

# SUPPRESSION OF A LAMINAR OPPOSED-FLOW NATURAL GAS/AIR DIFFUSION FLAME WITH C<sub>3</sub>HF<sub>7</sub>

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## ABSTRACT

An investigation of the opposed flow diffusion flame system has been performed with consideration of the products resulting from chemical flame suppression. The experimental study examined the chemical composition profiles in the natural gas/air flame with addition of C<sub>3</sub>HF<sub>7</sub> (FM-200) suppressant to the air stream. Numerical simulations of the flame system were performed using the Sandia Oppdif flame code and kinetic mechanisms for the natural gas flames suppressed with FM-200. Composition profiles were measured in the opposed flow natural gas flame with 2% addition of FM-200 to the air stream. A specially designed sampling probe consisting of an alumina tube coupled with a 200 μm ceramic tip probe was used for sampling the suppressed flame. The composition measurements using gas chromatographic analysis gave reasonable agreement between measurements for the major species profiles and those predicted from the Oppdif model.

## INTRODUCTION

Fire protection for technologically sensitive applications has in the past been well served by halon fire retardants. The ozone-depleting nature of these chemicals has led to them being phased out under the Montreal Protocol, and the search for suitable replacements continues in earnest.

Diffusion flames are characterised by an initial separation of fuel and oxidiser with combustion proceeding near the zone of impingement between the flows of fuel and oxidant. The diffusion type flame occurs in many industrial and practical situations where the degree of mixing between fuel and oxidant is limited. In the diffusion flame, the chemical reaction rate is generally much faster than the diffusion velocity of the reactant gases. Consequently, the chemical reaction occurs in a narrow zone between the fuel and oxidiser, the concentration of reactants in the reaction zone is low, and the combustion rate is controlled by the rate at which fuel and oxidiser flow into the reaction zone through the combustion products [1]. Many fires are characterised by diffusion flame behaviour, and the study of this flame regime can yield important insight into the behaviour of fires in a broader context.

The chemical structure and behaviour of various flame suppressant compounds on the methane/air flame system has attracted a large amount of research. Linteris [2], Hamins et al. [3], Masri et al. [4] and Westmoreland et al. [5] (among others) have investigated flames inhibited with CF<sub>3</sub>Br. Alternative inhibition agents have also been investigated by Babushok et al. [6], Hamins et al. [3], Milne et al. [7], Chelliah et al. [8], Wang et al. [9], Suet al. [10], and Womeldorf et al. [11]. Some of the alternative compounds studied include CHF<sub>3</sub> (HFC-23, FE13), CH<sub>2</sub>F<sub>2</sub>, CH<sub>3</sub>Br,

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$C_2F_6$ , and other halogenated hydrocarbons such as  $CH_3Cl$ . The bulk of the flame inhibition studies reported in the literature have used the premixed flame regime, and the primary concern has largely been with fire extinguishment efficiency and net toxic generation rather than flame structure. The opposed flow diffusion flame burner (Figure 1) is an ideal apparatus to examine the structure of flames undergoing chemical suppression. There is considerable scope to investigate the nature of many flame systems and additive compounds.

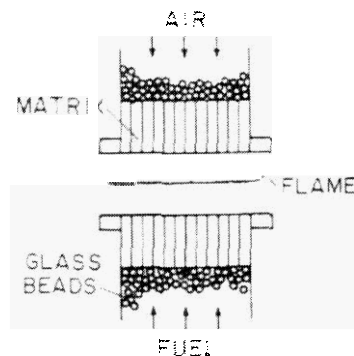


Figure 1. Opposed flow diffusion flame burner [1].

A limited number of studies have been performed using alternative fire suppressants with the opposed flow burner configuration. An experimental study by McNesby et al. [12] incorporated spectroscopic measurement of counterflow diffusion flames as part of a wider halon replacement assessment program. The suppressants studied included  $CF_3Br$  (Halon 1301) and a halon alternative  $C_3HF_7$  (FM-200, HFC-227ea). Reinelt and Linteris [13] conducted an experimental study of diffusion flames inhibited using the toxic, yet highly effective, suppressant iron pentacarbonyl. The objective of this study was to examine the flame structure of an opposed-flow diffusion flame during chemical suppression through both experimental measurements and numerical simulation in order to gain greater insight into the processes driving combustion product formation.

