Jahresbericht 2004, 09. Dezember 2005

Projekt

Optimierung der Brennstoffstufung im ALSTOM EV-Brenner

Schadstoffreduktion durch Teilvormischung

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BFE Projekt-/Vertrag-Nummer	47735 / 87855
Dauer des Projekts (von – bis)	6 Januar 2003 – 30 Juni 2006

ZUSAMMENFASSUNG

Verbrennungssysteme der neuesten Generation mit tiefen Emissionswerten und hoher Brennstoffnutzung werden durch ein kombiniertes Konzept von den zwei Hauptverbrennungskategorien (Diffusion- und Vorgemischte Verbrennung) realisiert, welches teilvorgemischte Verbrennung genannt wird.

Die heute gängigen Verbrennungsmodelle sind hingegen nicht in der Lage, diesen Grenzbereich Diffusion/Teilvorgemischte Verbrennung sinnvoll abzubilden.

Am LTNT wurde ein instationäres Flamelet Modell entwickelt, welches gemäss bisherigen Untersuchungen ein grosses Potential besitzt, diese Verbrennung zu modellieren.

Ziel dieses Projektes ist die Weiterentwicklung des vorhandenen instationären Flamelet-Modells um diesen interessanten Bereich zwischen diffusions- und teilvorgemischter Verbrennung besser zu simulieren.

Während des zweitens Jahres dieses Projekts wurde einen neuen Ansatz entwickelt um die transiente Zeitkonstante des Models besser zu definieren. Die resultierende neue numerische Methode heisst „Flame Age Model“ (FEM). Diese neue Modellvariante wurde in dem ersten Teil dieses Jahres weiter verbessert und gegen die experimentellen Daten von einer hochturbulenten Flamme geprüft. Die Resultate von dieser Arbeit wurden in einer internationalen Konferenz präsentiert.

Die Kollaboration mit der privaten Firma *ALSTOM* wurde hervorgehobt und zwischen Mai und Oktober habe ich ein Praktikum in dieser privaten Firma absolviert. Während dieser Arbeitserfahrung, wurde das neue FAM verwendet um die Flamme des neuen *ALSTOM* Brenners zu berechnen. Die Simulationsresultate haben gezeigt dass, der neue FAM eine grosse Elastizität beweist. Das neue Modell kann, neben Diffusionsflammen, auch teilvorgemischte und gemischte Verbrennungsprozesse vernünftig simulieren.

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Goals of the project

General aims of the project

Pollutant Emissions are still a dominating subject of the worldwide energy supply based on fossil fuels. The cheapest way to prevent the production of pollutants is to avoid them in the combustion process itself.

Turbulent combustion can be classified into two main categories: non-premixed combustion (or diffusion combustion) and premixed combustion. Premixed combustion is a concept for the reduction of nitrogen oxides, but it leaves a safety problem because a flammable mixture is present where no combustion is supposed to take place.

The newest generation of combustion systems, with low pollutant emission and high efficiency, are realized trough a combination of the mentioned two combustion categories; which is called partially premixed combustion.

Today simulation of combustion systems is a powerful tool to achieve burner optimization and in comparison with the pure experimental method it turns out cheaper. This fact is particularly true for high pressure burners.

The combustion models in use nowadays are not able to represent correctly this type of combustion (area between diffusion- and partially premixed combustion). At LTNT we have developed a transient flamelet model which, according to the last investigation, has got a great potential to model this new combustion area.

The Goal of this PhD thesis is to improve the transient laminar flamelet model (TLFM) developed by J. Ferreira [1] in order to simulate better this very interesting area between diffusion- and partially premixed combustion. The improved Flamelet-Model should be validated with experimental data taken from the literature and later should be used to simulate and optimize the new *ALSTOM* burner.

Goals for the year 2005

During the first two years of this project I focused my attention on the improvement of our transient laminar flamelet model. The characteristics of the numerical approach have been analyzed in depth and new ideas have been implemented. From these studies a complete new model for the turbulent residence time has been developed. For this year almost concluded, instead, the goals fixed up were:

- Improvement and validation of the new Flame Age Model (FAM) against the experimental data of the piloted Sandia jet flames (D, E, and F).
- Internship at *ALSTOM*.
- Analysis of the behavior of the slow chemicals reactions involved in the combustion process (CO and CO_2 chemistry) and development of an adequate model for those phenomenons.

Work and Results

In this section I summarize the work done during this year and show briefly the achieved results.

