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Observation, analysis and modelling in complex fluid media

Significance of DNS in combustion science

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Abstract

The recent advancement in numerical calculations provides us with a new scientific approach to combustion phenomena, that is, numerical experiment. The authors have succeeded in capturing a hydrogen jet lifted flame by DNS (Direct Numerical Simulation) approach with detailed chemistry and exact transport properties. The simulation made clear that the flame is not a single flame, but a complex flame composed of three flame elements. Some aspects of the flame elements showed the properties of laminar flames and some showed very complicated and unsteady nature of turbulent flames that cannot be described by the conventional laminar flame theory. In this article, the problems of this kind of study are identified and the direction of study is suggested throughout the DNS studies on the hydrogen jet lifted flame. ***To cite this article: T. Takeno, Y. Mizobuchi, C. R. Mecanique 334 (2006).***

Résumé

Signification des DNS en combustion. Les avancées récentes dans le domaine des calculs numériques nous procurent un nouvel outil scientifique pour appréhender les problèmes liés à la combustion, à savoir l'expérimentation numérique. Les auteurs ont réussi à produire par DNS (Simulations Numériques Directes) une flamme de jet d'hydrogène décollée du brûleur, en incluant des schémas détaillés de chimie et des propriétés exactes pour le transport. Ces simulations ont démontré clairement que la flamme n'est pas une flamme unique, mais une flamme complexe composée de trois éléments de flamme. Quelques aspects de ces éléments de flamme ont montré des propriétés comparables à celles des flammes laminaires, alors que d'autres se sont révélés comparables à la nature complexe et instationnaire des flammes turbulentes, qui ne peuvent pas être décrites par la théorie classique des flammes laminaires. Dans cet article, les problèmes rencontrés lors de telles études ont été identifiés et les directions à suivre pour de telles études sont suggérées, au travers d'études par DNS de flammes de jet d'hydrogène décollées du brûleur. ***Pour citer cet article : T. Takeno, Y. Mizobuchi, C. R. Mecanique 334 (2006).***

Keywords: Combustion; DNS; Hydrogen jet lifted flame

Mots-clés : Combustion ; Simulations Numériques Directes ; Flamme de jet d'hydrogène décollée du brûleur

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1. Introduction

The recent advancement in numerical calculations is remarkable, and this advancement will have a profound impact on combustion science. It has generated a new scientific approach of numerical experiment, which has been proved so successful in understanding the physics and chemistry of complicated combustion phenomena. Now 3D DNS of real size flames with detailed chemistry and exact transport properties is coming possible. Some pioneering studies in this direction have shown that there is a novel field of combustion research [1,2]. In this article, we try to identify the problems to be made clear and suggest the possible direction of this kind of large scale DNS calculation.

2. New findings

In our studies, a hydrogen jet lifted flame has been successfully simulated, with detailed chemistry and exact transport properties. The space and time resolution is fine enough to reproduce the turbulent combustion. The overview of the simulated flame is presented in Fig. 1. The studies have made clear that the lifted flame is not a single flame, but is a complex flame composed of a leading edge ring flame, many small diffusion flame islands and of a vigorous rich premixed turbulent flame as shown in Fig. 2. On the one hand, they have revealed interesting properties of laminar flames, and on the other, they also have demonstrated the very complicated nature of turbulent flame structures. The former findings include time-dependent 3D structures of partially premixed flames, as well as of conventional premixed and diffusion flames. The latter findings should be very useful to construct successful LES subgrid scale