## EXPERIMENTAL

### Apparatus

The apparatus developed for the study included an opposed flow burner, sample probe and transfer mechanism, and chemical analysis equipment. The burner configuration used in this application was based on the design of Puri and Seshadri [14]. This burner is characterised by a very stable disc of flame established in the space between two vertically aligned ducts issuing a fuel (natural gas) and an oxidiser stream (anhydrous air). The flow of air was regulated by a rotameter and the natural gas by a mass flow controller unit. A diagram of the opposed-flow burner and flame configuration is shown in Figure 1.

Chemical composition of the flame gases was determined by withdrawal and analysis of sampled gas from the flame space. The device used to extract gases from the flame region must cause minimal disturbance of the flame whilst removing sufficient volume of gases for representative chemical analysis. The probe device must also quench the combustion reactions in the sampled gases in order to “freeze” the gas composition as at the sampled flame position. The probe

design adopted for the study satisfied these requirements by utilising a short section of ceramic tubing of 200  $\mu$ m diameter as the invasive tip. The capillary section is attached to a 1.6 mm (OD) alumina tube to affect a supersonic expansion thus quenching the sampled gases. The gases are further cooled by a water jacket surrounding the larger tube section. A diagram of the sample probe is shown in Figure 2.

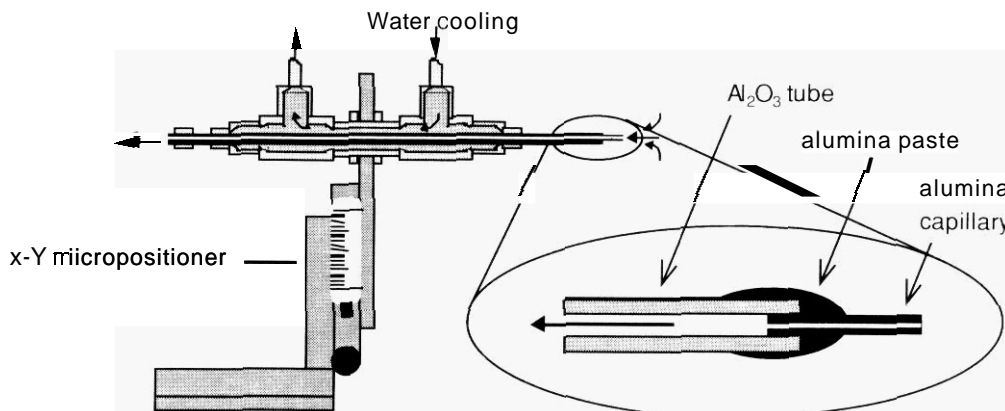


Figure 2. Diagram of sampling probe, cooling jacket, and micropositioner.

The position of the probe in the flame was varied using a micropositioner device. The probe tip was positioned to extract sample from the stagnation (centreline) axis. A partial vacuum was developed in the sample line to facilitate movement of gases into the probe and through the sample line to the chemical analysis equipment. The sample line consisted of 3.125 mm (OD) teflon tubing (heated) that connected the sample probe and the chemical analysis devices. The teflon tubing provided a chemically inert transport pathway: the small diameter of the tube promoted plug flow of sample gases, minimising distortion of sampled composition during transfer.

Chemical analysis of the sampled gases has been performed using gas chromatographic analysis. Gas chromatography allows fast, accurate, and reproducible quantitation of gas composition, and this technique is well suited to the analysis of the major stable species present in the flame system. A Shimadzu GC-17A gas chromatograph equipped with a thermal conductivity detector (TCD) was used in this study. An Alltech AT-Molesieve capillary column was used to give separation of  $O_2$ ,  $N_2$ ,  $CH_4$  and  $CO$  species. A J&W Scientific GS-Q capillary column allowed quantification of  $CH_4$ ,  $CO_2$  and  $C_3HF_7$ . An illustration of the apparatus configuration is given in Figure 3.