Introduction

Flamelet models are per definition designed for diffusion flames at high Damköhler numbers, where the reaction zone consists of a thin flame sheet. The basic idea of these models is to assume that a small instantaneous diffusion flame element embedded in a turbulent flow has the structure of a laminar counter flow flame. This laminar flame structure is also called flamelet. The structure of the laminar flamelets (temperature and species distribution) may be computed independently of the turbulent code and stored in “flamelet libraries”.

In the Transient Laminar Flamelet Model (TLFM) developed by Ferreira [1] the different flamelets are correlated with the turbulent flow by four parameters: the mixture fraction (Z), the scalar dissipation rate (χ), the reaction progress variable (c) and the turbulent time (τ). These four parameters together with transient flamelet libraries give also the possibility to simulate the unsteady extinction and re-ignition phenomenon in a diffusion flame. The transient flamelet libraries in the TLFM are generated using detailed chemistry and a one dimensional laminar code named *FLATRA* [2], which computes the exact transient state solution of the species concentration and the temperature.

In Fig. 1 we can see a flow-chart representation of the Ferreira-TLFM.

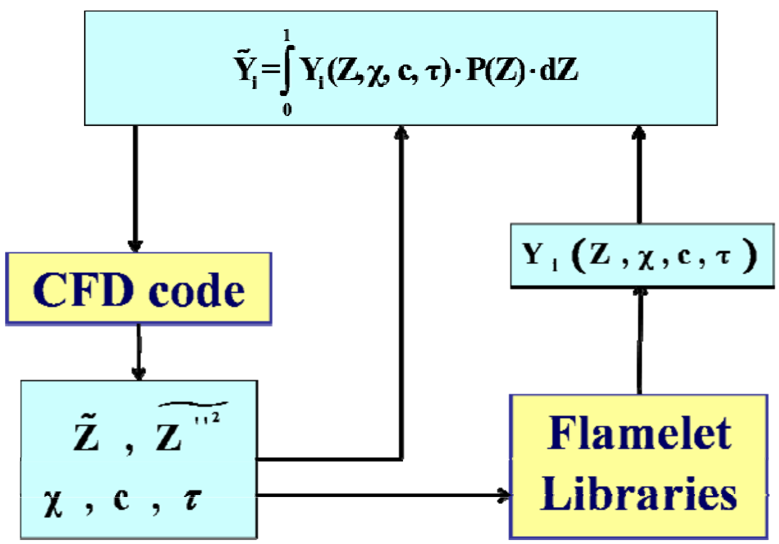

Fig. 1: flow-chart representation of the Ferreira-TLFM

For more detailed information about flamelet models and the Ferreira-TLFM refer to [1, 3, 4].

In the two years after the beginning of this project several improvements have been implemented on the TLFM of Ferreira. These activities are documented in last two “Jahresberichte” of this project [5, 6].

Besides these refinements and readjustments on the TLFM, together with my supervisor, Dr. J. Gass, we have developed a new transient laminar flamelet approach: the so called Flame Age Model (FAM). In this new numerical model the time evolvement in the turbulent flow field is modelled in a proper way and the reaction progress variable is no more needed as a linking parameter. In this way the new FAM appears less complex but more physical consistent then the previous TLFM.

During this last year I've refined and validated the new FAM. After this validation the new method was applied to simulate the behaviour of the new *ALSTOM* gas turbine burner. In the next subchapters a more detailed description of the activates undertook this year can be found.

New Coupling Strategy

The numerical procedure to compute turbulent diffusion and partially premixed flames with both our transient laminar flamelets model is split in two parts. As shown in Fig. 1, the local laminar flame structure is computed and stored with an in-house build *FORTRAN* code. The conservation equations of the turbulent flow field are instead computed with a commercial flow solver (in our case *CFX-5* [7]). The two scales of the combustion problem are then linked together with some additional coupling *FORTRAN* routines, which build the Beta-PDF and compute the mean species mass fraction quantities in the turbulent flow field.

Last year, together with my colleague S. Baykal, we had adjusted the different coupling subroutines and the simulation setup in order to be able to use correctly the *CFX-5* commercial flow solver together with our combustion model. In doing this we have immediately noticed that during a complete simulation of a turbulent flame the most time-consuming numerical steps were the calculation of the presumed distribution functions (PDFs) and the solution of the integral to compute the mean combustion variables. These two steps in the original codes were performed during every iteration of the flow solver, consuming a dramatic amount of computational resources. Simulations with numerical grids containing more then 1 Mio grid points turned out to be prohibitive and a new coupling strategy was needed.

