

Sampling Measurements of Nitric Oxide in Methane + Oxygen + Nitrogen Flames Doped with Ammonia

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Abstract

Probe sampling measurements of the concentrations of nitric oxide in the post-flame zone of methane + oxygen + nitrogen flames doped with ammonia (0.5 % of the fuel) are reported. The goal of this work was to analyze formation of NO_x from fuel-N under well-controlled conditions. A Heat Flux method was used for stabilization of non-stretched flames on a perforated plate burner at atmospheric pressure. Dilution ratios of oxygen, O₂/(O₂+N₂), were varied from 0.16 to 0.209. The concentrations of O₂, CO, CO₂ and NO_x were measured by means of a non-cooled quartz probe at different axial distances from the burner. Measured burning velocities for these flames and concentrations of the major species (O₂, CO, CO₂) agree well with those of the flames of methane + oxygen + nitrogen within an experimental accuracy. The concentrations of NO_x in the post-flame zone have a maximum near the stoichiometry. These measurements were compared to model predictions and to similar experiments in flames of methane + oxygen + carbon dioxide doped with ammonia. In (CH₄+NH₃) + O₂ + CO₂ mixtures the modeling over-predicts the measured concentrations of NO_x however the experimental trends are well reproduced. In (CH₄+NH₃) + O₂ + N₂ mixtures the plots of the concentrations of NO_x in the post-flame zone as a function of the stoichiometric ratio differ qualitatively from that in (CH₄+NH₃) + O₂ + CO₂ mixtures. The modeling is in satisfactory agreement with the experiments in lean flames, while in rich flames it is not.

Introduction

A detailed reaction mechanism for small hydrocarbons combustion [1] was extensively validated against experimental data available for oxidation, ignition, and flame structure of hydrogen, carbon monoxide, formaldehyde, methanol, methane, ethane, propane, and some of their mixtures. A series of dedicated experimental and modeling studies of laminar premixed flames has been performed to extend the basis of the mechanism validation, e.g. [2 - 4]. Adiabatic stabilization on flat flame burners is attractive for laminar premixed planar flame studies since it facilitates comparison with theoretical models; therefore a Heat Flux method was used to determine flame propagation speeds under conditions when the net heat loss of the flame is zero. This method also allowed for sampling measurements of the NO_x concentrations in the post-flame region of the premixed adiabatic flames [2, 4 - 6].

In most cases good agreement has been observed between the predictions of the current version of the reaction mechanism (Release 0.5) [1] and experimentally measured burning velocities and concentrations of the major species (O₂, CO, CO₂) and NO_x formed in the flame front. Sometimes comparison of the experiments and modeling revealed remaining uncertainties in the rate constants employed [4]. One should note that this reaction mechanism has been validated with experimental data mostly related to NO_x formation from atmospheric nitrogen. Recent study of NO_x formation in CH₄ + O₂ + CO₂ flames doped with ammonia [7] demonstrated good qualitative agreement

between experiments and modeling, although measured concentrations of NO_x were over-predicted. This encouraged further validation of the mechanism and this attempt to study methane + oxygen + nitrogen flames doped with ammonia.

Numerous experimental and modeling studies of the flames doped with ammonia reviewed recently by Glarborg et al. [8], were motivated by the concern of nitrogen oxides emission from combustion of biomass and other solid fuels. During initial stages of biomass combustion fuel nitrogen is released as volatile components mostly in form of ammonia; the biomass itself is converted into a combustible mixture of low- to medium-heating value, as compared to typical natural gas, due to presence of water vapor and carbon dioxide. Instead of varying the composition of the fuel to represent volatiles formed from biomass, the content of oxygen in the artificial air was varied in the present work from 0.209 down to 0.16 to modify burning velocity and flame temperature of the (CH₄+NH₃) + O₂ + N₂ mixtures. Premixed adiabatic flames were studied using a gas mixture of methane doped with 5000 ppm of NH₃ as a fuel. In the following these measurements are presented and compared to model predictions and to similar experiments in flames of methane + oxygen + carbon dioxide doped with ammonia [7].

