INVESTIGATION OF A COMBUSTOR USING A PRESUMED JPDF REACTION MODEL APPLYING RADIATIVE HEAT LOSS BY THE MONTE CARLO METHOD

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Abstract

In order to predict the stability limits of a model gas turbine combustion chamber, a non-adiabatic presumed-pdf reaction model applying a global chemical kinetics scheme has been developed. Radiative heat loss in the combustor has been taken into account by means of the Monte Carlo Method.

The investigations are carried out for aerodynamically stabilised flames under high turbulence and lean mixture conditions applying modern airblast nozzles. Such applications cover a wide range of operation conditions where stable combustion has to be guaranteed. Therefore, a growing demand exists for the knowledge of lean blow out limits, which is an important design parameter for the dimensioning of combustor air flows.

The reaction kinetic of the combustion process is influenced by the state of mixing as well as by the temperature distribution in the flow field. Hence, to consider the influence of the temperature distribution on the chemical reaction process in turbulent flames, in terms of the spatial temperature distribution and temperature fluctuations is essential for flame stability. The claim for numerical models to predict stability, thus, is very challenging.

In contrast to many stability models which mainly are based on global quantities, numerical models using local quantities offer the highest possible flexibility concerning variation of examined geometry and operating conditions.

In case of confined diffusive swirl-flames, the consideration heat transfer processes is crucial but, the exclusive consideration of convective heat transport has proven to be unsuitable.

Thus, for an adequate prediction of the temperature distribution in a combustor and on the combustor walls, respectively, both phenomena have to be accounted for.

Both of these processes, heat release and heat transfer, are described by statistical approaches in this work due to the high accuracy that can be achieved by these model types.

Nomenclature

C	constant	[-]
D	diameter	[m]
D	diffusion coefficient	[m^2/s]
P	thermal power	[kW]
R	radius / random number	[m] / [-]
Sc	turbulent Schmidt-No.	[-]
T	temperature	[K]
Y	radial coordinate	[m]
Y	species mass fraction	[kg/kg]
Z	element mass fraction	[kg/kg]
c	reaction progress	[-]
d	reaction progress variance	[-]
f	mixture fraction	[-]
g	mixture fraction variance	[-]
h	specific enthalpy	[J/kg]
h_N	enthalpy-index	[-]
p	pressure	[N/m^2]
$\vec{u}$	velocity vector	[m/s]
r	radial coordinate	[m]
t	time	[s]
x	axial coordinate	[m]
ε	emissivity	[-]
κ	absorption coefficient	[1/m]
λ	air equivalence ratio	[-]
ν_t	turbulent kinematic viscosity	[m^2/s^2]
ρ	density	[kg/m^3]
σ	Stefan-Boltzmann constant	[W/(m$^2 \cdot$T^4)]
χ	scalar dissipation rate	[1/s]

$\dot{\omega}$ reaction rate   [kg/(m^3·s)]

Subscripts
F   fuel stream
Ox   oxidizer stream
R   Reaction
ad   adiabatic
b   blackbody
c   referring to reaction progress mean value
d   referring to reaction progress variance
f   referring to mixture fraction mean value
g   referring to mixture fraction variance
loc   local
ref   at reference temperature
ν spectral

Operators
$\sim$ Favre average
$.''$ Favre fluctuation

1 Introduction

One of the main challenges in modelling turbulent premixed and non-premixed combustion processes is the numerically treatable description of the interaction of turbulent mixing processes and combustion. For this purpose, presumed shape Joint-Probability-Density-Function (JPDF) approaches [1,2] provide the possibility to cover the coupling of mixing and chemical reaction. Moreover, as the basis of such models consists of a set of few additionally solved transport equations for statistical moments, similar to the conventional equations for the transport of momentum and mass, their application together with high resolution methods like Large-Eddy-Simulation seems promising. Up to now available turbulent reaction models, capable of taking effects of local heat-losses on the chemical reaction into account are very scarce.

However, investigations of advanced problems in high-tech applications (e.g. industrial gas-turbines and aircraft-engines), like combustion instabilities, crucially depend on the modelling of the conjugate heat transfer.

The claim for the determination of radiative heat losses necessitates the evaluation of the divergence of the radiative heat flux, which generally is known as radiative source term in the energy transport equation. Hence, the quantities to be modelled are the radiative properties of the examined media as well as the variation of the spectral intensity, which is conventionally modelled by solving the radiative transfer equation applying discrete approaches. In contrast to those discrete methods, the radiative heat flux can also be determined by means of the Monte-Carlo method, which is a statistical approach and offers highest accuracy. Compared to non-statistical approaches, the Monte-Carlo approach is not restricted to discrete spatial resolution and is thus applicable on complex geometries.

