Numerical Prediction of the Dynamic Behaviour of Premixed Flames Using Systematically Reduced Multi-Step Reaction Mechanisms

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ABSTRACT

Environmental compatibility requires low emission burners for both gas turbine power plants and jet engines. In the past, significant progress has been made in the development of low NOx and CO burners by introducing lean premixed techniques. Unfortunately these burners often have a more pronounced tendency than conventional burner designs to produce combustion driven oscillations. The oscillations may be excited to such an extent that strong pulsation may occur, and this is associated with a risk of engine failure.

In order to describe the acoustical behaviour of the complete burner system, it is crucial to determine the unit function response of the flame itself. Using a new method which was presented in 1996 by Bohn et al. [1] the dynamic flame behaviour can be predicted by means of a full Navier-Stokes-simulation of the complex combustion process for both the steady-state and transient case.

The authors have successfully used this method to obtain the frequency response of turbulent diffusion flames which are mainly controlled by the mixing process. Chemical kinetics become dominant for premixed flames. Therefore, the combustion process of a premixed methane-air mixture is modelled using a systematically reduced 6-step reaction mechanism which takes account of a set of 25 elementary reactions. This reduced mechanism was implemented in the 3D-Navier-Stokes solver in order to perform a combined flow and combustion computation.

The dynamic combustion process of a laminar premixed methane flame in a matrix burner configuration has been investigated. At first, the steady-state combustion process was simulated using the code described above. The results are compared with experimental data. Very good agreement over a wide range of equivalence ratios has been found for quantities such as laminar burning velocity or adiabatic flame temperature. The steady state results are then used as an operating point from which the transient flame behaviour after a sudden jump in the mass flow at the burner inlet has been obtained. Finally, these data lead to the unit function response which can be transferred into frequency space by a Laplace transformation.

The frequency response of the premixed methane flame obtained by a Navier-Stokes simulation has been compared with both experimental as well as analytical solutions. It must be stressed that a pure delay time element which is often used as an analytical formulation is not suitable to describe the dynamic flame behaviour in detail. The frequency response shows the characteristics of a higher order delay time element with several important details.

Parametric studies on the influence of equivalence ratio and the flow pattern of the internal burner fluid flow which are of interest for gas turbine applications, show the importance of the detailed knowledge of the dynamic flame behaviour for the stability analysis of a gas turbine combustor.

NOMENCLATURE

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<thead>
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<th>Symbol</th>
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<td>specific heat capacity</td>
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<td>E</td>
<td>activation energy</td>
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Due to the need for environmental compatibility, combustion is a very important field of research in gas turbine development. In the past, significant progress has been made in the development of low NO\textsubscript{x} and CO burners by applying lean premixed combustion. In addition, the power output of heavy-duty gas turbines has increased significantly with the result that the thermal power of the combustion chamber is greater as well. Unfortunately these advanced burners and combustion chambers often have a more pronounced tendency to produce combustion driven oscillations than conventional burner designs. The oscillations may be excited to such an extent that pronounced pulsation may occur, and this is associated with a risk of engine failure. The oscillations can lead to higher levels of pollution and result in very high noise emissions. Therefore, there is an urgent need to develop a design tool for predicting these instabilities.

Bohn et al. [1] have introduced a new method to predict the dynamic flame behaviour by means of a full 3D-Navier-Stokes simulation of the complex combustion process. This method has been used successfully for turbulent diffusion flames which are mainly controlled by mixing effects using a simple mixed is burnt model which neglects chemical kinetics. However, chemical kinetics are the most important issue when predicting premixed flame systems and their dynamical behaviour.

This paper presents the numerical simulation of steady and unsteady combustion processes of premixed methane flames using systematically reduced mechanisms integrated into a 3D-Navier-Stokes solver. The principal reducing mechanism has been described by Peters [5], Paczko et al [6] and Peters and Rogg [7]. The implementation of the mechanism into the Navier-Stokes solver of the Institute of Steam and Gas Turbines, RWTH Aachen, has already been verified and tested successfully [Bohn et al. [8],[9]].

The dynamics of premixed flame combustion can be investigated in detail using this multi-step mechanism and the method for obtaining the frequency response of flame systems. The results can be compared with both analytical [Deuker [4]] and experimental work [Matsui [17]] in this area.