Experimental Details

Experiments have been performed in premixed flames stabilized on the perforated plate burner using the Heat Flux method. The detailed descriptions of the

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method, burner and experimental set-up can be found elsewhere [3, 5]. The most essential details are described in this paper. The burner consists of a plenum chamber and the burner head. The outlet of the burner head is the plate perforated with small holes, with six thermocouples soldered into the plate surface at the upstream side. The burner head has a heating jacketed with thermostatic water supply. In these experiments it was kept at 353 K. The plenum chamber has an independent thermostatic jacket and its temperature was kept at 298 K. Thus, during the measurements the burner plate temperature is higher than the initial gas temperature and the unburned gases passing through it are heated up. If the flame is stabilized under sub-adiabatic conditions, the gas velocity is lower than the adiabatic flame burning velocity and the sum of the heat loss and heat gain is higher than zero, there is a net outgoing heat flux from the plate. Then the center of the burner plate is hotter than the heating jacket. If the unburned gas velocity is higher than the adiabatic burning velocity (super-adiabatic conditions), the net heat flux is lower than zero and the center of the burner plate is cooler than the heating jacket. By changing the flow rate of the gas mixture an appropriate value of the gas velocity can be found to nullify the net heat flux. In this case the radial temperature distribution in the burner plate is uniform and equal to the temperature of the heating jacket. The series of thermocouples attached to the burner plate allow for measuring the temperature distribution in it. The flow rate at which the net heat flux is zero was shown to be an adiabatic flame burning velocity [9].

The gas supply system of the burner consists of three ducts for the fuel, oxygen and diluent gas. Each duct is connected to the appropriate gas cylinder and has a buffer vessel and a mass flow controller. Two water thermostats were used to provide the water supply to the thermostatic jackets of the burner. Dilution ratios of oxygen in the artificial air, $D = O_2/(O_2+N_2)$, were varied from 0.16 to 0.209. The pure gases were used as delivered by the supplier. The stated purity of methane, oxygen, and nitrogen were 99.995 % or better. Gas mixture of methane with 5000 ppm of NH_3 was prepared and delivered by the supplier with nominal accuracy of ± 500 ppm of ammonia.

Concentration measurements were made using a non-cooled quartz probe. It has a 0.9 mm inlet diameter, 6 mm external diameter and 1 mm wall thickness. The sample gas was directed to gas analyzers through the gas line via a conditioning unit, a membrane pump and a filter. Moisture was separated in the conditioning unit by rapid chilling at the dew point of water 5°C, without dissolution of gases in the liquid phase. Consequently, the measured concentrations were compared to the results of modeling recalculated to the dry basis.

The Fisher Rosemount Model 951A NO/NO₂ chemiluminescence analyzer was used for measuring the concentrations of NOx as a sum of NO and NO₂, because in the present study the measurements of NO or

NOx were indistinguishable within the experimental accuracy. Therefore the NOx concentrations measured in the post-flame zone presented here were attributed to the concentrations of NO. An overall accuracy in these measurements was better than 10 %. Ranges of measurements, instrumental errors of the analyzer, properties of calibration mixtures, calibration procedure, probe sampling errors and possibility of conversion of NO to NO₂ inside the probe were discussed elsewhere [5].

Modeling Details

The CHEMKIN - II collection of codes [10 – 12], including transport properties [13] from Sandia National Laboratories, were used for the flame modeling. Multi-component diffusion and thermal diffusion options were taken into account. The adaptive mesh parameters GRAD and CURV were respectively 0.05 and 0.5. Detailed C/H/N/O reaction mechanism for the combustion of small hydrocarbons [1] was implemented. The current version of the mechanism (Release 0.5) consists of 1200 reactions among 127 species. Modeling was carried out for free propagating adiabatic flames.