2 Turbulent presumed JPDF reaction model

The numerical investigation of highly turbulent combustion processes requires the modelling of the interaction of turbulent mixing processes and chemical reactions. In the present work, a joint-probability-density-function (presumed JPDF) approach is applied to evaluate the governing quantities for these reaction processes. The model is based on two variables, of which there are the mixture fraction variable f and the reaction progress variable c.

$$f = \frac{(Z_C + Z_H) - (Z_C + Z_H)_{Ox}}{(Z_C + Z_H)_F - (Z_C + Z_H)_{Ox}} \qquad (1)$$

$$c = \frac{Z_{O,local} - Y_{O_2}}{\min(Z_{O,stoich}, Z_{O,local})} \qquad (2)$$

As stated in the definitions of f and c (eqn.(1) and eqn.(2)), both variables can take values in the range of zero to unity.

The specified range for f covers the mixing state of an air-fuel mixture from pure air ($f=0$) to pure fuel ($f=1$). To acquire the progress of the reaction within the chemical reaction mechanism, c characterises the progress from unburned mixture ($c=0$) to totally burned mixture ($c=1$).

The shape of the PDFs used for modelling the mixture fraction and reaction progress is presumed to be of clipped-Gaussian type [1]. Based on the assumption that these two vari-

ables are statistically independent from each other, each PDF is characterised by the statistical moments, variance and mean value, of the corresponding variable. This implies that a set of additional transport equations (eqn.(3) through eqn.(6)) for mean values and variances of both, mixture fraction and reaction progress variable, must be derived.

$$\frac{\partial(\overline{\rho}\,\widetilde{f})}{\partial t} + \nabla\cdot\left(\overline{\rho}\,\widetilde{u}\,\widetilde{f}\right) - \nabla\cdot\left(\overline{\rho}\left(D + \frac{v_t}{Sc_f}\right)\nabla\widetilde{f}\right) = 0 \qquad (3)$$

$$\frac{\partial(\overline{\rho}\,\widetilde{g})}{\partial t} + \nabla\cdot\left(\overline{\rho}\,\widetilde{u}\,\widetilde{g}\right) - \nabla\cdot\left(\overline{\rho}\left(D + \frac{v_t}{Sc_g}\right)\nabla\widetilde{g}\right)$$
$$= C_{g,1}\,\overline{\rho}\,\frac{v_t}{Sc_g}\left(\nabla\widetilde{f}\right)^2 - C_{g,2}\,\overline{\rho}\,\chi_t\,\widetilde{g} \qquad (4)$$

$$\frac{\partial(\overline{\rho}\,\widetilde{c})}{\partial t} + \nabla\cdot\left(\overline{\rho}\,\widetilde{u}\,\widetilde{c}\right) - \nabla\cdot\left(\overline{\rho}\left(D + \frac{v_t}{Sc_c}\right)\nabla\widetilde{c}\right) = \overline{\dot{\omega}_c} \qquad (5)$$

$$\frac{\partial(\overline{\rho}\,\widetilde{d})}{\partial t} + \nabla\cdot\left(\overline{\rho}\,\widetilde{u}\,\widetilde{d}\right) - \nabla\cdot\left(\overline{\rho}\left(D + \frac{v_t}{Sc_d}\right)\nabla\widetilde{d}\right)$$
$$= C_{d,1}\,\overline{\rho}\,\frac{v_t}{Sc_d}\left(\nabla\widetilde{c}\right)^2 - C_{d,2}\,\overline{\rho}\,\chi_t\,\widetilde{d} + 2\,\overline{\dot{\omega}_c c''} \qquad (6)$$

Closure of the production- and dissipation terms in those transport equations is obtained by classical gradient approaches. The reaction source terms appearing in the transport equations for the reaction progress are obtained by an appropriate chemical kinetics scheme.

2.1 Chemical kinetics scheme

Using a chemical reaction mechanism, that is based on a single reaction progress variable, is realised by applying the concept of the semi-global 2-domain-1-step chemical kinetics scheme [3],[4]. The concept of this reaction scheme is both the division of the combustion process into 2 domains, which are the fuel-consumption domain, and the CO/H_2-oxidation domain, and the assumption that all chemical reactions in each domain are specified by 1-step kinetics. Thus, stable intermediate component concentrations, like CO or H_2, are evaluated and the complete reaction progress is covered by a single reaction progress variable, which is, as stated above in eqn.(2), the normalised mass