## Procedure

The flame studied in this investigation resulted from a natural gas flow rate of 0.5 L/min and an air flow rate of 6.4 L/min. The diameter of each burner duct was 50 mm, and a separation of approximately 12 mm between the fuel and oxidiser ducts was adopted for the study. Once a stable flame was established, the micropositioner (with the sample probe) could be adjusted to give the desired measurement position in the flame space. The position and thickness of the luminous flame zone was estimated visually by relating the probe tip position to each edge of the visible flame zone.

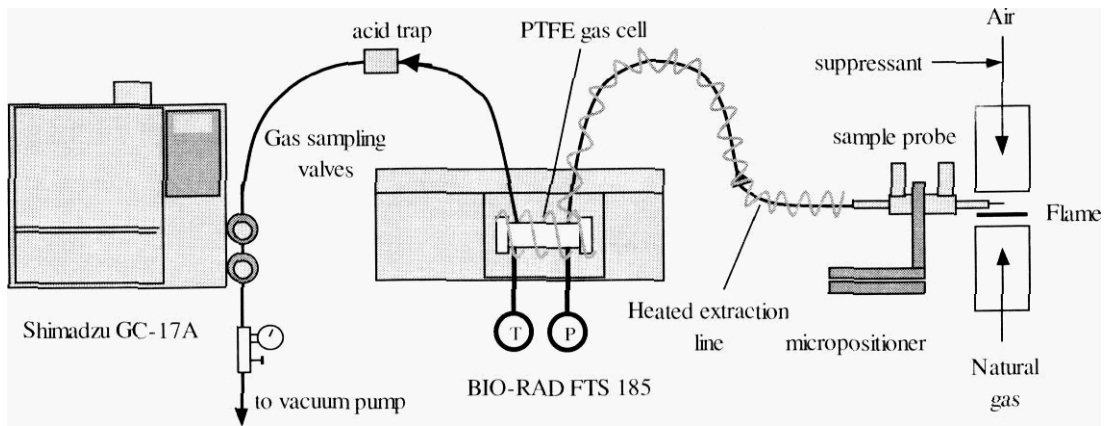


Figure 3. Diagram of the apparatus configuration.

The chemical composition experiments involved positioning the sample probe at various points along the centreline (stagnation axis) of the burner (initial position directly above fuel duct surface) and extracting a continuous stream of sampled gases through the probe and sample line. An extraction pressure of 60kPa was adopted to minimise composition distortions in the sample [15]. The sample extraction for a given position was allowed to proceed for at least 1 min to ensure the sample had reached the gas chromatograph. After this time, the sample was injected (via sample loop arrangement) into the gas chromatograph and the resulting chromatogram recorded. The probe was then moved to the next position along the stagnation axis, where the sampling procedure was repeated. The chemical composition for each position was found from analysis of the associated chromatogram. Detector response factors from Dietz [16] and Height et al. [17] were used for gas chromatography mole fraction calculations.

## Modelling

Computer modelling of the flame system was performed using the Sandia Oppdif opposed flame diffusion flame software [18]. Initial modelling of the natural gas/air flame used the GRIMech 2.11 kinetic mechanism and associated thermodynamic and transport data [19]. Modelling of the experimental system of flames inhibited with FM-200 were performed using the mechanism and transport data developed by Hynes et al. [20] for premixed hydrogen-air flames inhibited with FM-200. The mixture averaged diffusion velocity formula was used for most calculations. The computation parameters GRAD and CURV were each typically set to 0.5.

## RESULTS AND DISCUSSION

### Major Species Composition Profiles

The major species analysed in the study included the oxidiser stream compounds  $N_2$ ,  $O_2$ , and  $C_3HF_7$  (FM-200) along with the primary fuel component  $CH_4$  and the combustion products  $CO$  and  $CO_2$ . The concentration profiles for the major species were determined using gas chromatographic analysis. The measured and predicted composition profiles for the oxidiser stream species are shown in Figure 4.