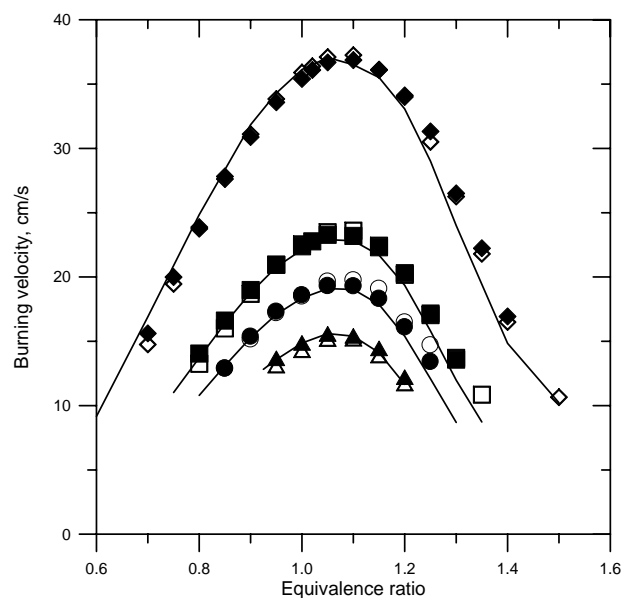


Figure 1. Adiabatic burning velocities measured at atmospheric pressure and initial gas temperature of 298 K. Solid symbols: present results in $(CH_4+NH_3) + O_2 + N_2$ flames; open symbols: results in $CH_4 + O_2 + N_2$ flames [3]. Diamonds: dilution ratio $D = 0.209$; squares: $D = 0.18$; circles: $D = 0.17$; triangles: $D = 0.16$. Solid lines: modeling.

Results and Discussion

Figure 1 shows adiabatic burning velocities measured at atmospheric pressure and initial gas temperature of 298 K in $(CH_4+NH_3) + O_2 + N_2$ mixtures. Also shown are earlier results in $CH_4 + O_2 + N_2$ flames [3] and calculated adiabatic burning velocities. An accuracy of the burning velocity

measurements (± 0.8 cm/s, double standard deviation with 95 % confidence level) and relative accuracy of the equivalence ratio (± 0.54 %) were estimated from calibration data as described earlier [3]. No influence of the ammonia admixture on the flame burning velocities was experimentally found within an experimental uncertainty. The same conclusion was made in the study of $(\text{CH}_4+\text{NH}_3) + \text{O}_2 + \text{CO}_2$ mixtures [7]. This experimental observation was also substantiated by the modeling: calculated burning velocities in $\text{CH}_4 + \text{O}_2 + \text{N}_2$ mixtures and in corresponding mixtures doped with ammonia are indistinguishable within an uncertainty of the numerical calculations, which is about ± 0.2 cm/s.

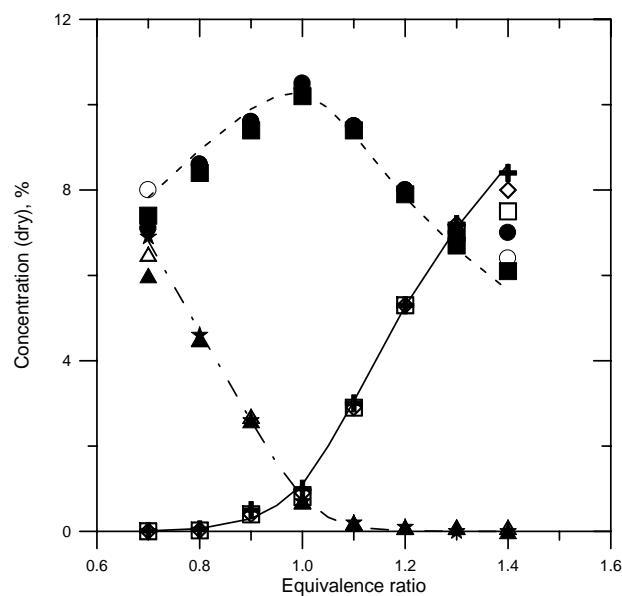


Figure 2. Concentrations of CO , CO_2 , and O_2 in $(\text{CH}_4+\text{NH}_3) + \text{O}_2 + \text{N}_2$ flames at different distances from the burner. Dilution ratio $D = 0.209$. Crosses, diamonds and open squares: $[\text{CO}]$ at 10, 15 and 20 mm from the burner, respectively; solid squares, open circles and solid circles: $[\text{CO}_2]$ at 10, 15 and 20 mm; open triangles, solid triangles and stars: $[\text{O}_2]$ at 10, 15 and 20 mm. Lines: model predictions in adiabatic flames with downstream heat losses at 10 mm. Solid line: $[\text{CO}]$; dashed line: $[\text{CO}_2]$; dash-dot line: $[\text{O}_2]$.

