Numerical Study of Radiation Reabsorption Effect on NOx Formation in Flames(火炎のNOx生成におけるふく射再吸収の影響に関する数値解析的研究)

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論文内容要旨

Chapter 1. Introduction

In this chapter, the background and the objectives of this study are stated, and the organization of the dissertation is described. Moreover, previous researches related to this study are also reviewed.

The principal oxides of nitrogen, NO, NO_2 and N_2O, abbreviated as NO_x, is one of the main pollutants emitting from combustion. It has been known that NO_x contributes to photochemical smog in the troposphere, participates in a chain reaction that removes ozone from the stratosphere with the consequence of increased ultraviolet radiation reaching the earth's surface. In addition, it affects the human's nervous system, causes anxiety and reduces blood pressure. Therefore, minimization of NO_x production has become a very important topic and target in the field of combustion. To achieve the goal of minimizing NO_x emission, the comprehension of chemical kinetic mechanisms that generate NO_x and understanding of the interaction of chemical kinetic mechanisms, fluid dynamics, mass transfer and heat transfer in combustion processes are needed.

On the other hand, thermal radiation is an important, often dominant, heat transfer mechanism in flames. It is well known that radiative heat transfer leads to a decrease in flame temperature, which may induce large variations of some flame properties such as extinction limits. Moreover, since chemical production of NO_x is very sensitive to temperature, a small temperature decrease can lead to important changes in NO_x formation. Although some studies have been conducted to investigate the influence of radiation heat loss on the extinction limits, the effect of radiation heat loss on NO_x formation has received less attention. To date, there are only several studies in which the influence of radiation heat loss on NO_x formation in flames has been investigated. Nevertheless, the Optically thin model was adopted to evaluate the radiation heat loss and the reabsorption was ignored in almost all the studies. In addition to radiation reabsorption, the spectral characteristics of radiative gas are also not taken into consideration in the simple optically thin model.

Furthermore, exhaust gas recirculation, which has been proved to be an effective measure to suppress NO emission and improve heat transfer in combustion chambers, is an important technique in industrial applications. For the flames with exhaust gas recirculation such as "High-temperature Air Combustion Technology (HiCOT)", the thickness and the optical thickness of flame are increased and radiation reabsorption is enhanced, since CO_2 is the main species in flue gas and is also a major absorbing and emitting species in flames. Until now, however, no numerical study using an accurate non-gray radiation model has been reported concerning the effect of radiation on NO_x formation in flames with exhaust gas recirculation. Therefore, it is necessary to further study the effects of radiation heat transfer on NO_x formation in flames by using more accurate radiation model in which radiation reabsorption is taken into account.

Based on the above considerations, the objectives of this study are to develop a numerical program scheme in which the NO_x formation was calculated by using detailed chemistry and non-gray gas radiation model, and then to use it to systematically investigate the influence of radiation and reabsorption on the NO_x formation process in fundamental CH_4/air and CH_4/air/CO_2 counterflow diffusion and premixed flames and HiCOT flames as well.

Chapter 2. Numerical Models and Computation Methods

In this chapter, a numerical program scheme for simulating NO_x formation in counterflow flames with detailed chemistry and taking the radiation reabsorption into account was developed. The numerical program scheme includes three parts: a part for simulating NO_x formation; a part for calculating the spectral properties of radiative gases and radiative intensities issued from an isothermal and inhomogeneous column containing mixture of H_2O, CO_2, CO and transparent gases; and a part for solving the wavenumber averaged radiative transfer equation and for evaluating the volume radiation heat loss. The governing equations of models and their computational methods were described. The governing equations of combustion model were solved by a combination of the time-dependent method and the steady state method, namely, **damped modified Newton's method**. The statistical narrow-band model is used to calculate the spectral properties of radiative gas, in which the narrow-band width is 25 cm^{-1} and the total numbers of H_2O, CO_2 and CO bands are 367, 96 and 48, respectively. The considered spectral and temperature ranges are respectively 150～9300 cm^{-1} and 300~2900 K. The wavenumber averaged radiative transfer equation was solved by the **discrete ordinate method** and **S_6 quadrature scheme** was used. Finally in this chapter, the effectiveness of the developed numerical scheme was examined. It is found that the flame temperature and the fraction of the major species and NO mole fraction predicted by the developed numerical scheme are in good agreement with experimental results.