**NUMERICAL SIMULATION**

**FLUID FLOW MODEL**

The transient Navier Stokes equations are used to model the fluid flow. They comprise equations for conservation of mass (1), momentum (2) and enthalpy (3):

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{1}
\]

\[
\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v} - \mu \nabla \mathbf{v}) = -\nabla p + \nabla \cdot (\mu (\nabla \mathbf{v})^T) \tag{2}
\]

\[
\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho \mathbf{v} h_t - \left( \frac{\lambda}{c_p} \right) \nabla T) = \frac{\partial p}{\partial t} \tag{3}
\]
This set of 5 coupled partial differential equations is closed by
the equation of state for ideal gases (4) and the constitutive
equation of ideal gases (5):

\[\rho = \frac{p}{RT}\] (4)

\[h = \int c_p(T) dT\] (5)

For ideal gas mixtures, the specific gas constant and the specific
heat capacity are defined as:

\[R = \frac{\sum_i R_i}{M} = \frac{\sum_i \frac{Z_i}{M_i}}{M}\] (6)

\[c_p(T) = \sum_i c_{pi}(T)\] (7)

The values for the specific heats are taken from Kee et al. [10],
where the temperature dependence is approximated by 4th degree
polynomials.

A simplified transport model according to Smooke et al. [11]
has been used to define thermal diffusion and laminar viscosity:

\[\lambda = 2.58 \cdot 10^{-5} \left(\frac{T}{298}\right)^{0.7} \left(\frac{kg}{sm}\right)\] (8)

Setting the Prandtl number to \(Pr = 0.75\), the viscosity is then
defined as:

\[\mu = 0.75 \cdot 2.58 \cdot 10^{-5} \left(\frac{T}{298}\right)^{0.7} \left(\frac{kg}{sm}\right)\] (9)

COMBUSTION MODEL

In order to accurately simulate chemistry-driven premixed
flame combustion, a detailed model of the oxidation process in
the flame is crucial. By means of sensitivity analyses it has been
identified in Peters [5] and Paczko et al. [6] that the set of 25
elementary reactions given in table A1 in the Appendix is a
sufficiently good representation of the elementary kinetics for
lean to stoichiometric methane flames and pressures up to 50
atm. However, a combined flow and combustion simulation using
all of the 25 elementary reactions would far exceed the
limitations of hardware and time. Therefore, a systematically
reduced 6-step reaction mechanism has been derived:

\[
\begin{align*}
I & \quad \text{CH}_4 + O \quad \leftrightarrow \quad \text{CO} + 2 \text{H}_2 \\
II & \quad \text{CO} + \text{OH} \quad \leftrightarrow \quad \text{CO}_2 + \text{H} \\
III & \quad \text{H} + \text{H} + \text{M} \quad \leftrightarrow \quad \text{H}_2 + \text{M} \\
IV & \quad \text{H} + \text{O}_2 \quad \leftrightarrow \quad \text{OH} + \text{O} \\
V & \quad \text{O} + \text{H}_2 \quad \leftrightarrow \quad \text{H} + \text{OH} \\
VI & \quad \text{OH} + \text{H}_2 \quad \leftrightarrow \quad \text{H} + \text{H}_2\text{O}_2 \\
\end{align*}
\] (11)

To do so, 6 species, namely \(\text{CH}_3, \text{CH}_2\text{O}, \text{CH}_3\text{O}, \text{HCO}, \text{HO}_2,\) and \(\text{H}_2\text{O}_2\), have been considered to be in steady state throughout
the reaction. This means that the time derivative of these species
concentrations is set to zero. This is straightforward when
assuming much higher consumption rates than production rates,
which lead to much smaller concentrations than initial reactants
and final products. Since the concentrations always stay very
small, the time derivatives also stay small in comparison to
dervatives of other species.