So, with the help of my colleague S. Baykal, we have reorganized all the coupling routines and used another procedure to interpolate the flamelet structures during a simulation of turbulent flame. Instead of computing the Beta-PDF during every iteration we have decided to calculate the PDFs before the numerical procedure to compute the Navier-Stokes equations. After the flamelet generation, the flamelet profiles are convoluted with the assumed-shape PDFs as in Fig. 1, and then tabulated in look-up tables in the memory of the commercial flow solver. Therefore with this method the PDFs are computed only once and during the iterations of the flow solver only “small” interpolation steps are needed. A similar numerical strategy is also implemented in the commercial code *FLUENT* [8].

Refinements and Validation of the Flame Age Model

As already mentioned above, the new FAM was developed from the previous Ferreira's TLFM. The two models differ from each other in the way they simulate the transient effects of turbulent flames. The FAM uses only one time variable to describe these phenomenons. This linking parameter, the flame age time (τ), is not modelled using variables of the turbulent empiric κ-ε model. The time evolvement in the turbulent flow field, instead, in the FAM is simulated with the help of an additional transport equation:

$$\frac{\partial(\tau\cdot\rho)}{\partial t}+\nabla\bullet\left(\vec{v}\cdot\rho\cdot\tau\right)-\left(\frac{\mu_t}{Sc_t}\nabla\tau\right)=S_\tau \qquad (1)$$

The first two terms on the left hand side correspond to the Eulerian derivative (D/Dt), the third term instead represents the effect of the turbulent diffusion. The source term of the flame age time is the right hand term of equation (1). The way to capture correctly the unsteady effects and the ignition point of a turbulent flame consists exactly in modelling well this source term. The version of the FAM developed this spring assumes the fallowing relationship to model the flame age source term:

$$S_\tau = \rho\left[1-\left(\frac{\chi}{\chi_{ext}}\right)^n\right] \tag{2}$$

where ρ is the density of the flow, n a dimensionless integer number, χ the scalar dissipation rate and χ_{ext} its extinction limit. S_τ is activated only for positive values. In this way if the local scalar dissipation rate is bigger than its extinction limit the source of the flame age time is equal to zero.

The definitive FAM with its appropriate flamelet libraries was later tested and validated against the Sandia piloted jet Flame D [9]. Fig. 2 shows, for instance, the temperature distributions along the dimensionless axial direction of the jet burner computed with a classical steady state laminar flamelet model (SLFM, dashed line) and the Flame Age Model (FAM, line).

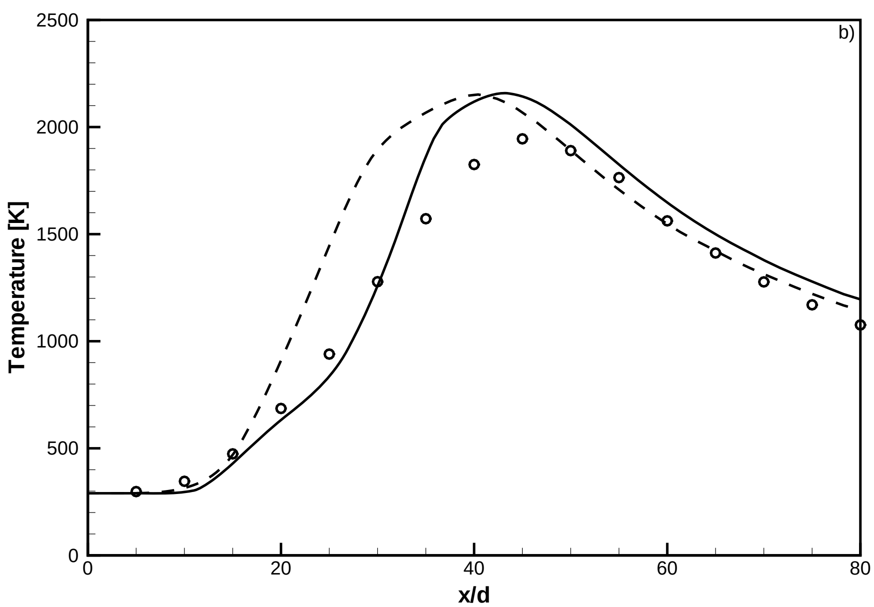

Fig. 2: Axial temperature distribution of the piloted Sandia Jet burner [8]. (Circles: experimental data, line: FAM data, dashed line: SLFM data).