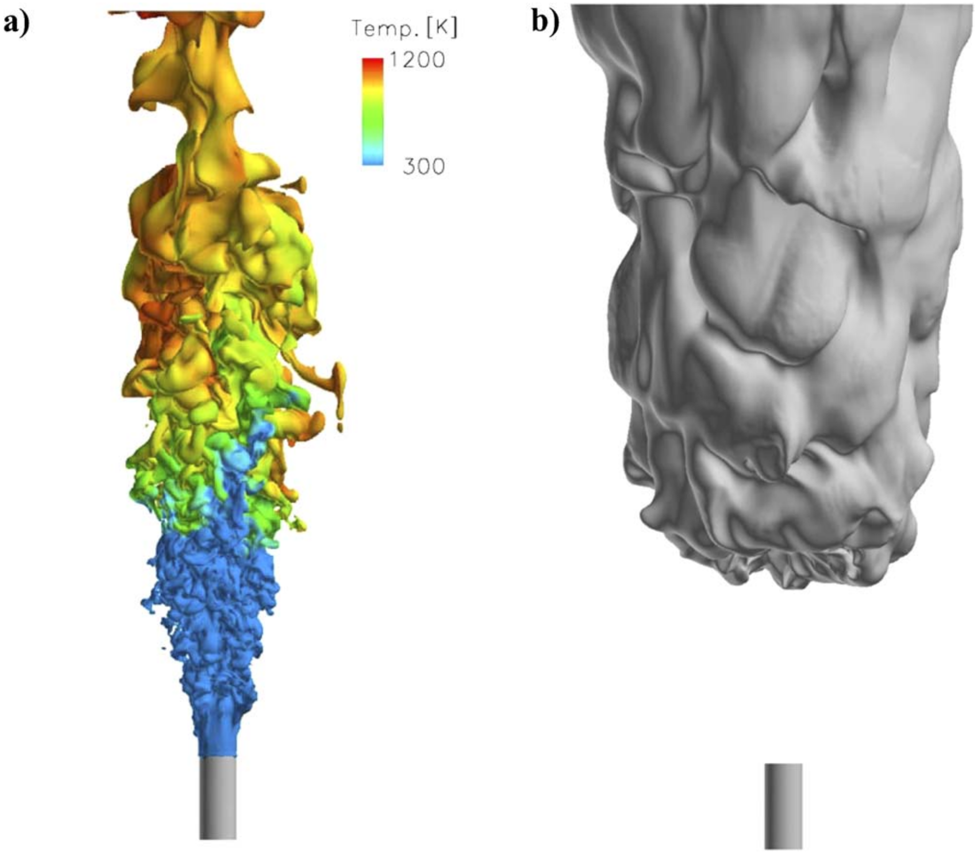

Fig. 1. Overview of the simulated hydrogen jet lifted flame, (a) instantaneous iso-surface of hydrogen mole fraction at 70% with temperature distribution, (b) instantaneous iso-surface of temperature at 1000 K.

Fig. 1. Vue globale d'une flamme de jet d'hydrogène obtenue par simulation numérique, (a) iso-surface instantanée de la fraction molaire d'hydrogène à 70% avec la distribution de température, (b) iso-surface instantanée de la température à 1000 K.

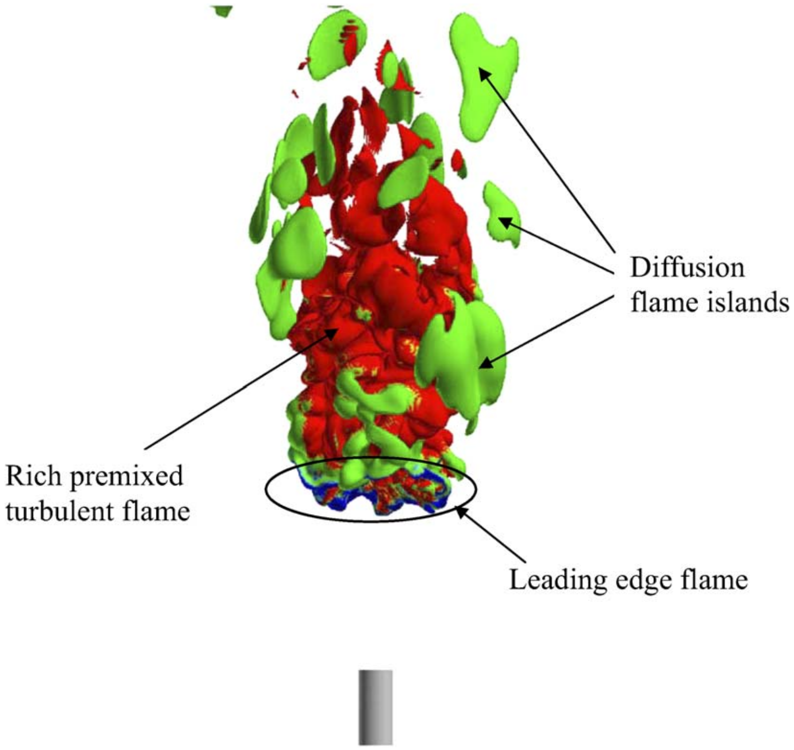

Fig. 2. Global structure of simulated lifted flame. Instantaneous iso-surfaces of hydrogen consumption rate at 10^4 $\mathrm{mol/s/m^3}$ are shown, with combustion modes, red: rich premixed, blue: lean premixed, green: diffusive. The flame is composed of a leading edge flame, diffusion flame islands and a rich premixed turbulent flame.