The reaction rates of the global mechanism (11) are defined as
follows by the effective rates of the skeletal mechanism (see table
A1 in the appendix):

\[
\begin{align*}
w_1 &= w_1 + w_{11} + w_{12} \\
w_2 &= w_9 \\
w_{11} &= w_5 + w_{10} + w_{16} + w_{24} + w_{25} \\
w_{12} &= w_1 + w_6 \\
w_9 &= w_2 + w_4 + w_6 \\
w_{16} &= w_3 + w_4 + w_8 + w_{12} + w_{15} + w_{24} \\
\end{align*}
\] (12)

These rates of the starting mechanism are approximated by the
Arrhenius Ansatz:

\[w = \frac{\partial[A]}{\partial t} = -A T^k \cdot e^{-E/RT} [A] [B] \quad (A + B \rightarrow C + D)\] (13)

The reaction rates of the reduced mechanism defined in (12) are
needed as source terms in the conservation equations of six
components - one of each for every reaction (I-VI) - to be solved
simulating reduced flame kinetics:

\[\frac{\partial \rho \xi_i}{\partial t} + \nabla \left( \rho \nabla \xi_i - \frac{\mu}{L e} \nabla \nabla \xi_i \right) = M_i \sum_j v_{ij} w_j \] (14)

The Lewis numbers are set constant and are listed in table A2.

Finally, heat release is taken into account by a new definition
of the static enthalpy:

\[h = \int c_p(T) dT + \sum_i \xi_i h_{fi} (T_{ref})\] (15)

SOLUTION METHOD

A fully implicit Finite-Volume scheme has been used for
solving the coupled equations (1)-(3) and (14). The SIMPLEC
pressure-correction algorithm [12] is adapted on a non-staggered
grid, whilst avoiding the checkerboard oscillations by using the
improved Rhie-Chow interpolation method [13], [14]. A central
difference scheme is used for diffusion terms, whilst advection
terms are discretised by upwind differencing, because of the
higher stability. A fully backward difference time stepping
procedure is employed. Therefore, the time step is not bound to
CFL restrictions in principle, and this is a very important feature
for numerical investigations of transient combustion phenomena.

STEADY-STATE RESULTS

The fundamentals of self-induced combustion driven
oscillations and the dynamic flame behaviour have been
investigated experimentally at the Institute of Steam and Gas
Turbines, RWTH Aachen, using a 2D matrix burner system as
shown in figure 2. The combustor is built up from a diffusor with
a small circular end and a wide rectangular end, a mixing
chamber, a matrix burner with 7 or 16 channels with a 2.2 x 40 mm cross section producing small plane conical flames of premixed type, and a combustion chamber comprising a straight tube with a 92 x 46 mm cross section and a length of 400 mm. To obtain optical access, the tube is made from quartz glass in the region of the flames. The flow in the burner channels was found to be laminar over a wide range. This is very important in order to separate the influence of reaction kinetics from turbulence effects. The Mach numbers are smaller than 0.04. The flow rates of fuel (methane or propane) and air are measured and adjusted separately. The exhaust temperature is measured by a PtRh-Pt thermocouple at a distance of 100 mm from the matrix burner exit.

The burner can be operated in the range of equivalence ratios between 0.7 to 1.5. In order to obtain informations on the stability concerning combustion driven oscillations of the burner a 1/2-inch microphone is set up at a distance of 1 m from the test assembly. The noise is analysed with a FFT-analyser. The combustion chamber produces noise with frequency of about 225 Hz depending on the length of the exhaust duct.

In order to simulate the combustion process inside the burner, only a section measuring 52 mm x 2.65 mm is considered as indicated by the rectangle in figure 3, where a schlieren picture of the steady-state flames taken from the experimental apparatus is shown. The computational mesh is divided into 300 x 36 meshpoints, equidistant in y direction, whereas the resolution is increased in x direction close to the inlet. The left and right-hand boundaries are defined by conditions of symmetry. The bottom is divided up into a wall region and an inlet. The inlet conditions are characterised by a stoichiometric to lean - the equivalence ratio is varied between 1.0 to 0.77 - air-methane mixture at a temperature of T= 293.15 K entering with a homogeneous velocity \( u_0 = 10.0 \) m/s. There is also one set in which the inlet velocity profile is considered to examine the influence of this relevant case on the dynamic flame behaviour. The outlet is defined by a constant pressure \( p = 1 \) atm.

In figure 4, the calculated flame shape represented by the mass fraction of CO and the temperature T is shown for four different equivalence ratios. As the temperature and CO-level fall the length of the flame grows with decreasing equivalence ratios. The distribution of the CO mass fraction also shows clearly the very thin combustion zone of this laminar premixed flame.

The combined simulation of both aerodynamic and combustion phenomena gives an insight into the very important
stabilizing mechanism near the burner port. The flame is stabilized by a strong vortex, which is induced at the sharp edge at the exit of the burner channel. This vortex also grows significantly with decreasing $\phi$ as shown in figure 5 where the streamlines near the burner port are given together with the distribution of the O-radical. This intermediate is also a good indicator of the combustion zone.