From the graph above one can immediately recognize that the steady state flamelet model is not able to capture the dynamic of the flame in the rich part of the burner and as a consequence the temperatures in this area are always over predicted. The FAM, instead, with the help of its flame age variable is able to mitigate the combustion processes where the integral residence time of the fluid particles is low and therefore simulate better the transient phenomenon. The simulated temperatures with the new model are closer to the measured ones.

The complete results of the validation were presented in the ECCOMAS thematic conference on computational combustion, which was held in Lisbon. The paper presented there [8] contains besides the simulation results a more detailed description of the new FAM.

Internship in *ALSTOM*

After the development of the new FAM I've begun my internship in *ALSTOM*. This work experience lasted six month from May to the end of October. During this period I focused my work on the simulation of the *ALSTOM* gas turbine burner, and all the activities carried out in *ALSTOM* were reported in detail in [10]. The mentioned burner uses a swirl to stabilize and anchor its flame during the operation of the gas turbine. Even thought the reactants are introduced into the system separately, the particular geometry of this combustor device allows the user to create diffusion, premixed and partially premixed flames inside the combustion chamber. The main aim of the study was, exactly, to prove that the FAM is able to capture the ignition chemistry feature of premixed and partially premixed combustion inside the *ALSTOM* burner.

Four different cases where analyzed during the internship, each of these representing a particular flame configuration. Since no experimental data were available, the numerical results of the FAM were compared against the numerical results of a simple and well-known combined ED/FRC model. From this comparison emerge that the new FAM contains the right tools to predict reasonably well the behaviour of the ALSOM burner with any flow regime and to simulate well the right ignition points of the fuel elements. The flame age time together with well structured flamelet libraries give a great elasticity to this new transient laminar flamelet approach.

As an example in Fig. 3 the dimensionless temperature distribution inside the combustion chamber for the four different flame configurations is shown. These distributions are all normalized, i.e. the physical values are divided by an appropriate constant value. In order to keep clarity the eight contour plots show the same cross section of the combustor. The different cases are ordered in the rows starting from the pure non-premixed burner configuration to a situation where 95% of the fuel is already premixed before the combustion chamber (CASE_3). CASE_1 and 2 show two different partially premixed flame configurations. With both numerical approaches the temperature rises only in the combustion chamber of the *ALSTOM* burner. Besides this, the results of the temperature distributions computed with the two models, especially for CASE_0 and CASE_1, look quite similar. These observations confirm the fact, that the flame age time computed with the transport equation (1) and with an appropriate source term can mitigate correctly the reaction processes and represent the flame in a realistic position.

With the conducted simulations, also the robustness of the FAM was proofed. This means that the model behaves correctly also with a mash that satisfies the industrial standards; a numerical grid that was used extensively with the standard combustion models implemented in *ALSTOM*.

Besides these facts, during my *ALSTOM* internship, a new model for the scalar dissipation rate (χ) inside the flamelet structures was successfully implemented. The effects of this improvement on the flamelet structures was studied and documented. However in order to have a better understanding of this new model, results of turbulent flame simulations should be compared against experimental data (Sandia piloted jet flames).

During the simulation of the ALSOM burner some obscure qualities of the new FAM were also discovered; characteristics of the new approach that need to be further investigated.