fraction of O_2. Starting from this definition, the evaluated rate of O_2 is interpreted as reaction rate and implemented as reaction source term in eqn.(3) through eqn.(6). Fig. 1 shows the partition of a reactive-diffusive system in the mentioned fuel-consumption and CO/H_2-oxidation domain. Here the fuel-consumption domain covers both, preheating and reaction zone. The advantage of this approach is the possibility to easily adapt it to different types of fuel on basis of a chemical time scale that can be derived from measured or calculated laminar flame speeds.
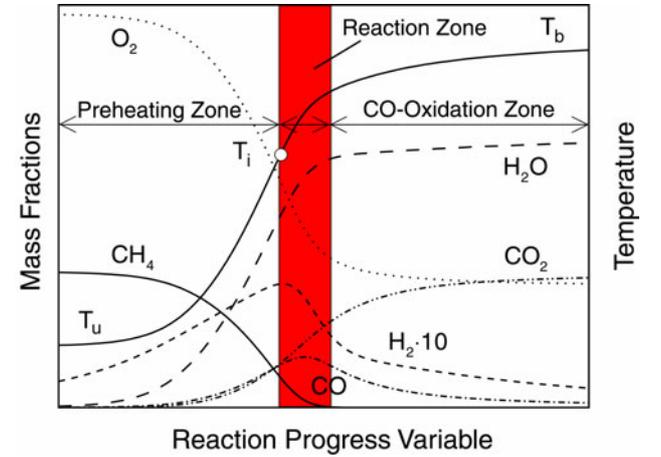
Fig. 1. The 2-domain concept for a reactive-diffusive system.

2.2 Non-adiabatic combustion processes

Adopting the combustion model to industrial applications makes it inevitable to account for non-adiabatic combustion processes. Hence, Wetzel et al. [5] extend the mixture fraction – reaction progress JPDF model, by introducing a dimensionless enthalpy which considers local heat losses. In the following, this dimensionless enthalpy is referred to as *'enthalpy-index'* h_N. The enthalpy-index is calculated according to:

$$h_N = \frac{h_{loc} - h_{ref}}{h_{ad} - h_{ref}}, \qquad (7)$$

where h_{loc} is the local enthalpy of the mixture, h_{ad} is the enthalpy of the local mixture at adiabatic conditions and h_{ref} is the enthalpy of the local mixture at a presumed reference temperature. Consequently, eqn.(7) is the ratio of the

effective local enthalpy-difference to the adiabatic enthalpy-difference. It is suitable to evaluate the reference enthalpy of the local mixture at the pre-heating temperature of air or fuel mass flow. Using the mentioned definitions, the enthalpy-index is zero for maximum heat loss and unity for adiabatic combustion, per definition. The local enthalpy of the mixture is determined by solving the energy transport equation, which is in turn affected by radiation exchange processes amongst the flame and surrounding walls.

2.3 Model implementation

To reduce computational costs the JPDF module, which contains information about the shape of the PDF, the number and distribution of integration points is executed in a pre-processor step. The JPDF module interacts with the 2-domain-1step kinetic sub-module, which provides information about reaction rates, species mass fractions, temperature and density. It evaluates the JPDF integrals and stores the results in a look-up table.
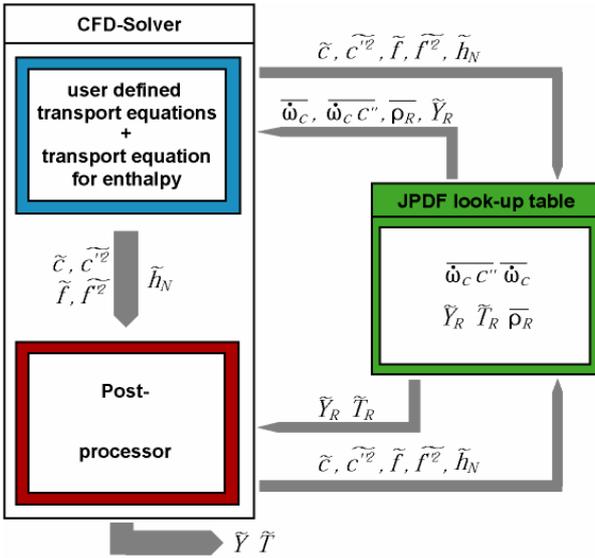
Fig. 2. Accessing the JPDF look-up table.

This JPDF look-up table contains the mean values of reaction source terms, species mass fractions, temperature and density as function of the independent tabulation variables, which are the mean values and variances of mixture fraction and reaction progress variable and, for the modelling of non-adiabatic combustion processes, the enthalpy-index. The above mentioned additional transport equations of mean value and variances of mixture fraction and reaction progress variables have to be solved by the CFD-solver. According to those solution fields, the required data is obtained out of the JPDF look-up table (see Fig. 2).