Fig. 2. Structure globale de la flamme simulée. Iso-surfaces instantanées du taux de consommation d'hydrogène à 10^4 $\mathrm{mol/s/m^3}$, et modes de combustion, rouge : prémélangée riche, bleu : prémélangée pauvre, vert : diffusive. La flamme est composée d'une flamme de bord d'entrée, d'ilôts de flamme de diffusion et d'une flamme turbulente prémélangée riche.

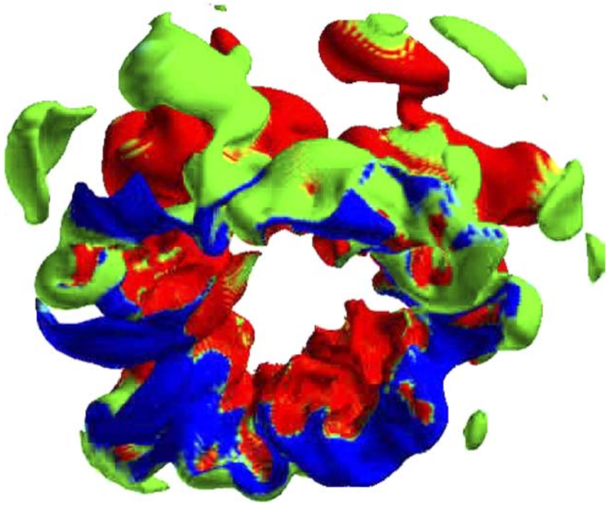

Fig. 3. Leading edge flame, the instantaneous view from below. The leading edge flame is composed of a diffusion flame (green) in the center and a lean premixed flame (blue) and a rich premixed flame (red) on both sides.

Fig. 3. Flamme de bord d'entrée, vue instantanée par dessous. Cette flamme est composée d'une flamme de diffusion (vert) dans le centre, d'une flamme de prémélange pauvre (bleu) et d'une flamme de prémélange riche (rouge) de chaque côté.

models. We have to develop new methodologies to understand the observed flame behavior. In the beginning, some examples of these findings will be explained briefly.

3. Subjects to be investigated

3.1. *Time-dependent complex laminar flame behavior*

The leading edge flame of ring shape, itself, is a complex flame composed of a number of triple flames. The respective triple flame is composed of a diffusion flame in the center and a lean premixed flame, and a rich premixed flame on both sides. These triple flames are connected together to form a single overall flame of ring shape as observed in Fig. 3. Each triple flame is always moving and rotating, yet they keep remaining in a single ring flame. In addition, the overall ring shape flame remains at a fixed position downstream of the jet exit. We have to understand why the leading edge flame has so complicated complex structure, in the beginning. We then try to understand why the respective triple flame is moving, and how the overall ring flame can stabilize at the fixed location.

3.2. *Behavior of flame islands*

At first, we thought that the diffusion flame island is a kind of flame, such as a flame ball [3], in which chemical reactions are balanced by the molecular diffusion. However, in the following study, we have now found that the fuel consumption rate in the islands near the leading edge flame (some are observed in Fig. 3) is too small and they do not have any definite organized structure, to be called a kind of flame. Some of the burning fuel in the triple flame is thrown out of the flame into the hot burnt gas stream, in the course of the interaction between the triple flame and the incoming unburnt fuel volume. The latter volume is produced in the fuel jet shear layer, upstream of the flame and is convected downstream. This process is discussed in our previous paper [2]. The combustion process of the island may not be interesting scientifically, but in the actual, premixed or diffusion, turbulent flames, the local flame extinction may often happen [4] to produce this kind of combustion and it should be useful to understand the process. We have