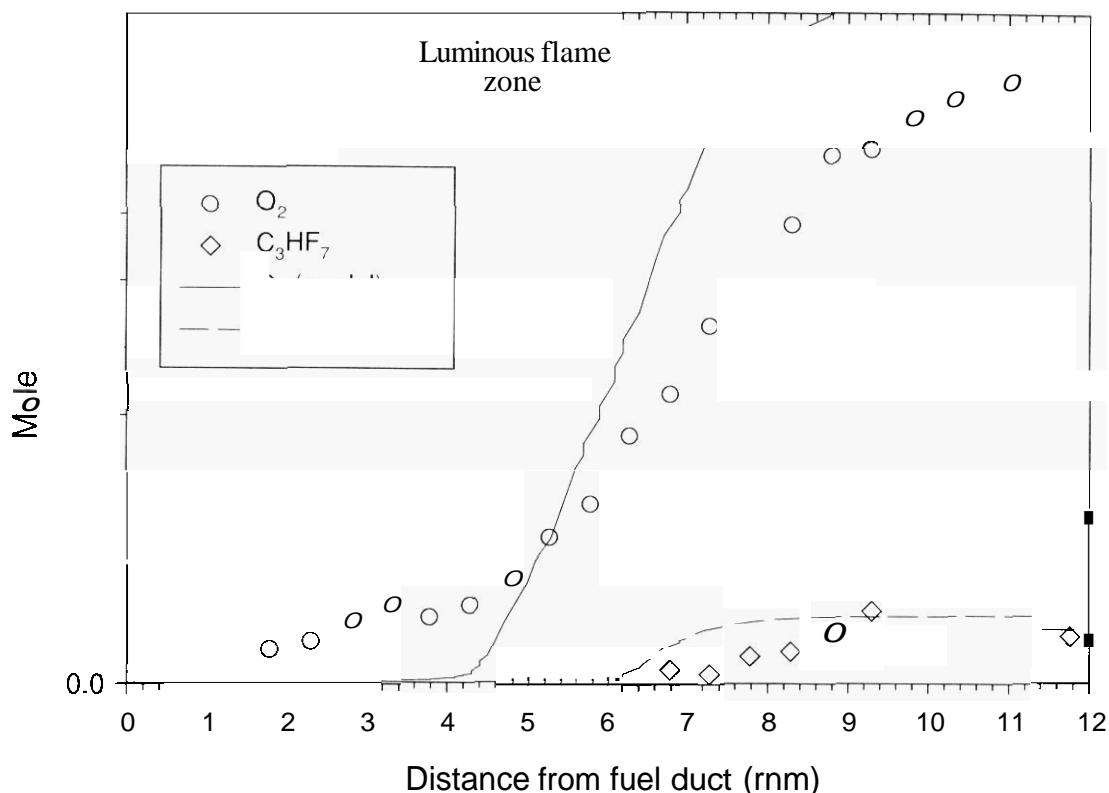


Figure 4. Species composition profiles for oxidiser stream

The oxygen ( $O_2$ ) profile shows the composition decreasing steadily as the air stream approaches the flame zone. This observation reflects the progressive consumption of oxygen through combustion reactions. The measured profile is lower than the theoretical profile on the air side of the flame zone. The over-prediction of the oxygen may result from neglecting moisture in the inlet parameters of the model. The concentration of  $C_3HF_7$  (FM-200) is observed to diminish as the air stream approaches the flame, illustrating the progressive reaction of the suppressant species. The measured profile shows close agreement to the model, with the measurements showing the concentration diminishing at a slightly earlier stage than that of the modelled profile. The prolonged concentration profile of the model may suggest the kinetic mechanism is deficient in  $C_3HF_7$  pyrolysis reactions. The fuel stream concentration plot is shown in Figure 5.