Concentrations of O_2 , CO , CO_2 and NO_x were measured by means of a quartz probe for all dilution ratios of oxygen in the artificial air, $D = \text{O}_2/(\text{O}_2+\text{N}_2) = 0.16, 0.17, 0.18$ and 0.209 . Figure 2 shows concentrations of CO , CO_2 , and O_2 in $(\text{CH}_4+\text{NH}_3) + \text{O}_2 + \text{N}_2$ flames with dilution ratio $D = 0.209$ at different axial distances from the burner. The concentrations of these major species agree well with those measured in the flames of methane + air [5] within an experimental accuracy. The measurements are compared with the model prediction in adiabatic flames recalculated to the dry basis. In the previous and present studies the concentration measurements of major stable species and comparison with the modeling were used to reveal the range of flames not affected by the air entrainment.

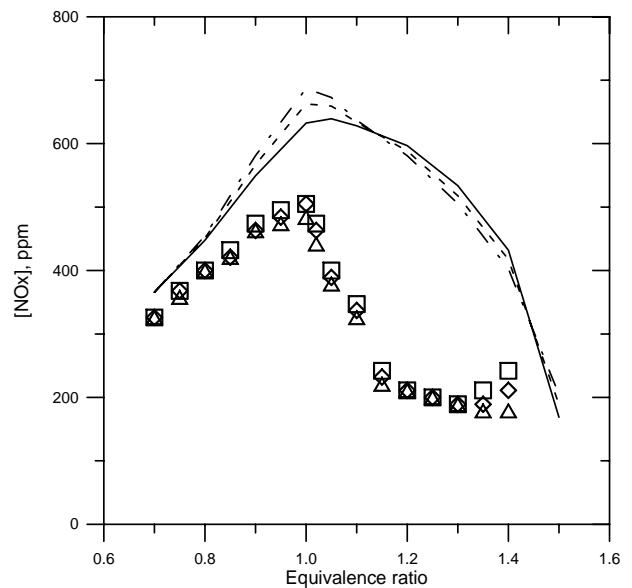


Figure 3. Concentrations of NO_x in $(\text{CH}_4+\text{NH}_3) + \text{O}_2 + \text{N}_2$ flames at different distances from the burner. Dilution ratio $D = 0.209$. Points: measurements, lines: calculations. Solid line and triangles: $[\text{NO}_x]$ at 10 mm from the burner; dashed line and diamonds: $[\text{NO}_x]$ at 15 mm; dash-dot line and squares: $[\text{NO}_x]$ at 20 mm.

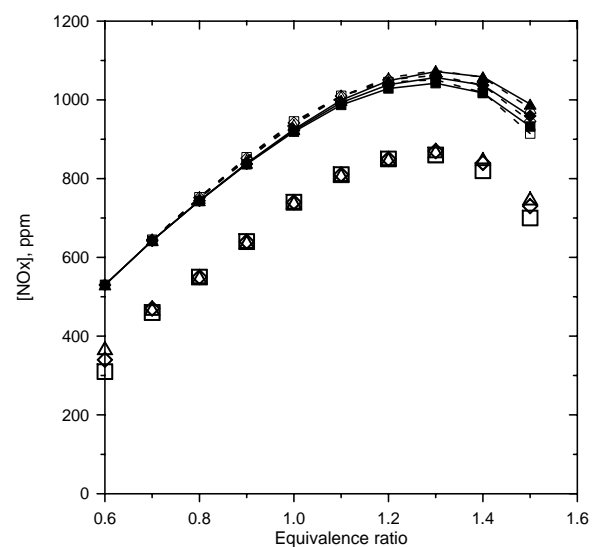


Figure 4. Concentrations of NO_x in $(\text{CH}_4+\text{NH}_3) + \text{O}_2 + \text{CO}_2$ flames at different distances from the burner. Dilution ratio $D = 0.35$. Measurements: open symbols; adiabatic flame modeling: solid symbols and solid lines. Modeling with downstream heat losses: open symbols and dashed line. Triangles: $[\text{NO}_x]$ at 10 mm from the burner; diamonds: $[\text{NO}_x]$ at 15 mm; squares: $[\text{NO}_x]$ at 20 mm.