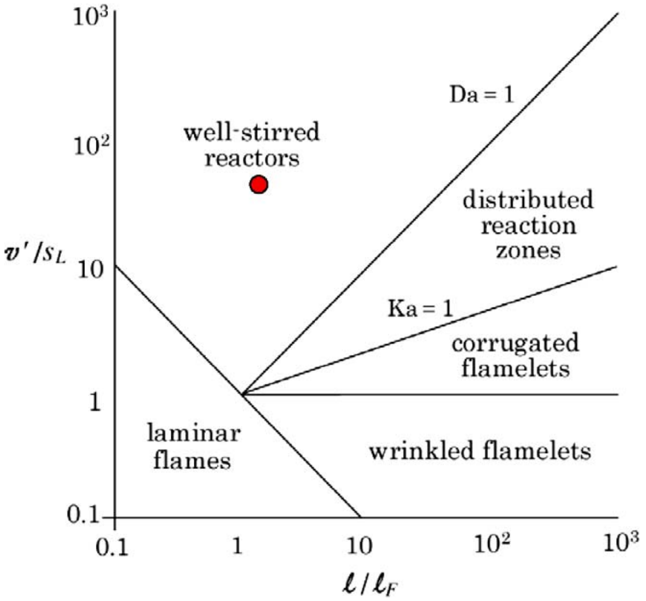

Fig. 4. Location of turbulent premixed flame in Borghi's diagram. The turbulence scale is estimated by the statistical post-processing of the simulated data as $v'/S_L = 33$, the flame scale is estimated by 1D simulation of a plane premixed flame of equivalence ratio 4.0 as $l/l_F = 2$.

Fig. 4. Positionnement de la flamme turbulente de prémélange dans le diagramme de Borghi. L'échelle de la turbulence est estimée par post-traitement statistique des données de la simulation numérique, ce qui donne $v'/S_L = 33$. L'échelle de la flamme est estimée par une simulation 1D d'une flamme de prémélange de rapport d'équivalence égal à 4, ce qui donne $l/l_F = 2$.

to understand if the chemical reactions proceeding in the island are identical with those of the normal flame. Further more, it should be important to clarify the criterion by which this burning fuel may reignite to produce the flame [4].

3.3. Turbulent premixed flame structure

The data analysis of turbulence characteristics has shown that the inner turbulent premixed flame is located in the well-stirred reactors regime in Borghi's diagram as plotted in Fig. 4. The analysis has been carried out about the point arrowed in Fig. 5, where the turbulence scale has been estimated by the statistical post-processing of the data and the flame scale is estimated by 1D simulation of a plane premixed flame of the corresponding equivalence ratio. On the other hand, the Flame Index ($\equiv \nabla Y_{H_2} \cdot \nabla Y_{O_2}$) analysis [4] of the hydrogen consumption region of the flame has shown rather large value of Normalized Flame Index [1] at the upstream edge as shown in Fig. 5(a), indicating a considerable amount of combustible mixture is supplied to the reaction zone by the molecular diffusion. Here, Normalized Flame Index of premixed flame has been normalized by Flame Index of the 1D plane premixed flame of equivalent mixture