The profile for primary fuel component, methane ( $CH_4$ ) is observed to decline from a high initial concentration at the fuel inlet to zero composition in the flame zone. This behaviour is anticipated as the methane is consumed through pyrolysis and combustion reactions as it approaches the flame region. The measured  $CH_4$  composition values lie below the theoretical profile. This observation may be attributed to more extensive fuel reaction than is accounted for by the mechanism or discrepancies in the boundary conditions of the model and those in the experiment. The composition profiles for  $CO$  and  $CO_2$  are shown in Figure 6.

The measured profiles for  $CO_2$  and  $CO$  show the concave distribution expected for diffusion of combustion products away from the flame zone. The measured profiles show close correlation with the model for both species. Good agreement is observed for the  $CO_2$  profiles from the fuel

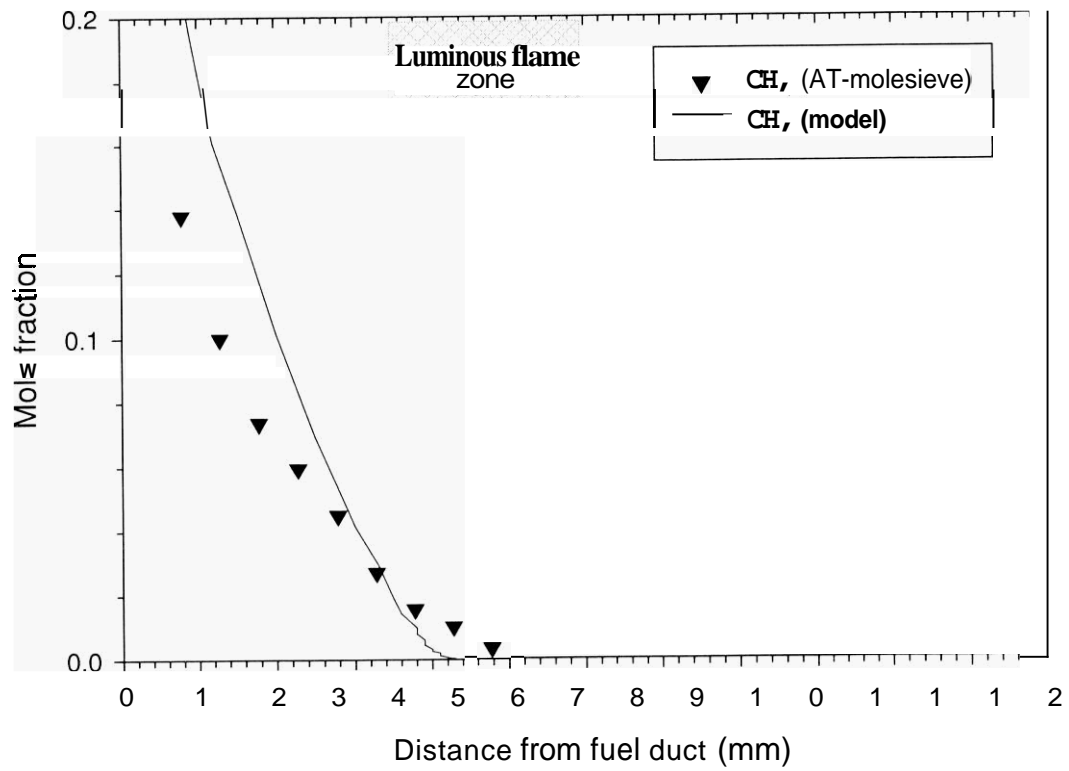


Figure 5. Fuel stream concentration profiles.