3 Modelling of radiation energy transfer

The radiation energy transfer in a non-grey non-scattering medium is specified by the radiative transfer equation [6]:

$$\frac{dI}{ds} = -\kappa_{abs}\left(I_\nu - I_{\nu,b}\right),\qquad(8)$$

where I_ν and $I_{\nu,b}$ are the spectral radiative intensity and black body intensity, s is the path-length coordinate and κ_{abs} the Planck mean absorption coefficient of the participating medium. According to [6] the mean absorption coefficient is defined as:

$$\kappa_{abs} = \frac{\pi}{\sigma T^4}\int_0^{4\pi} I_{\nu,b}\cdot\kappa_\nu\,d\nu\,.\qquad(9)$$

Here σ is the Stefan-Boltzmann constant, T the temperature of emission, ν the spectral wave number and κ_ν the spectral absorption coefficient. For the determination of the radiative source term in the energy transport equation, the divergence of the radiative heat flux

$$\nabla\vec{q}_{rad} = \kappa_{abs}\left(4\sigma T^4 - \int_0^{4\pi} I_\nu\,d\nu\right)\qquad(10)$$

has to be evaluated. In the present work this is done by means of the Monte-Carlo Method (MCM).

Several relationships within the Monte-Carlo approach are determined by random numbers. In the following, it is assumed that all random numbers are evaluated within the range from zero to unity. Numerically, the values of those random numbers are determined by a so called pseudo-random number generator RANECU.

3.1 Monte-Carlo formulation of radiation energy transfer

In contrast to other approaches for modelling radiative heat transfer, it is not necessary to solve an additional transport equation using the MCM. Instead the MCM directly evaluates the divergence of the radiative heat flux $\nabla \vec{q}_{rad}$. For this, each volume and surface element in the computational domain emits a sufficiently large number of energy bundles (photons) from randomly distributed locations within the particular element, in randomly chosen directions and wave numbers. The energy of photons that are emitted from volume elements is determined according to

$$\Delta E_{i,V} = \frac{4\kappa_{v,i}\sigma T_i^4 V_i}{N_{i,V}} \qquad (11)$$

and analogous for photons emitted from surface elements:

$$\Delta E_{i,A} = \frac{\varepsilon_i \sigma T_i^4 A_i}{N_{i,A}}, \qquad (12)$$

where $N_{i,V}$ and $N_{i,A}$ are the total numbers of photons that are emitted from the particular element type. The local amount of emitted energy bundles from within volume and surface elements, respectively are determined out of:

$$N_{i,V} = \frac{\kappa_{abs}\left(T^4 - T_0^4\right)\big|_{i,V}}{\sum_{j,V}\kappa_{abs}\left(T^4 - T_0^4\right)\big|_{j,V}} \cdot N_{max,V}, \qquad (13)$$

$$N_{i,A} = \frac{\kappa_{abs}\left(T^4 - T_0^4\right)\big|_{i,A}}{\sum_{j,V}\kappa_{abs}\left(T^4 - T_0^4\right)\big|_{j,A}} \cdot N_{max,A}. \qquad (14)$$

Here T is the local temperature, T_0 the minimum temperature for emission and $N_{max,A}$ as well as $N_{max,V}$ are the maximum numbers for photons emitted from the particular regions. With these formulations the emission from cold volume and surface elements is prevented. Contrary to similar approaches ([7]) that use the same expressions multiplied by the particular element volumes/areas, this approach is grid independent concerning the product of small element volumes/areas and the maximum number of emitted elements.

The energy bundles are tracked across the computational domain until they are either absorbed by volume elements due to attenuation in the medium and surface elements (surrounding walls), respectively or they leave the domain. The location of absorption within the medium is determined according to [6] and [8] respectively by:

$$R_{abs} = exp\left[-\int_0^{L_{abs}}\kappa_v ds\right] \qquad (15)$$

where R_{abs} is the random number for the determination of the flight distance L_{abs}. In this context the random number can be interpreted as the transmissivity along the direction of flight s of the particular energy bundle. When the transmissivity becomes larger than the randomly determined threshold, the bundle is absorbed within the medium. If the bundles approach a wall, the bundle is absorbed when the probability of absorption is larger than the absorptivity of the wall. Else the photons are diffuse reflected. Here, the wall absorptivity is assumed to be equal to the wall emissivity.

For each element, the sum of the emitted energy and the absorbed energy divided by the particular element volume directly corresponds to the divergence of the radiative heat flux. A detailed description of the MCM is given in [8].

3.2 Radiative properties of radiative active species

According to the applied reaction mechanism within the JPDF model it is assumed that the mixture of the exhaust gases is composed out of the radiative active species CO, CO_2 and H_2O. To evaluate the spectral absorption coefficient of the gas mixture a Single Line Group approach is applied. Within this approach it is assumed, that all spectral lines contained in the particular spectral intervals are characterised by a representative absorption coefficient and a representative line density. Initially, for calculating the effective transmissivity an exponen-

tial line strength distribution with randomly distributed line frequencies is adopted (Goody statistical model [9]). Spectral absorption coefficients as well as line densities are tabulated in literature for wavelength dependent spectral intervals and at discrete temperatures. Intermediate values for temperatures are linearly interpolated. This method assumes that the determination of the transmissivity is based on effective optical depths. Both, the representative spectral absorption coefficients and line densities for each component are tabulated at discrete temperatures and wave numbers ([10] or [11]).