This comparison and analysis shows that ambient air can dilute the post-flame gases, especially in very lean or very rich mixtures. This is indicated by small decrease of the $[\text{CO}_2]$ in the very lean mixture with equivalence ratio 0.7 and small decrease of the $[\text{CO}]$ in the very rich mixture with equivalence ratio 1.4 for the

flames with dilution ratio 0.209 (Fig. 2). This effect becomes more pronounced with decrease of the dilution ratio of oxygen. The flames having dilution ratio 0.16 were weak, the dilution by the ambient air was observed in the whole range of equivalence ratios.

Concentrations of NO_x in (CH₄+NH₃) + O₂ + N₂ flames with dilution ratio D = 0.209 at different distances from the burner are shown in Fig. 3. Also shown are NO concentrations calculated in free propagating adiabatic flames. The modeling is in satisfactory agreement with the experiments in lean flames, while in rich flames it is not. It is also notable that in (CH₄+NH₃) + O₂ + N₂ mixtures the plot of the concentrations of NO_x in the post-flame zone as a function of the stoichiometric ratio differs qualitatively from that in (CH₄+NH₃) + O₂ + CO₂ mixtures. Concentrations of NO_x in (CH₄+NH₃) + O₂ + CO₂ flames with dilution ratio D = 0.35 [7] are shown in Fig. 4 for comparison. In (CH₄+NH₃) + O₂ + CO₂ mixtures the modeling over-predicts the measured concentrations of NO_x however the experimental trends were well reproduced.

Significant qualitative discrepancy between experiments and modeling in rich (CH₄+NH₃) + O₂ + N₂ mixtures was an unexpected result of the present study. One can assume that conversion of ammonia into NO and formation of NO from atmospheric nitrogen are independent processes as soon as the structure of the flame (concentrations of the major species and radicals) is not affected by the admixture of ammonia. In fact in the study of (CH₄+NH₃) + O₂ + CO₂ flames carbon dioxide was used as an inert diluent to avoid NO_x formation from atmospheric nitrogen. It was expected that in (CH₄+NH₃) + O₂ + N₂ flames additional NO could be formed from atmospheric nitrogen in the quantities comparable with those observed in CH₄ + O₂ + N₂ flames [2, 6]. Absence of any cumulative effect calls for detailed analysis of the experimental and modeling uncertainties.

Influence of the air entrainment on the measured concentrations was discussed above; it is also observed in Fig. 3 in very rich mixtures with equivalence ratio 1.35 - 1.4. It was therefore concluded that the flames with dilution ratio 0.209 are not affected by the ambient air within equivalence ratio range from 0.8 to 1.3. Probe sampling errors and possibility of conversion of NO inside the probe were discussed elsewhere [5]. Although the possibility of NO reduction in the probe cannot be ruled out completely, one should note that sampling procedure in (CH₄+NH₃) + O₂ + CO₂ flames and in (CH₄+NH₃) + O₂ + N₂ flames was exactly the same. Additional errors could be caused by the uncertainties in the initial NH₃ content in the fuel (\pm 10%). Also the calibrating gas mixture of 100 ppm NO in nitrogen for the gas analyzer had a stated accuracy 5 %, and the gas analyzer itself had a precision of \pm 0.5 % of the full scale (1000 ppm for the cases studied). On the other hand, these potential uncertainties could be only of systematic nature over the range of equivalence ratios, because the same calibrating and fuel mixtures

were used throughout the experiments. Thus the discrepancy between the modeling and experiments in rich (CH₄+NH₃) + O₂ + N₂ flames cannot be attributed to the sampling and calibration procedures.