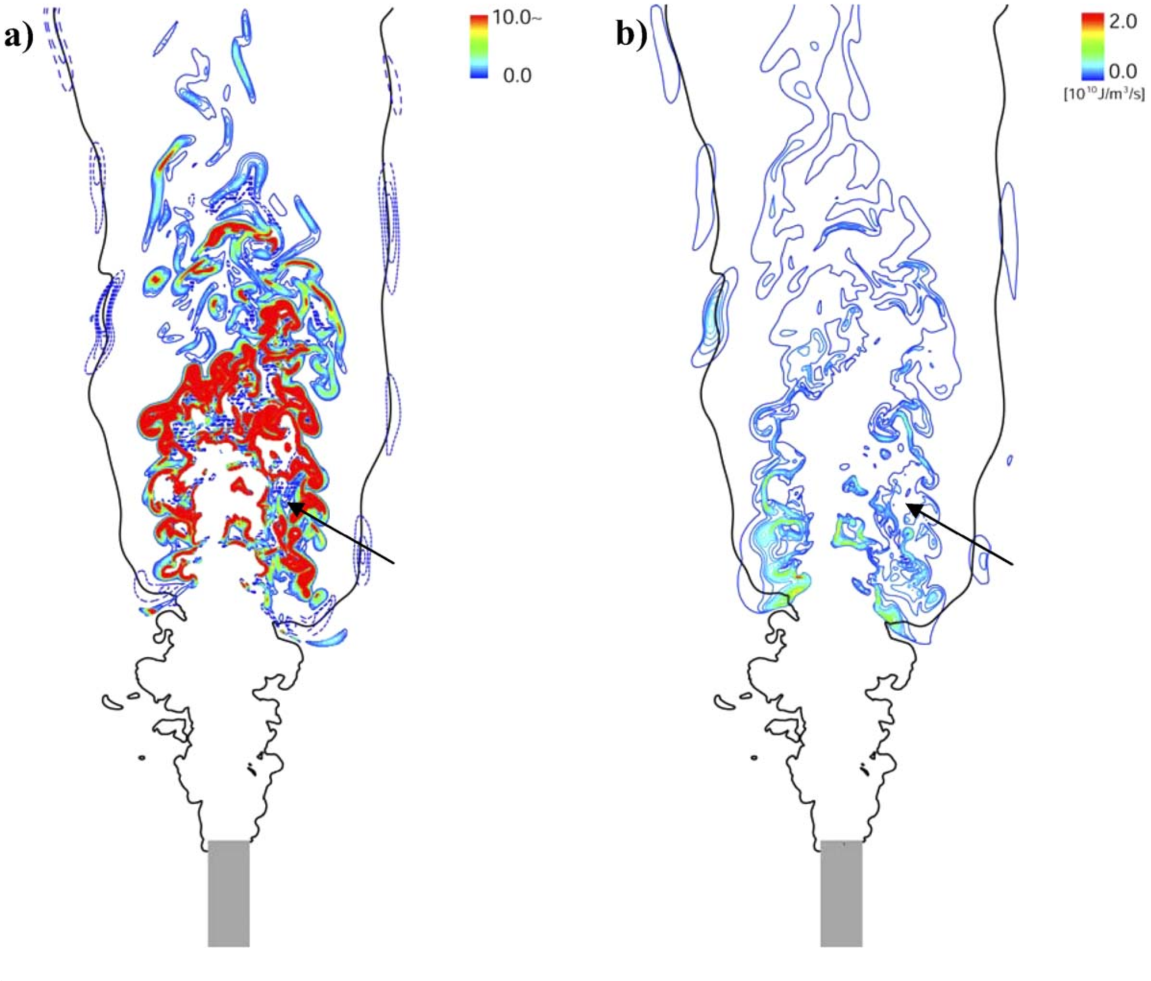

Fig. 5. Combustible mixture supply to the flame and reaction zone. (a) Normalized Flame Index (NFI) distribution in a cutting plane. The iso-lines of NFI of premixed flame is drawn with rigid lines from 0.5 to 10 with a step of 0.5 (region of NFI > 10 is painted red), and diffusion flame by dashed lines from −0.001 to −0.005 with a step of 0.001. (b) Heat release rate distribution. In both figures, the rigid black lines are stoichiometric lines.

Fig. 5. Alimentation de la flamme et de la zone de réaction en mélange combustible. (a) Index de Flamme Normalisé (IFN) dans un plan. Les lignes d'iso-niveaux de l'IFN pour la flamme de prémélange sont tracées en lignes continues de 0,5 à 10, par pas de 0,5 (les régions avec un IFN > 10 sont en rouge), et, pour la flamme de diffusion, elles sont en lignes pointillées, de −0,001 à −0,005 avec un pas de 0,001. (b) Taux de dégagement de chaleur. Pour ces deux figures, les lignes noires continues sont les lignes stochiométriques.

fraction. The possible explanation of this apparent contradiction is that the turbulent flame has a double structure; a rather thin upstream edge governed by the molecular diffusion and a thick reaction zone. In the upstream molecular diffusion layer, the convection by 3D turbulent flow is balanced by the molecular diffusion, and in the downstream reaction zone the chemical reactions are balanced by 3D turbulent flow convection. However, more detailed analysis of the obtained numerical data must be required to make clear this structure.

4. Some concluding remarks

DNS is a very useful means to understand the physics and chemistry of complicated combustion phenomena. However, we have to develop a novel methodology to bring its potential into full play.

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