3.3 Model implementation
Using the possibility of parallel computation of the CFD-solver and to ensure that its computational speed up is not influenced by the MCM-code, the radiation module is executed in parallel to the CFD-solver (see Fig. 3).
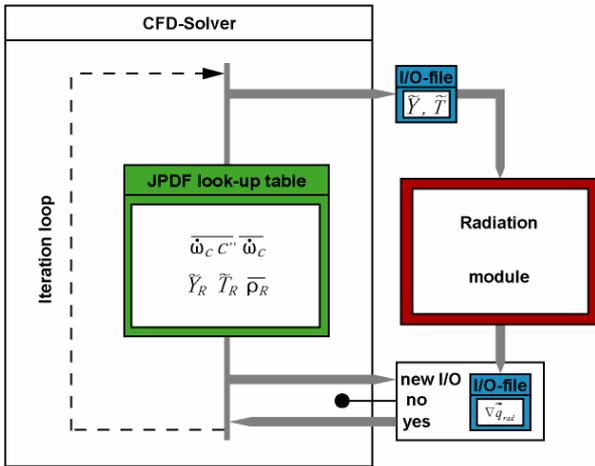
Fig. 3. Combined model implementation of JPDF and MC radiation module.

Both programs communicate via IO-files. The IO-files provided by the CFD-solver cover the required mesh information, the temperature field and species mass fractions. In a pre-solver step, the required connectivity lists for the ray-tracing algorithm are once computed out of the provided mesh data and stored in a look-up table. Temperature and species data are updated each time the radiation module is executed. The IO-file returned by the radiation module contains the radiative source term. This procedure

guarantees that the computational time needed for the solution of the flow field is not influenced by the time needed for the determination of the radiative source term.

4 Results and Discussion
To demonstrate the influence of heat loss processes on the chemical kinetics scheme, the temperature and reaction rate distributions resulting from a series of computations is shown below. To illustrate the predictability of the applied approaches, the particular distributions will be compared to results obtained from an adiabatic computation.

4.1 Heat loss prediction assuming an adiabatic chemical reaction scheme
Preliminary studies have shown that the chemical reaction mechanism is strongly influenced by local heat losses due to radiation. To consider those heat losses, the adiabatic reaction model is extended by a dimensionless enthalpy-index that can be referred to as heat loss ratio comparing the local enthalpy to the enthalpy of combustion under adiabatic conditions as stated in (7). Applying this approach, it is possible to account for non-adiabatic combustion processes.

As stated above, the influence of the heat loss on chemical kinetics is neglected, corresponding to $h_N = 1$. The temperature and reaction rate distributions are given in Fig. 4 and Fig. 5 for a flame with a thermal load $P_{th} = 10kW$ and an air equivalence ratio $\lambda = 1.75$ burning under atmospheric conditions. Both quantities are shown as functions of combustor radius r and axial burner distance x.

As expected, the non-adiabatic calculation results in significantly colder temperature levels compared to adiabatic conditions. Contrary, the reaction rate for the non-adiabatic computation (adiabatic chemistry) is not influenced by the colder flame temperatures in a relevant way. The maximum value of the reaction rate is slightly reduced, but the shape of the flame is not significantly changed. To cover the expected effects on the reaction mechanism, the influence
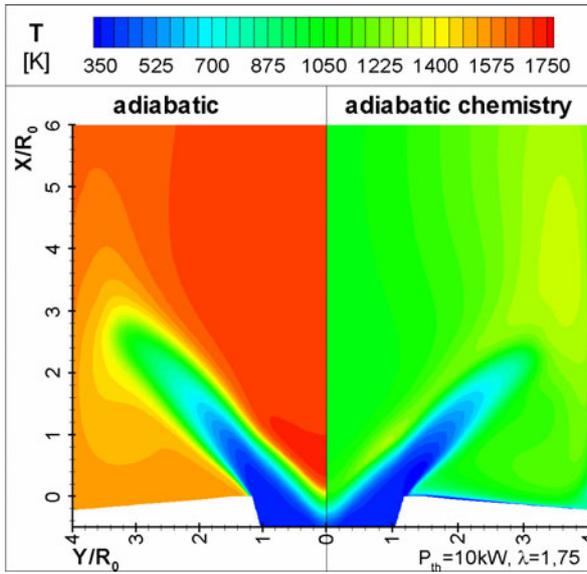
Fig. 4. Influence of heat loss on chemical kinetics – Temperature distribution.
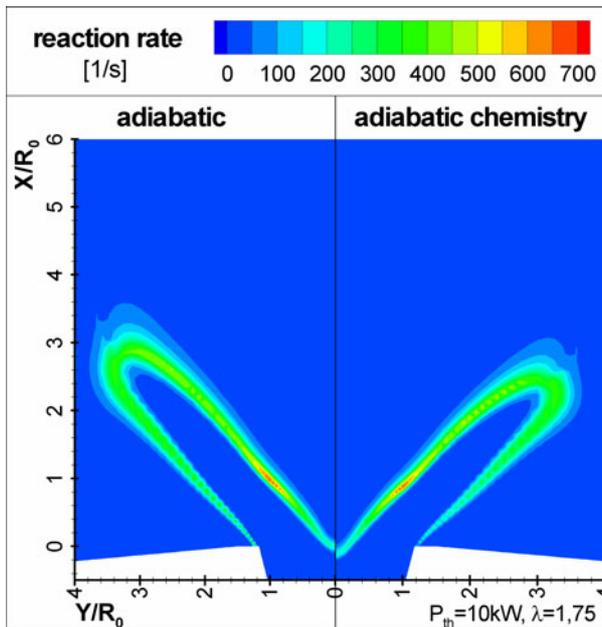
Fig. 5. Influence of heat loss on chemical kinetics – Reaction rate distribution.