Chapter 3. Effects of Radiation Reabsorption on NO Formation in CH_4/Air and CH_4/Air/CO_2 Counterflow Diffusion Flames

In this chapter, the combined effects of radiation reabsorption with stretch rate, amount of CO_2 added to air and pressure on the flame structure and NO formation in CH_4/air and CH_4/air/CO_2 counterflow diffusion flames were numerically investigated and discussed.

Qualitatively, the radiation effects on counterflow CH_4/air and CH_4/air/CO_2 diffusion flame have the same tendency for both the statistical narrow-band model and the optically thin model. Radiation heat loss causes a decrease in flame temperature, flame thickness and production of NO, and causes the NO emission index to appear as a maximum value at a certain stretch rate. The addition of CO_2 to air drastically decreases the NO emission and flame temperature, and significantly enhances the effect of radiation and reabsorption on NO formation. The reduction of NO emission caused by CO_2 consists of three parts: in addition to the thermal and chemical effects, the radiation heat loss from CO_2 causes a further reduction of NO emission, namely, radiation effect.

The radiation and reabsorption effects on NO formation become important as the stretch rate decreases. For CH_4/air flames, the effects of radiation and reabsorption on NO formation are relatively small, except for low stretch rates. However, radiation and reabsorption considerably influence NO formation for CH_4/air/CO_2 counterflow diffusion flames, even at high stretch rates. The reabsorption influence on the NO emission index increases with increasing pressure. A new fact that contrary variation of the NO emission index with pressure was respectively indicated by the calculation with and without consideration of radiation reabsorption was discovered. Therefore, non-reabsorption models such as the optically thin model are unable to correctly predict NO formation in flames with high pressure both qualitatively and quantitatively.

The effects of radiation and reabsorption on the contribution of respective mechanisms (thermal and prompt) to NO_X formation in counterflow diffusion flames were also clarified. Radiation and reabsorption have remarkable effects on thermal NO formation at small stretch rates but almost no effect at large stretch rates. At large stretch rates, the relatively small influences of radiation and reabsorption on total NO formation are through the prompt mechanism. A wrong conclusion might be reached by using the adiabatic flame model to analyze and identify the role of the respective mechanisms in NO formation.

Chapter 4. Effects of Radiation Reabsorption on NO_x Formation in CH_4/Air and CH_4/Air/CO_2 Counterflow Premixed Flames

In this chapter, the effects of radiation and reabsorption combined with equivalence ratio, stretch rate and amount of CO_2 added to air on the flame structure and NO_x formation in CH_4/air and CH_4/air/CO_2 counterflow premixed flames were numerically investigated and discussed, with special emphasis on premixed lean flames. In premixed flames, the radiation and reabsorption has more obvious effects on flame thickness than that in diffusion flames. Different from diffusion flames in which radiation and reabsorption have only large effects on NO formation, radiation and reabsorption have more significant influences not only on NO but also on N_2O production in premixed flames. For CH_4/air/CO_2 premixed flames, radiation and reabsorption also has an obvious influence on the NO_x emission at the stretch rate extinction side in addition of the effects at low stretch rate. The ranges of equivalence ratio at which the radiation and reabsorption effects on NO_x formation are important, and the influence of radiation and reabsorption on flame extinction limit resulted from CO_2 addition are obtained. Furthermore, the validity of the optically thin model for predicting the nitric oxide formation in counterflow premixed flames is examined.