Figure 6 shows some fundamentals of the shape of premixed flames. As indicated, it is possible to calculate the laminar burning velocity $A$ by knowing the homogeneous inlet velocity $u_0$ and the length of the flame $L_F$. The length of the flame can be predicted by the distribution of fuel (i.e. CH$_4$) along the burner axis as shown in figure 7 together with the temperature rise in the combustion zone. The flame length is defined as the point where methane is completely oxidized. The calculated burning velocities and adiabatic flame temperatures are summarized in figure 8. In order to verify the numerical procedure and the 6-step-mechanism, the data are compared with measurements in figure 9. The grey triangles represent the calculation, and it can be concluded that the numerical data are in very good agreement with various measurements referenced by Law [15] and Wamatz [16].

To sum up, it can be said that the 6-step-reaction mechanism is suitable for calculating lean premixed flames considering the main characteristics which are important for the dynamic flame behaviour, i.e. the temperature distribution, the burning velocity and the length of the flame.

The steady-state results shown above are not only used to validate the numerical code, but also to obtain the operating point for the transient procedure as described below.

Because the influence of the flow pattern of the burner itself on the dynamic flame behaviour is of interest, one more steady-state calculation has been established in which the inlet velocity is not homogeneous. A parabolic velocity profile at the inlet is used to best represent the real internal fluid flow. This velocity profile has been measured using the LDA-technique and has been calculated by a numerical simulation of the cold internal flow of the matrix burner. The profile is determined in such a way that the average velocity $\overline{u}_0$ is equal to the homogeneous velocity of 10 m/s. This yields the same mass flow rate through burner and flame for both boundary conditions. In figure 10, the two different inlet boundary conditions can be identified in the velocity vector plot near the burner port. The flow pattern has a considerable influence on the stabilizing vortex at the sharp edge of the burner port. This can be seen clearly in figure 11, in which the temperature and CO-distribution of the whole flame as well as the O-distribution and streamlines at the burner exit are shown once again. The flame length is not affected by the different velocity profiles, however
the stability vortex in the region near the burner slot is influenced to a large extent. This should have an effect on the dynamic flame behaviour as described in the next chapter.

TRANSIENT RESULTS

The new method, first presented by Bohn et al. [1], to predict the dynamic flame behaviour is summarized in Figure 12. For more details see Bohn et al. [1]. The steady-state results described above formed the operating point on which the transient calculations are based. Therefore, the mass flow rate at the inlet is increased suddenly to 115% of the steady-state mass flow, in other words a jump of 15%. Investigations have showed that up to a jump of 20% the frequency response of the flame has a linear character which is important for the validity of the stability criteria for the entire burner system.
The frequency response of a premixed flame can be defined as the ratio of the transient mass flow increase at the exit, downstream of the flame, and the jump in mass flow at the inlet:

$$F_{Fh}(j\omega) = \frac{\Delta m_{exit} - \Delta m_{steady}}{\Delta m_{inlet}}$$

(16)

Four different transient calculations will be discussed in this paper. In order to study the principal dynamical behaviour of premixed flames and in order to investigate the characteristics of the frequency response, one calculation with a homogeneous velocity profile and $\phi=0.91$ (weak lean conditions) will be presented. In order to discuss the influence of the equivalence ratio, this parameter is varied and thus two more calculations - the first with $\phi=1.0$ (stoichiometric condition) and the second with $\phi=0.83$ (lean condition) - are presented. Finally, the influence of the flow pattern of the burner nozzle is investigated by a further transient calculation with a parabolic velocity profile at the inlet (see figure 10 for details) and stoichiometric conditions.

CHARACTERISTICS OF THE DYNAMICAL FLAME BEHAVIOUR OF PREMIXED FLAMES

How does a steady-state, well-stabilized premixed flame react to a sudden jump in mass flow at the burner port? The flame shape for several time steps is shown in figure 13. During the calculation the increase in time was 0.1 ms. Additional analyses run with smaller time steps show no significant difference. It can be seen that up to a time of 1 ms the flame shape only differs close to the burner port. The length of the flame, however, does not change during this period. Then, the flame grows up to its maximum length after about 3 ms. For periods larger than 4 ms the flame shape does not vary. This indicates that the steady-state point is reached again. The new flame cone corresponding to the new inlet velocity is established.