of heat loss processes on the chemical kinetics have to be modelled. This is accomplished by applying JPDF look-up tables which are evaluated for non-adiabatic chemical reaction as function of the enthalpy-index.

4.2 Influence of the enthalpy index on the chemical reaction mechanism

Assuming a constant value for the enthalpy-index all over the combustion chamber has shown its influence on the combustion system. The significant influence of the enthalpy-index on the temperature distribution and the reaction rate are shown in Fig. 6 and Fig. 7. Both figures show the influence on the particular variables starting from adiabatic conditions (top) to a presumed heat loss of 20% (bottom). The contour levels in these figures are the same as those in Fig. 4 and Fig. 5, respectively.
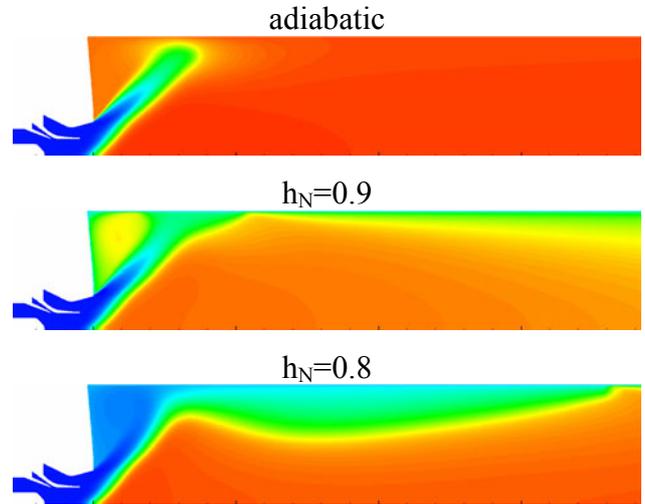
Fig. 6. Presumed enthalpy index – Temperature distribution.
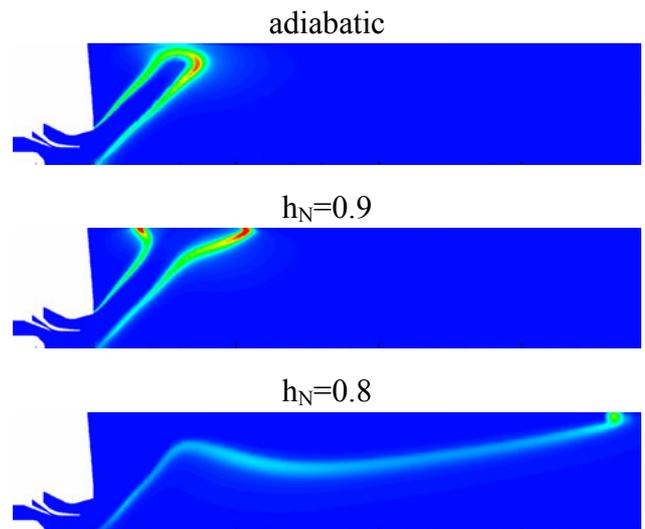
Fig. 7. Presumed enthalpy index – Reaction rate distribution.