Chapter 5. Effects of Radiation Reabsorption on NO Emission from CH_4/High-temperature Air Counterflow Diffusion Flames

In this chapter, the effects of radiation and reabsorption on NO emission from "High-temperature Air Combustion Technology (HiCOT)" were numerically investigated by using counterflow diffusion flames. A mixture of N_2 and CO_2 was used to model the exhaust gas. The effects of radiation and reabsorption on NO emission with varying some flame characteristics such as preheated temperature of oxidizer, stretch rate of flame, CO_2 and the O_2 concentrations in oxidizer and the exhaust gas recirculation rate as well were clarified. The effects of radiation and reabsorption on NO emission from high temperature counterflow diffusion flames become significant and important as the temperature of the oxidizer increases and the flame stretch rate decreases. The increase of CO_2 concentration and decrease of O_2 concentration in gas mixture caused by exhaust gas recirculation further enhance these effects. This means that the reabsorption effect should be considered in actual HiCOT generally operated under conditions of low oxygen concentration resulting from exhaust gas recirculation.

It is firstly clarified that radiation and reabsorption play a very important role in creation of the uniform temperature distribution in HiCOT. The mechanism of radiation and reabsorption is distinctly different between the flames with low oxidizer temperature and those with very highly preheated oxidizer temperature. The absorption zone on the fuel side and the emitting zone on the high temperature oxidizer side that both increase with increasing oxidizer temperature and exhaust gas recirculation contribute to spreading the reaction region and flatting the temperature distribution. Although NO emission greatly increases with increasing preheated temperature of oxidizer, it is numerically demonstrated that low NO emission can be indeed achieved in HiCOT from the results obtained in this study.

Chapter 6. Summary and Conclusions

In this chapter, the main conclusions obtained through this study were summarized.

論文審査結果の要旨

ふく射は火炎の伝熱における重要な因子の一つであり、NO_x生成メカニズムなどの燃焼過程に大きな影響を与える。火炎中のCO_2やH_2Oなどのふく射およびふく射再吸収は強いバンド特性を持ち、火炎のふく射を正確に求めるためには、バンドふく射特性を考慮した非灰色ふく射モデルが必要である。本論文は、非灰色狭域ふく射モデルと詳細反応機構を用いて、NO_x生成と火炎構造に対するふく射再吸収の影響に関する数値解析的研究結果をまとめたもので、全編6章よりなる。

第1章は序論であり、本研究の背景と目的について述べている。

第2章では、詳細反応機構を用いて、ガスふく射のバンド特性と再吸収を考慮した火炎のNO_x生成解析コードを開発している。その数学モデル及び数値解析法について詳述している。これは火炎のNO_x生成に関する研究に大きな進展を与える。

第3章では、CH_4/Air とCH_4/Air/CO_2対向流拡散火炎の解析を行って、NO_x生成メカニズム及び火炎構造に対する、ふく射再吸収、伸長率、CO_2添加率、圧力などの複合効果を明らかにしている。その中で、非灰色ガスふく射モデルで解析したNO_x生成に対する圧力の効果が、従来とは全く異なった傾向を持つことをはじめて明らかにしている。これらは新しい知見であり、重要な成果である。

第4章では、CH_4/Air とCH_4/Air/CO_2対向流予混合火炎の解析を行って、ふく射並びにふく射再吸収のNO_x生成と火炎構造に及ぼす影響を明らかにしている。拡散火炎と異なって、ふく射とふく射再吸収はNO生成にだけではなくN_2O生成にも大きな影響を与えている。これらは予混合燃焼におけるNO_x生成を低減する上で実用的に極めて重要な知見である。

第5章では、高温空気燃焼技術におけるNO_x生成の解析を行っている。酸化剤予熱温度、排ガス再循環率、火炎伸長率及び酸化剤中のCO_2とO_2の濃度などのパラメータを変化させ、高温空気の使用にもかかわらず、NO_xの低減が実現できることを理論的に明らかにしている。これらは高温空気燃焼技術の研究を進展させる上で重要な結果と知見である。

第6章は結論である。

以上要するに本論文は、ガスふく射のバンド特性と再吸収を考慮した火炎のNO_x生成解析コードを開発し、拡散火炎、予混合火炎、高温空気燃焼の場合を解析し、ふく射とふく射再吸収がNO_x生成と火炎構造に及ぼす影響を明らかにしたもので、航空宇宙工学及び燃焼工学の発展に寄与するところが少なくない。

よって、本論文は博士（工学）の学位論文として合格と認める。