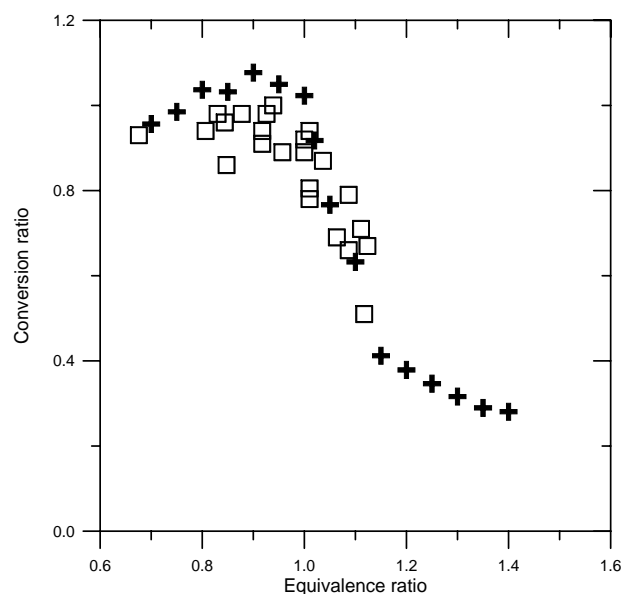


Figure 5. Conversion of NH₃ into NO_x in (CH₄+NH₃) + O₂ + N₂ flames with dilution ratio D = 0.209. Crosses: this work; squares: conversion in similar flames with 1% ammonia in the fuel [14].

Additional evidence of the correctness of experimental procedures is illustrated in Fig. 5. Conversion ratio of NH₃ into NO_x at 10 mm from the burner in (CH₄+NH₃) + O₂ + N₂ flames with dilution ratio D = 0.209 is compared with conversion in similar (CH₄+NH₃) + air flames with 1% ammonia in the fuel [14]. The agreement between two independent experimental studies is very good; it is also consistent with the conclusion of Wendt and Sterling [14] that the fractional conversion of ammonia into NO_x decreases with increasing concentration of NH₃ in the initial gas mixture. Similar observations were reported by Kato et al. [15] and summarized by Glarborg et al. [8].

One can conclude that the measurements of NO in mixtures doped with ammonia are likely correct within experimental uncertainties described above, and that it is the kinetic model which is responsible for the discrepancies discussed. It is well known that predictions of the kinetic model validated within a certain temperature range could be wrong outside this range. Adiabatic temperatures in premixed flames with different inerts were calculated. Although (CH₄+NH₃) + O₂ + CO₂ flames with dilution ratio D = 0.35 are the hottest, the temperature ranges of the flames with carbon dioxide and with nitrogen as diluents overlap.

The flame front stabilized by the Heat Flux method is adiabatic with respect to the burner, however downstream heat losses to the environment may affect predicted concentrations of NO formed in flames as it was demonstrated in methane + air flames [5].

Concentrations of NO_x in CH₄ + air flames at different distances from the burner are shown in Fig. 6. Also shown are NO concentrations calculated in free propagating adiabatic flames and in flame with downstream heat losses. The influence of the heat losses on the calculated [NO] was pronounced at equivalence ratios close to the stoichiometric one, where thermal-NO mechanism is mostly important. In rich flames with equivalence ratio higher than about 1.2 the impact of this phenomenon vanished. Similar modeling was performed in (CH₄+NH₃) + O₂ + CO₂ flames with the oxygen dilution ratio D = 0.35, when the temperature gradient of 100 K/cm associated with the downstream heat losses was applied, Fig 4 [7]. The difference between the predictions of NO concentrations for the adiabatic flames and for the flames with the downstream heat losses was negligible, within 2-3 ppm for the lean and rich mixtures and slightly increased up to 15 - 25 ppm near the stoichiometric equivalence ratio. Therefore one can conclude that in the premixed flames of methane + oxygen + carbon dioxide doped with ammonia the heat losses in the post-flame zone do not remarkably affect the formation of NO_x. Comparison of the experimental results and calculations presented in Figs. 3, 4 and 6 shows that significant discrepancy (over 300 ppm) in rich (CH₄+NH₃) + O₂ + N₂ mixtures cannot be attributed to the uncertainties in the modeling of the thermal-NO due to possible heat losses in these flames.