Increasing the heat loss in the combustor, by decreasing the enthalpy-index, results in growing flame lengths. As shown in Fig. 6 and Fig. 7 the flame length increases until it impinges onto the wall and the reaction zone breaks up into two branches. The corresponding temperature plot shows in general reduced temperature levels. By increasing the heat loss even more, the flame extinguishes in the corner of the combustor (left branch) and burns lifted off from the nozzle, stabilised at the combustors wall. Resulting from these computations, the necessity of considering the influence of the local heat loss on the chemical reaction mechanism is getting obvious.

4.3 Reaction field prediction applying a globally varying enthalpy index

For the tabulation of the JPDF quantities as a function of the enthalpy index, preliminary investigations concerning the influence of the actual heat loss within the combustor were carried out by [5]. Hence, in a first simple approach the radiative source term in the energy transport equation is determined as the heat flux resulting from the emissivity of the particular CFD-elements, their temperatures and the temperature at the combustor's wall. Within this approach the absorption by gas is neglected, but it has shown that the reaction mechanism is significantly influenced by the spatial distributed enthalpy-index. Fig. 8 and Fig. 9 show a comparison of the adiabatic reaction mechanism and the non-adiabatic reaction mechanism (variable enthalpy-index).

It can be seen, that considering the local heat loss in the chemical reaction significantly influences the temperature distribution and the reaction rate of the flame. Considering a varying enthalpy-index, the temperature distribution (Fig. 8) shows obviously reduced values all over the combustion chamber. Concerning the flame shape, the corresponding reaction rate illustrated in Fig. 9 points up a flame, that burns lifted off from the edge of the nozzle and thus may cause lean blow out. Coming up from these computations the demand for an appropriate radiation module is obvious.
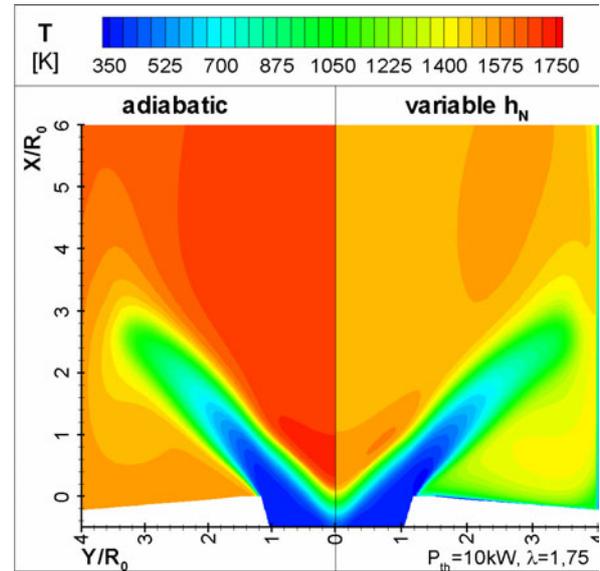
Fig. 8. Adiabatic and variable enthalpy-index computation - Temperature distribution
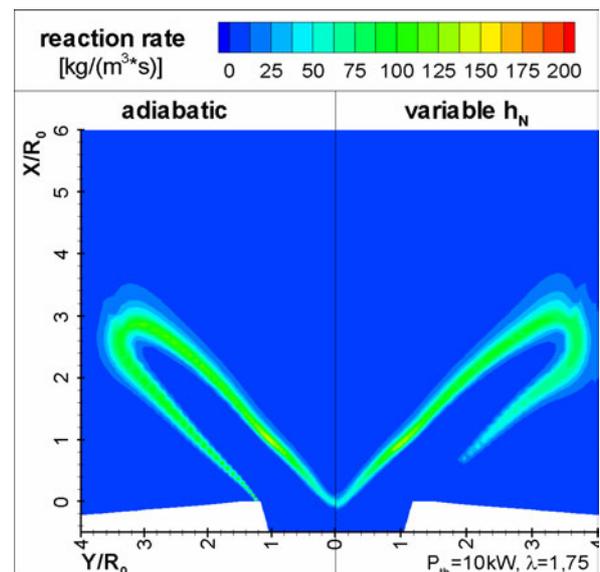
Fig. 9. Adiabatic and variable enthalpy-index computation - Reaction rate distribution.

4.4 Radiative heat loss prediction by means of the Monte-Carlo Method

For the examined case, the distribution of the resulting radiative net heat flux and the corresponding mean absorption coefficient are illustrated in Fig. 10. For the net heat flux, a strong emitting region can be seen in the center of the combustion chamber, while the region of cold,