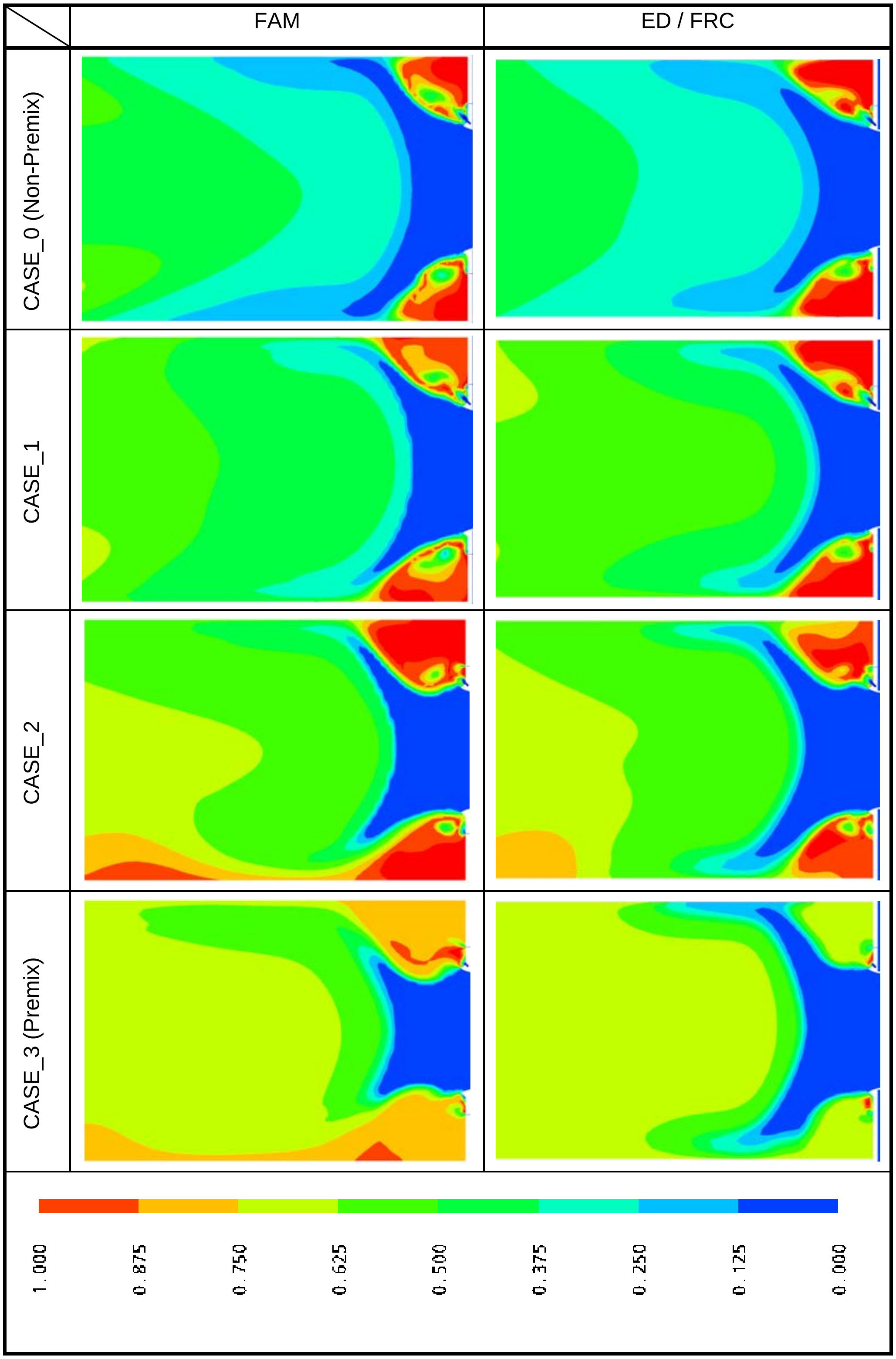

Fig.3: Temperature distributions inside the combustion chamber of the *ALSTOM* burner.

National Collaboration

This project is done in collaboration with *ALSTOM* (Switzerland) and during this year this collaboration has become more active. I've accomplished an internship of six month in this private company (start: 1 May 2005, end: 31 October 2005). Under the supervision of Dr. H. Lübcke I've worked in the combustion technology group of the combustor department located in Baden, Switzerland. The activities carried out during this work experience are documented in detail in [10].

Evaluation 2005 and Outlook 2006

The goals fixed up for the year almost concluded are listed in the first chapter of this report. This spring the Flame Age Model (FAM) was improved and validated against the Sandia piloted jet flame (flame D). Afterwards the new FAM, together with a new coupling strategy, was applied successfully to simulate the behaviour of the *ALSTOM* gas turbine burner. Burner that can establish diffusion, partially premixed and premixed flame configurations inside its combustion chamber. These simulations have demonstrated the elasticity our transient laminar flamelet model, which was developed to capture the characteristics of diffusion flames but turned out to be able also to represent in a reasonable way premixed and partially premixed combustion phenomenon. Finally, during my internship in *ALSTOM*, our new numerical approach was further improved and a new model for the scalar dissipation rate (χ) inside the flamelet structures was successfully implemented.

Although I wasn't able to simulate with the new FAM the other flames of the Sandia set (flame E and F) I'm happy with the results achieved this year. The computation of the two jet flames is obviously postponed to the first months of the fallowing year.

For the next year I've planned the fallowing works:

- Evaluating the differences and the performance of the two versions of transient flamelet model (Ferreira's TLFM and FAM) simulating the three piloted Sandia flames (D, E, and F).
- Analysis of the behavior of the slow chemicals reactions involved in the combustion process (CO and CO_2 chemistry) and development of an adequate model for these phenomenons.
- Finish writing the thesis for my PhD.

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