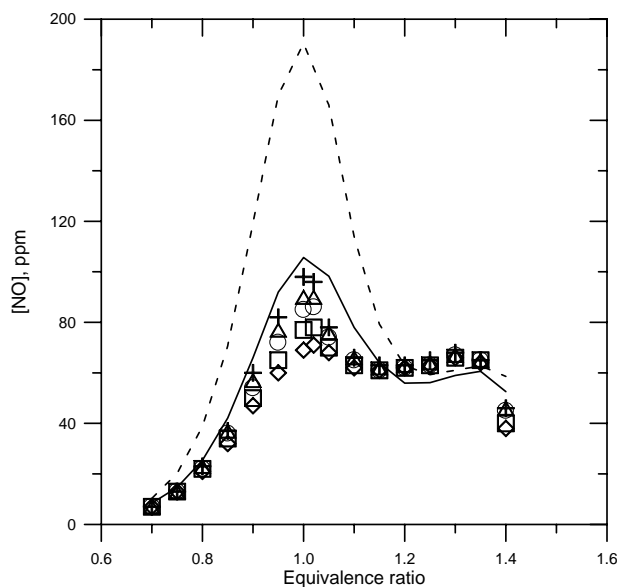


Figure 6. Concentrations of NO in CH₄ + air flames at different distances from the burner [5]. Points: measurements, lines: calculations. Diamonds: 10 mm from the burner; squares: 12 mm; circles: 15 mm; triangles: 17 mm; crosses: 20 mm. Dashed line: [NO] in the adiabatic flame at 20 mm; solid line: [NO] in the flame with downstream heat losses at 20 mm.

Concentrations of NO_x in (CH₄+NH₃) + O₂ + N₂ flames with dilution ratio D = 0.18 and 0.17 at different distances from the burner are shown in Figs. 7 and 8 respectively. Also shown in Figs. 7 and 8 are NO

concentrations calculated in free propagating adiabatic flames. The flames with dilution ratio 0.16 were weak, the dilution by the ambient air was observed in the whole range of equivalence ratios. The concentrations of NO_x in the post-flame zone have a maximum near the stoichiometry. Changes of the dilution ratio from 0.209 down to 0.17 reduced flame front temperature from about 2220 K down to 1980 K. The dilution was accompanied by the decrease of the maximum [NO] from about 500 ppm (Fig. 3) down to 400 ppm (Figs. 7 and 8). The concentration of NO in stoichiometric mixtures, therefore, was quite insensitive to the changes of the dilution ratio and temperature. In rich mixtures, however, these variations led to increase of [NO] from less than 200 ppm (Fig. 3) up to 330 ppm (Fig. 8). Transformation of the plots of the concentrations of NO_x in the post-flame zone as a function of the stoichiometric ratio led to the apparent improvement of agreement between experiments and modeling.

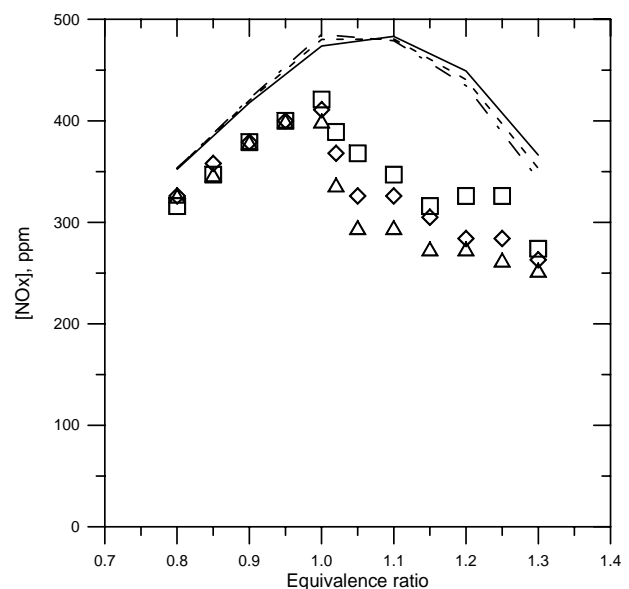


Figure 7. Concentrations of NO_x in (CH₄+NH₃) + O₂ + N₂ flames at different distances from the burner. Dilution ratio D = 0.18. Points: measurements, lines: calculations. Solid line and triangles: [NO_x] at 10 mm from the burner; dashed line and diamonds: [NO_x] at 15 mm; dash-dot line and squares: [NO_x] at 20 mm.

