results from one-dimensional flat-flame modeling.

The results of the OH and S_2 density measurements are summarized in Table 1 and in Fig. 2. Profile measurements at heights <2 mm were inhibited because the burner began to block the input beams and beam steering effects due to density and temperature gradients led to lensing effects. The overlap of the signal generating beams and the signal passing through the flame was therefore disturbed and led to a significant reduction of the DFWM efficiency. Consequently, data were obtained above 2 mm at 0.25-mm height increments. Since the reaction zone for the $H_2/air/SO_2$ flame is very close to the burner surface, the region of maximum OH radical concentration could not be mapped completely. However, the OH concentration profile indicates the flame front position below a height of 2 mm. Further downstream, the hydroxyl radical concentration decreases from 116 ppm to the equilibrium value of 28 ppm at a height of 2.5 mm, in agreement with the equilibrium value of the numerical simulation. In general, the OH profile in the postflame region agrees reasonably well with the theoretical calculations. The discrepancies are due to the roughness of the model and the uncertain kinetic data for many sulfur chemical reactions (see below).

Likewise, the results of the S_2 concentration profile measurements in the $H_2/air/SO_2$ flame are in qualitative agreement with the calculations. S_2 and other reduced species (SH and H_2S) are formed downstream of the OH radical peak. In this region of the flame the temperature and the major radicals are decreasing and S_2 is formed in the presence of S_2O. After

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TABLE 1

Concentration profiles in ppm for OH and S_2 above flat-flame burner

Height Above Burner (mm)	$[OH]_{EXP}$ (ppm)	$[OH]_{SIM}$ (ppm)	$[S_2]_{EXP}$ (ppm)	$[S_2]_{SIM}$ (ppm)	$TEMP_{SIM}$ (K)
Experimental and simulated data for the H_2/air/SO_2 flame ($\phi = 1.13$)*					
2.0	116 ± 35	84.5		1.0	1576
2.25	64 ± 19	66.2		1.3	1577
2.5	31 ± 9	53.2	210 ± 126	1.8	1578
2.75	26 ± 8	43.6	509 ± 305	2.2	1577
3.0	28 ± 8	36.4	637 ± 382	2.7	1577
3.25			721 ± 433	3.9	1576
Experimental results for C_3H_8/air/SO_2 flame ($\phi = 1.4$) for comparison					
1.0	210 ± 63				
1.5	299 ± 90				
2.0	284 ± 85				
2.5	205 ± 62		273 ± 164		
3.5	138 ± 41		568 ± 341		
4.5	121 ± 36		621 ± 373		
5.5	121 ± 36		677 ± 406		
6.5			699 ± 419		

* Simulated temperature in K is also shown.

formation, the diatomic sulfur species diffuse back toward the burner and undergo exothermic reactions to form the oxidized species [9]. However, the quantitative concentrations that were experimentally obtained for the S_2 profiles differ from those of the numerical simulation by more than two orders of magnitude. It is interesting to consider some implications based on the comparison between the experimental and calculated sulfur dimer profiles.

The reaction scheme for the numerical simulation of sulfur laden flames describes the H_2/O_2/SO_2 at low pressure (100–150 Torr) rather well [9]. However, in this work, the measurements were performed at atmospheric pressure and air was used as oxidizer, as opposed to oxygen. In fact, at atmospheric pressure many fundamental three-body reactions begin to occur at significant rates. Such reactions usually do not affect the modeling of low-pressure flames significantly, because their rates are too slow to be important. But at the increased pressure of 1 atm, the use of unrefined rate parameters or unknown three-body reactions can cause significant disagreement between model and experiment.

Furthermore, the sulfur subsystem has been established for a hydrogen/oxygen flame and does not adequately represent the hydrogen/air subsystem. In particular, the nitrogen/sulfur chemistry is omitted from the model and can cause significant discrepancies. In fact, previous work has indicated that the SO_x and NO_x interactions are quite complex. Under fuel-rich conditions sulfur species like SO, H_2S, SH, S_2, and S are formed and these may well interact with nitrogen-containing species. Wendt et al. [34] have studied SO_2-doped CO/Ar/O_2/C_2N_2 flames and were able to model the experiments successfully by a reaction scheme that included the Zeldowich mechanism (thermal NO_x formation)

$$O + N_2 \leftrightarrow NO + N$$

$$N + O_2 \leftrightarrow NO + O$$

$$N + OH \leftrightarrow NO + H$$

and five direct sulfur/nitrogen reactions

$$N + SO \leftrightarrow NO + S$$

$$S + NO \rightarrow NS + O$$

$$O + NS \rightarrow SO + N$$

$$N + NS \rightarrow N_2 + S$$

$$N + SH \rightarrow NS + H$$

Note that the reactions involve the O and OH radicals, which also play an important role in the fuel oxidation mechanism. Hence, in general, it is necessary to couple the thermal NO reactions and the sulfur/nitrogen reactions to the sequence describing oxidation of the fuel. AQ: 2 Unfortunately, Corley and Wendt [7] have not been able to predict SO_2-doped $CH_4/He/O_2/C_2N_2$ flames by applying the same model, indicating that important intermediates and reactions could have been omitted. Since a more complete reaction scheme is not available from the literature, the nitrogen/sulfur chemistry is omitted in the applied model and could account partially for the discrepancy of the theoretical and measured OH and S_2 concentrations. Obviously, further theoretical and experimental work is required to establish a valid mechanism for the sulfur chemistry in combustion processes.

For comparison, MULTIPLEX measurements were performed on a $C_3H_8/air/SO_2$ flame at the same equivalence ratio of $\phi = 1.4$. For this hydrocarbon flame the flame front is located ≈1.5 mm and could be mapped by monitoring the OH profile. The equilibrium value of ≈120 ppm for OH is significantly higher as compared to the hydrogen fueled flame. On the other hand, S_2 concentrations in this flame are very similar to those for the $H_2/air/SO_2$ flame.

SUMMARY AND CONCLUSION

A novel spectroscopic technique (MULTIPLEX spectroscopy) [11] was applied to measure S_2 and OH concentration profiles in $H_2/air/SO_2$ flames stabilized on a flat-flame burner at atmospheric pressure, in conjunction with numerical simulations for a one-dimensional flat-flame. An established reaction mechanism for hydrogen oxidation was extended by the sulfur chemistry reactions proposed by Zachariah and Smith [9] for low-pressure $H_2/O_2/SO_2$ flames.

The experimental results for the OH and S_2 concentration profiles are in good qualitative agreement with the numerical simulations. The S_2 abundance increases downstream of the maximum OH concentration (indicating the position of the flame front) as predicted by the model. However, the model calculations underestimate the S_2 concentrations by two orders of magnitude. This result is rationalized by considering two effects that have not been treated completely by the relatively simple reaction mechanism. First, the model of Zachariah and Smith [9] has been established and tested for low-pressure conditions only. At atmospheric pressure however, three-body reactions are increasingly important. In the applied model this class of reactions might be ill characterized or missing. Second, nitrogen/sulfur interactions are not implemented in the mechanism and can produce significant discrepancies between model and experiment.

We conclude that further theoretical and experimental investigations are required to shed more light on the sulfur chemistry in combustion systems. Quantitative MULTIPLEX spectroscopy could be applied on important sulfurous intermediates, like SO, SH, NS, in conjunction with numerical modeling to reduce the lack of information in the sensible field of the sulfur chemistry in flames.

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