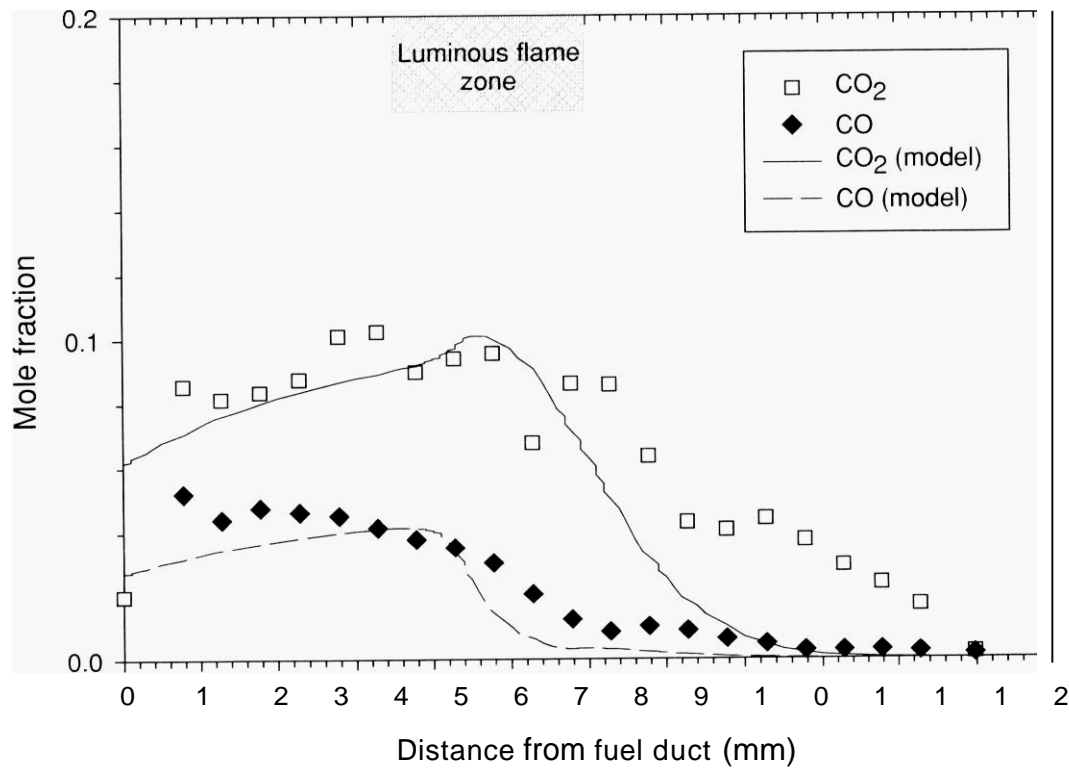


Figure 6. Concentration profiles for  $\text{CO}_2$  and  $\text{CO}$ .

duct up to approximately 7 mm from the fuel duct. The CO<sub>2</sub> measurements in particular confirm the significant level of diffusion of combustion products back towards the fuel duct. This is an observation that could be discounted as a shortcoming in the transport model; however, the measurements confirm the accuracy of the model in this respect. The close correlation of the CO and CO<sub>2</sub> profiles to the model is also encouraging as it indicates that distortion of these species in the sampling probe, as reported by Hynes et al. [21], is not a significant concern for the probe used in this study. Another interesting observation is that the measurement of the secondary CO peak on the air side of the flame zone (6-7 mm from fuel duct) is in agreement with the model.

A significant deviation from the CO<sub>2</sub> model is observed on the air side of the flame zone (7-10 mm from fuel duct) with an elevated concentration of measured CO<sub>2</sub> in this region. A more thorough analysis of the model output shows that a significant level of CF<sub>2</sub>O formation is predicted to occur in this vicinity. A possible explanation for the elevated CO<sub>2</sub> concentration may be that C<sub>3</sub>HF<sub>7</sub> is pyrolysing and reacting to give CF<sub>2</sub>O, which in turn reacts with H<sub>2</sub>O to release CO<sub>2</sub> (Equation 1). This observation may also account for the earlier than anticipated decline in C<sub>3</sub>HF<sub>7</sub> concentration commented on in relation to Figure 4. It is possible that this reaction is an internal probe rather than a flame effect.