The unit function response of this flame (figure 14a), which is defined in the same manner as the frequency response, can be split up into five major parts:

Part I: acoustical behaviour ($0 < t \leq 0.15$ ms)
The disturbance at the inlet is transported with acoustical velocity; the mass flow at the exit increases by about 22.5% of the mass flow jump at the inlet.

Part II: delay time due to chemical reasons ($0.15$ ms $< t \leq 1.1$ ms)
In spite of the increasing flame surface, this can be identified in figure 13 exemplary for a time of 0.7 ms, the mass flow at the outlet does not change. Two main effects seem to be responsible for this behaviour: The area of the cold, unburnt mixture is growing due to the increased flame surface. Therefore more mass can be stored inside the control volume. In addition, the integral heat release in the flame does not change strongly during this period. Due to chemical kinetic effects the combustion is disturbed locally leading to a smaller burning velocity compared to the steady-state one and therefore smaller heat release.

Part III: strong amplification ($1.1$ ms $< t \leq 2.9$ ms)
In this period the influence of both effects described above is
decreasing, whilst the mass flow at the outlet is increasing up to a maximum of about 122\% of the jump at the inlet.

**Part IV: fade-away period (2.9 ms < t ≤ 4.2 ms)**

This part is characterized by the fade-away of the overshooting. Now the flame surface is decreasing to its steady-state value corresponding to the new inlet velocity. The disturbances in the flame zone diminish and finally the flame reaches its typical steady-state cone shape. The unit function response is decreasing monotonously to the limiting value of 1 for $t \to \infty$.

**Part V: steady-state ($4.2 < t < \infty$)**

With regard to the mass flow rate at the exit the flame is burning in steady-state mode again.

There are some characteristics which represent the dynamics of a flame: the delay time of part II, the slope of the curve in part III, the time at which the bending point is reached and the height of the overshooting. Many authors (for example: Deuker [4]) have tried to come up with an analytical solution for the unit function response of premixed flames. All these attempts assume a linear increase of mass flow with time up to a delay time $t_{\text{max}}$, which is a function of the geometry, the inlet velocity and a constant laminar burning velocity. For purposes of comparison, this analytical unit function response is also plotted in figure 14a. It can be concluded that many important features of the dynamical flame behaviour cannot be prescribed with this solution. Only the bend of the analytical solution, which is determined by the laminar burning velocity, is found at the same time as the maximum of the numerical solution.

The consequences of this on the important frequency response are illustrated in figure 14b, in which Bode's diagram for both the analytical and numerical solution is shown. Whilst the differences in the amount do not seem to be very significant, the differences for the phase angle, which is the most important parameter for the prediction of the stability of an entire burner system, are well worth mentioning. The difference is significant especially in the region between 150 and 600 Hz. Most of the known combustion oscillations are in this order of frequency and this is marked by the grey window in figure 14b. Whilst the analytical solution jumps between 0° and 180°, the phase angle of the numerical solution passes the whole range from 0° to 450°. The solution obtained by the numerical method agrees better with experimental data. This is proved by figure 15 in which the frequency response in Bode's diagram is shown for a laminar premixed flame.

---

**FIG. 13: Transient Behaviour of a Premixed Flame**

$\phi = 0.91$ (Contours of CO Mass Fraction)

**FIG. 14a: Unit Function Response of Premixed Flame**

($\phi = 0.91$, $Re_h=2500$)

**FIG. 14b: Frequency Response of Premixed Flame**

($\phi = 0.91$, $Re_h=2500$)
measured by Matsui [17] and Sugimoto et al. [18]. This measured frequency response shows qualitatively the same characteristics as the one obtained here by the full Navier-Stokes analysis using the reduced 6-step-reaction mechanism, especially for the important phase angle. Only the frequency range is shifted to lower values. This can be explained by the fact that the authors have used a completely different geometry.

From this point of view, it can be summarized that it is possible to predict the dynamical behaviour of premixed flames very accurately with the new method described above.