One should note that in (CH₄+NH₃) + O₂ + CO₂ flames the discrepancy between measured and predicted concentrations of NO varied in a different way [7]. For the whole range of equivalence ratios of the flames with oxygen dilution ratios 0.3155 and 0.35 and for equivalence ratios from 1.0 to 1.2 of the flames with oxygen dilution ratio 0.29 these discrepancies were very close (about 150 ppm). The difference significantly increased in the lean (equivalence ratios 0.8, 0.9) and rich (equivalence ratio 1.3) flames with oxygen dilution ratio 0.29 probably due to the dilution by the ambient air. The analysis of the discrepancies between experimental results and calculations performed by Dyakov et al. [7] and extended in the present work

clearly demonstrated that performance of the current version of the Konnov's mechanism (Release 0.5) [1] in rich $(\text{CH}_4+\text{NH}_3) + \text{O}_2 + \text{N}_2$ flames is not satisfactory. In lean flames and also in $(\text{CH}_4+\text{NH}_3) + \text{O}_2 + \text{CO}_2$ flames the discrepancy is above the experimental uncertainty, although qualitative agreement is good. These deficiencies of the kinetic model should be resolved by extended modeling study, which is an objective of the authors.

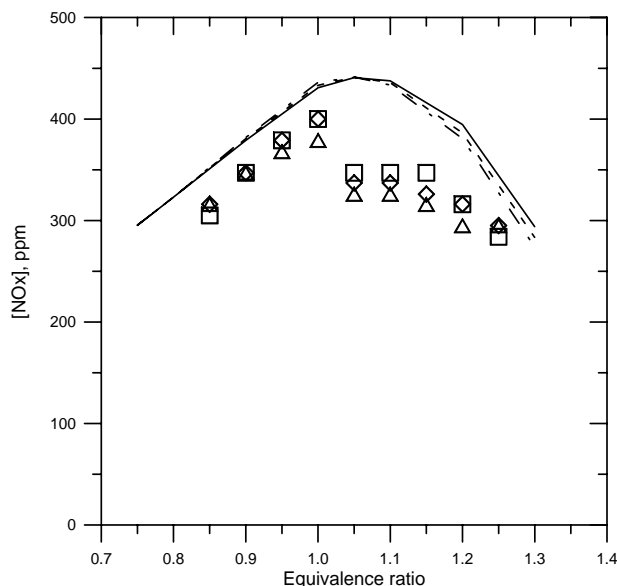


Figure 8. Concentrations of NOx in $(\text{CH}_4+\text{NH}_3) + \text{O}_2 + \text{N}_2$ flames at different distances from the burner. Dilution ratio $D = 0.17$. Points: measurements, lines: calculations. Solid line and triangles: [NOx] at 10 mm from the burner; dashed line and diamonds: [NOx] at 15 mm; dash-dot line and squares: [NOx] at 20 mm.

Conclusions

An experimental study of methane + oxygen + nitrogen flames doped with ammonia (0.5 % of the fuel) has been performed. A Heat Flux method was used to determine flame burning velocities at atmospheric pressure under conditions when the net heat loss of the flame is zero. Adiabatic stabilization facilitates comparison with calculations. Probe sampling measurements of the concentrations of nitric oxide in the post-flame zone are reported. The concentration measurements of major stable species (O_2 , CO , CO_2) and comparison with the modeling were used to reveal the range of flames not affected by the air entrainment. Measured burning velocities for these flames and concentrations of the major species agree well with those of the flames of methane + oxygen + nitrogen within an experimental accuracy. It was concluded that the measurements of NO in mixtures doped with ammonia are likely correct within experimental uncertainties. These measurements were compared to model predictions and to similar experiments in flames of methane + oxygen + carbon dioxide doped with ammonia. In $(\text{CH}_4+\text{NH}_3) + \text{O}_2 + \text{CO}_2$ mixtures the

modeling over-predicts the measured concentrations of NOx however the experimental trends are well reproduced. In $(\text{CH}_4+\text{NH}_3) + \text{O}_2 + \text{N}_2$ mixtures the plots of the concentrations of NOx in the post-flame zone as a function of the stoichiometric ratio differ qualitatively from that in $(\text{CH}_4+\text{NH}_3) + \text{O}_2 + \text{CO}_2$ mixtures. The modeling is in satisfactory agreement with the experiments in lean flames, while in rich flames it is not. It was concluded that it is kinetic model which is responsible for the discrepancies observed.

Acknowledgements

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