## MODEL PREDICTIONS

The principal toxic species of concern for flame suppression studies using a hydrofluorocarbon such as C<sub>3</sub>HF<sub>7</sub> is the acid gas HF. The Oppdif code coupled with a suitable kinetic mechanism is able to predict the spatial concentration of species, including HF, produced during suppression. The concentration profiles of other species such as H<sub>2</sub>O and COF<sub>2</sub> can also be predicted, as shown in Figure 7.

## FUTURE DIRECTIONS

The authors propose to use the FTIR coupled with the MALT synthetic calibration analysis [22] to quantify HF, COF<sub>2</sub>, and H<sub>2</sub>O species produced in the suppressed flame. The MALT software will be used to analyse the spectra obtained at various probe positions throughout the suppressed flame region, and quantify products that we were not able to analyse through chromatographic analysis.

## CONCLUSIONS

Chemical composition measurements were obtained for the natural gas/air opposed flow diffusion flame with 2% C<sub>3</sub>HF<sub>7</sub> (FM-200) added to the air stream. Measurements were performed using a 200 μm tipped ceramic probe, with gas chromatographic quantitative analysis. A numerical model using Oppdif software and suitable kinetic mechanisms was also used to simulate the experimental system.

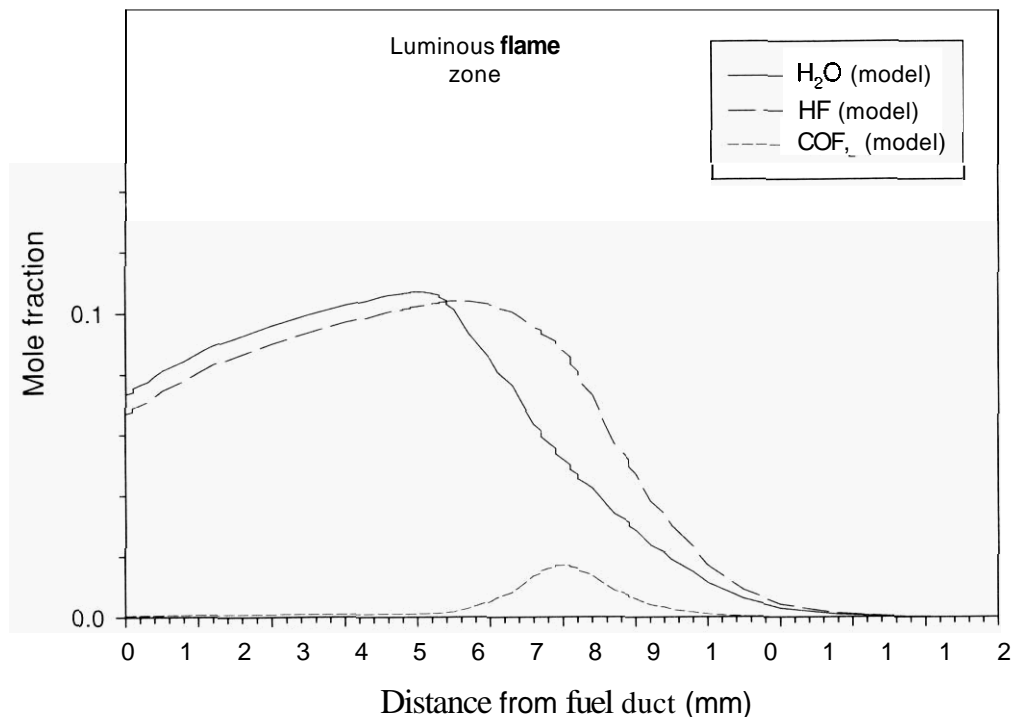


Figure 7. Predicted concentration profiles for toxic combustion by-products.

The measured concentration profiles on the whole showed very close agreement to the simulation profiles. Close correlation was observed for CO, CO<sub>2</sub> and CH<sub>4</sub> in particular. Concentrations below the predicted levels were found for O<sub>2</sub> and C<sub>3</sub>HF<sub>7</sub> and were rationalised by consideration of sampling effects. The close agreement between the experimental results for the major species and the model gives support to the validity of the model (and component kinetic mechanism) and in turn the experimental techniques.

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