INFLUENCE OF THE EQUIVALENCE RATIO

From the discussion above, it is clear that the equivalence ratio, respectively the burning velocity, is one of the most important parameters which influences the dynamical behaviour. Therefore, the unit function response and the frequency response for three different equivalence ratios $\phi = 1.0$, $\phi = 0.91$ and $\phi = 0.83$ are given in figure 16a and 16b. Four major differences between these three configurations should be mentioned. For lean flames, which is is the relevant case for gas turbine applications, the chemical delay time decreases with growing equivalence ratios as the burning velocity increases. Thus, the time at which the maximum is reached also becomes smaller. The third difference is the height of the banked curve, which decreases also for higher equivalence ratios. The final difference is the slope of the amplification which is similar for $\phi = 0.91$ and $\phi = 0.83$ but different for $\phi = 1.0$. This behaviour can be explained by the different chemical processes which become dominant for stoichiometric to rich flames, i.e. the CO-mechanism in particular. The differences are also very clear from Bode's diagram (figure 16b). Once again, the phase angle in particular differs significantly for different equivalence ratios. This is due to the chemical delay time which differs with the variation of the burning velocity.
INFLUENCE OF THE FLOW PATTERN OF THE BURNER NOZZLE

The influence of the flow pattern of the burner nozzle has been discussed for the steady-state-solution above. Figure 17a shows the unit function responses for both cases, i.e. homogeneous and parabolic inlet velocity profile. The velocity distribution at the burner inlet influences the dynamical flame behaviour greatly. The delay time for the parabolic profile is somewhat smaller, and therefore the flame reacts faster to the disturbance. This can be explained by the higher velocity at y=0. In addition, the slope of h(t) in the region of amplification is somewhat steeper than in the case with the assumption of homogeneous inlet velocity. Compared with the analytical solution, which also assumes homogeneous inlet velocity, the difference between the case with more realistic boundary conditions becomes more significant. However, the difference between the Navier-Stokes solution with more realistic inlet boundary conditions and the analytical solution are smaller in the relevant frequency case of 100 to 500 Hz concerning the phase angle of the frequency response (figure 17b).

Ankhow, the results show the importance of the burner nozzle fluid flow and the interaction between chemical processes and fluid flow.

SUMMARY AND CONCLUSION

The dynamical flame behaviour of premixed flames have been investigated based on full Navier-Stokes-calculations of the transient combustion process. In order to take account of the chemical kinetics, which control the combustion process of this kind of flame, a systematically reduced multi-step reaction mechanism has been developed and integrated into the numerical procedure. All important species, including CO, O, OH etc., are considered, so that the combustion can be predicted very precisely. It is worth mentioning that, in contrast to the analytical solutions, there is no need to specify any global parameters, such as the laminar burning velocity.

The steady-state results for different equivalence ratios show very good agreement between the numerical calculation and experimental data concerning the burning velocity. This is one of the major parameters which control the flame dynamics. In addition to varying the stoichiometrics, investigations have been carried out to study the influence of a more realistic inlet boundary condition at the burner port. The steady-state results show that this has a significant influence, especially on the vortex system near the burner rim where the flame is stabilized.

Transient calculations, based on the steady-state results as an operating point, yield the unit function response of the premixed flame, which finally can be transferred into the frequency space by a Laplace-Transformation in order to obtain the frequency response of the flame. The results obtained in this way agree very well with the experimental data of other authors.

The transient flame behaviour shows some typical characteristics of a delay time element with some important details which are controlled by the flame kinetics: as the analysis shows, the chemical delay time, the amplification and the overshooting are the main features which are important especially for the phase angle of the frequency response.

The interaction between the flow pattern of the burner nozzle and chemical kinetic processes also greatly influences the dynamical flame behaviour.

Up to now, most authors have used a simple analytical expression for the unit function response of premixed flames, with the assumption of a constant burning velocity. From the analysis here, it can be concluded very clearly that only a numerical simulation, which takes account of both the chemical kinetics and the flow pattern of the internal burner fluid flow, is able to accurately predict the dynamics of premixed flames.

Therefore, the numerical tool enables us to study the dynamics of real gas turbine flames. Further investigations will concentrate...
on the influence of pressure and turbulence as both of these factors should play an important role in the transient behaviour of flames.