unburned air/fuel mixture is characterised by slight absorption.
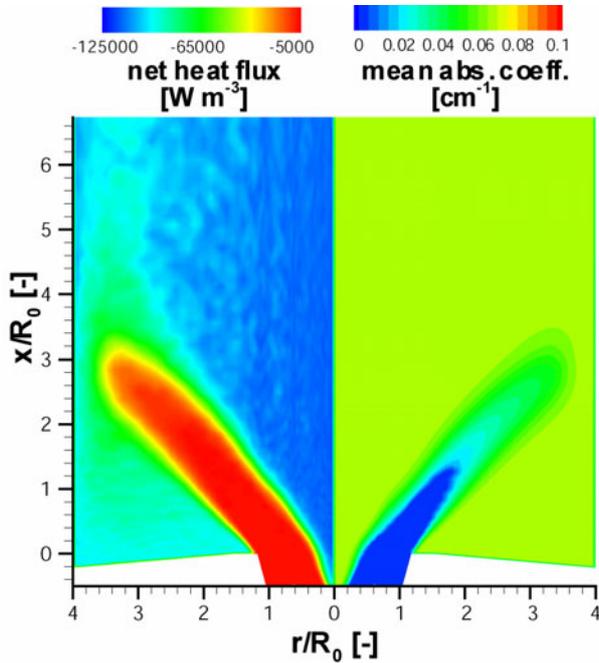
Fig. 10. Radiative net heat flux and mean absorption coefficient.

To determine the radiative source term it is assumed, that gas at temperatures lower than 600K is not emitting. Thus, the minimum temperature for emission T_0 in equations (13) and (14) is assumed to be 600K. Those regions are characterised by small mean absorption coefficients.

The corresponding species mass fractions of the radiative active components are illustrated in Fig. 11. From the figure it can be seen, that the contribution of CO is very small all over the combustion chamber and that the CO maximum values are restricted to the reaction zone within the flame. The overall homogeneous composition is reflected in the likewise homogeneous distribution of the absorption coefficient (Fig. 10).

5 Conclusions

The influence of local heat losses on the chemical reaction mechanism has been systematically investigated for a model gas turbine combustion chamber. Considering the radiative local heat loss in the chemical reaction, signifi-
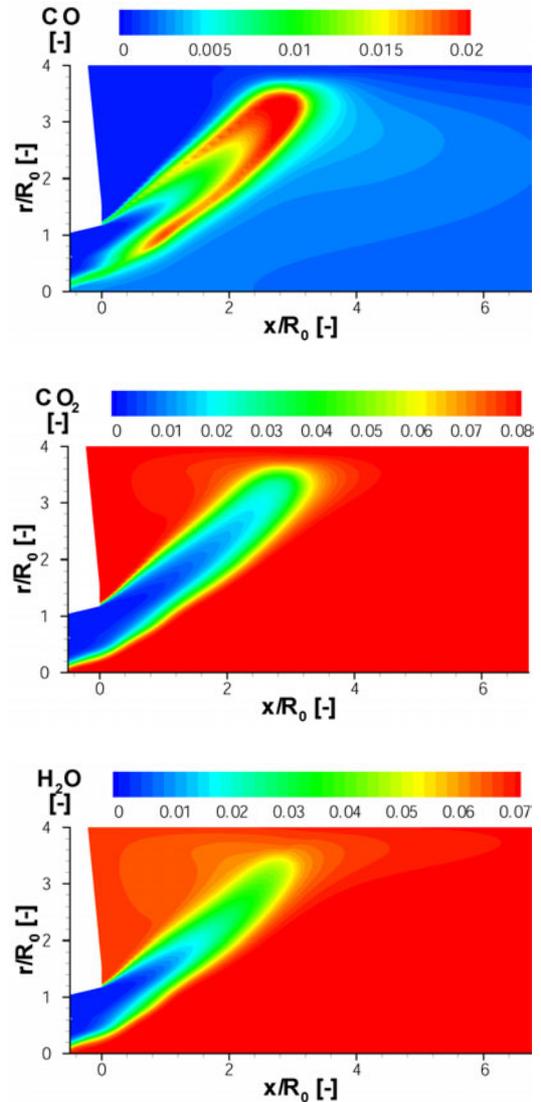
Fig. 11. Mass fractions of radiative active species a) CO b) CO_2 c) H_2O

cantly influences the reaction field compared to adiabatic conditions and thus the necessity of a non-adiabatic treatment of the reaction mechanism has been demonstrated. As a result of the investigations applying the simplified approach for modelling the radiative source term, the demand for an accurate radiation model has been proven.

Accounting for emission and absorption due to a non-gray, non-scattering medium, a Monte-Carlo radiation code has been developed. It has been shown that the radiation module is

capable for predicting radiative heat fluxes and mean absorption coefficients for the examined model combustion chamber. Starting from the preliminary results presented here, investigations concerning the influence of conjugate heat transfer will be carried out.

The investigations presented within the present paper will be used as basis for further investigations on combustors operating under lean mixture conditions at high pressures. For this purpose it will be necessary to extend the chemical kinetics scheme and to evaluate the properties of the radiative active components for combustion at high pressures.

Acknowledgments

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