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### APPENDIX

#### Table A1. Methane-air reaction mechanism [1]

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<th>Reaction</th>
<th>A</th>
<th>β</th>
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<td>H + O₂ → O + OH</td>
<td>2.0E14</td>
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<td>70.338</td>
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<tr>
<td>O + OH → O₂ + H</td>
<td>1.57E13</td>
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<td>1.8E10</td>
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<td>36.95</td>
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<td>1.0</td>
<td>28.30</td>
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<td>H + O₂ + M → HO₂ + M</td>
<td>2.3E18</td>
<td>-0.8</td>
<td>0</td>
</tr>
<tr>
<td>H + HO₂ → OH + OH</td>
<td>1.5E14</td>
<td>0.0</td>
<td>4.204</td>
</tr>
<tr>
<td>H + HO₂ → H₂ + O₂</td>
<td>2.5E13</td>
<td>0.0</td>
<td>2.93</td>
</tr>
<tr>
<td>O + HO₂ → H₂O + O₂</td>
<td>2.0E13</td>
<td>0.0</td>
<td>4.168</td>
</tr>
<tr>
<td>CO + OH → CO₂ + H</td>
<td>1.51E7</td>
<td>1.3</td>
<td>-3.17</td>
</tr>
<tr>
<td>CO₂ + H → CO₂ + OH</td>
<td>1.57E9</td>
<td>1.3</td>
<td>93.52</td>
</tr>
<tr>
<td>CH₄ + (+M) → CH₃H + (+M)</td>
<td>6.3E14</td>
<td>0.0</td>
<td>435.43</td>
</tr>
<tr>
<td>CH₄ + (+M) → CH₄H + (+M)</td>
<td>5.2E12</td>
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<td>-5.485</td>
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<tr>
<td>CH₄ + H → CH₃H + H</td>
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<td>3.0</td>
<td>36.63</td>
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<tr>
<td>CH₃H₂ → CH₄H + H</td>
<td>9.5E2</td>
<td>3.0</td>
<td>36.63</td>
</tr>
<tr>
<td>CH₄ + OH → CH₃H₂O</td>
<td>1.6E6</td>
<td>2.1</td>
<td>10.93</td>
</tr>
<tr>
<td>CH₃H₂O → CH₄ + OH</td>
<td>3.0E5</td>
<td>2.1</td>
<td>72.94</td>
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<tr>
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<td>0</td>
</tr>
<tr>
<td>CH₂H + H → HCO + H₂</td>
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<td>0.0</td>
<td>16.71</td>
</tr>
<tr>
<td>CH₂O + OH → HCO + H₂O</td>
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<td>5.003</td>
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<tr>
<td>HCO + H → CO + H₂</td>
<td>4.0E13</td>
<td>0.0</td>
<td>0</td>
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<tr>
<td>HCO + M → CO + H + M</td>
<td>1.6E14</td>
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<td>61.54</td>
</tr>
<tr>
<td>CH₃ + O₂ → CH₂O + O</td>
<td>7.0E12</td>
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<td>107.4</td>
</tr>
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<td>0</td>
</tr>
<tr>
<td>CH₂O + M → CH₂O + M</td>
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<tr>
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<td>0.0</td>
<td>0</td>
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<tr>
<td>H₂O₂ + M → O₂ + OH + M</td>
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<td>190.5</td>
</tr>
<tr>
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<td>-21.26</td>
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<td>7.536</td>
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<td>2.2E22</td>
<td>-2.0</td>
<td>0</td>
</tr>
<tr>
<td>H₂ + H + M → H₂ + M</td>
<td>1.8E18</td>
<td>-1.0</td>
<td>0</td>
</tr>
</tbody>
</table>

**a** Third body efficiencies: CH₄=6.5, H₂O=6.5, CO₂=1.5, H₂=1.0, CO=0.75, O₂=0.4, N₂=0.4

**b** Lindemann form k=k₀(1+k_fM)/(M)

Rate coefficients are defined as: k=kn₀exp(-E/kTV)

Units are: Moles, cubic centimeters, seconds, Kelvins, kJ/Moles

#### Table A2. Lewis numbers

<table>
<thead>
<tr>
<th>CH₄</th>
<th>O₂</th>
<th>H₂O</th>
<th>CO₂</th>
<th>H</th>
<th>O</th>
<th>OH</th>
<th>H₂</th>
<th>CO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Le</td>
<td>0.97</td>
<td>1.11</td>
<td>0.83</td>
<td>1.39</td>
<td>0.18</td>
<td>0.7</td>
<td>0.73</td>
<td>0.3</td>
</tr>
</tbody>
</table>