Numerical investigation of methane combustion under mixed air-steam turbine conditions—FLAMESEEK

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Abstract

Lowering emissions from power generating gas turbines, while retaining efficiency and power output, constitutes a formidable task, both at fundamental and technical levels. Combined gas turbine cycles involving air humidification are particularly attractive, since they provide additional power with improved efficiency. Water or steam addition promotes the reduction of nitrogen oxides emissions, for both the premixed and non-premixed modes of operation. Consequently, there is an urgent need for thorough understanding of the combustion chemistry and flow-chemistry interaction under high pressure and high humidity conditions as well as simulating the turbulent flow field with realistic chemistry. Both objectives require the development of reduced kinetic mechanisms.

Reduced mechanisms for methane combustion valid for high pressure and high humidity are developed here, using the CSP (computational singular perturbation) method. The effects of humidity and pressure on the dynamics of NO formation pathways are discussed. A reaction progress variable model for the simulation of turbulent combustion is also developed, valid for adiabatic, non-adiabatic, premixed as well as partly or non-premixed combustion of various fuels, including natural gas, hydrogen and syngas. The model utilizes the CSP methodology for accurate mapping of the pertinent thermochemical data on a set of two reaction progress variables. Preliminary results are displayed.
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Nomenclature

b	CSP-generated matrix (–)
C	reaction progress variable (–)
D	diffusion coefficient ($m^2 s^{-1}$)
E	number of elements (–)
F	mixture fraction (–)
H	enthalpy ($J kg^{-1}$)
M	number of steady-state relations in reduced mechanism (–)
N	number of species (–)
S	number of steps in reduced mechanism (–)
Sc	Schmidt number (–)
T	time (s)
U	velocity ($m s^{-1}$)
W	normalization function for a reaction progress variable (–)
Y	mass fraction (–)

Greeks

ρ	density ($kg m^{-3}$)
ω	chemical source term (s^{-1})
μ	molecular viscosity (Pa s)

Subscripts

i	species number (–)
j	species number (–)
T	turbulent (–)

Superscripts

s	slow subsystem (–)
u	unburnt (–)
eq	equilibrium (–)
in	inlet (–)
–	reynolds averaged (–)
$\sim$	favre-averaged (–)
c_i	belonging to ith Reaction progress variable (–)
r	fast subsystem (–)
$\wedge$	composed (–)

1. Introduction

Developing computational tools to support the design of gas turbines operating with significantly enhanced air humidity is a primary goal of the FLAMESEEK project. The FLAMESEEK (FLAME sensors for efficient gas turbine engine cycles) project is financially supported by the

European Commission and the participating partners are: Rolls-Royce Power Engineering plc (UK), Alstom Power Sweden AB (Sweden), Lund Universitet (Sweden), Imperial College, London (UK), Universiteit Twente (The Netherlands) and Foundation of Research and Technology Hellas/Institute of Chemical Engineering and High Temperature Chemical Processes (Greece). The specific objectives are to study the effect of air humidity and high pressure on gas turbines power output, efficiency and emissions.

Significant reduction in NO_x levels can be achieved by operating in the lean premixed combustion mode [1,2]. In addition, high pressure ratios present favourable conditions for increased NO_x emissions, e.g., [2,3]. Combined cycles involving air humidification, such as mixed air-steam turbine (MAST) cycles, are particularly attractive since they provide additional power, due to the increased mass flow of humid air and the enhanced thermal capacity of the mixture, with improved efficiency, since virtually no additional compression work is required [4,5]. Water or steam addition is also beneficial to the reduction of nitrogen oxides emissions from gas turbines operating both in the premixed and non-premixed modes [6,7]. This is mainly due to a reduction in temperature, caused by the steam addition, which directly affects the NO production rate due to the thermal mechanism, e.g., [6]. In addition, the presence of steam lowers the O radical levels, which in turn further suppresses the thermal mechanism [7]. The development of reduced mechanisms for methane combustion under high pressure and high humidity conditions is therefore of paramount importance, in order to improve the understanding of relevant phenomena and to make realistic simulations of turbulent flames feasible.

Several reduced mechanisms have appeared in the literature. These include the six-step mechanism for lean mixtures by Glarborg et al. [8] and the seven-step and 10-step mechanisms for atmospheric premixed flames of Massias et al. [9,10]. Higher order reduced mechanisms have also been developed for more complex systems, e.g., [11]. One of the turbulent flame models which allow the direct incorporation of realistic chemistry, such as reduced mechanisms, is the one based on the reaction progress variables (RPVs), see e.g., [12] for an overview.

The first objective of the present paper is thus to develop a reduced mechanism for methane combustion valid for high pressure and high humidity conditions. This mechanism is further validated here for a wide range of equivalence ratios, pressures and humidity levels. The reduction methodology is also employed in order to construct a two-step reduced mechanism, which can be used in turbulent flame calculations. A second objective of the paper is to describe the turbulent combustion model that is based on the transport of the RPVs, allowing for mixing and heat loss through radiation. The source terms of the RPV transport equations are calculated a priori and stored in a thermochemical database. For a stoichiometric, atmospheric premixed flame database results are shown for a two-step reduced mechanism and two RPVs, based on the GRI-3.0 Mechanism [13].

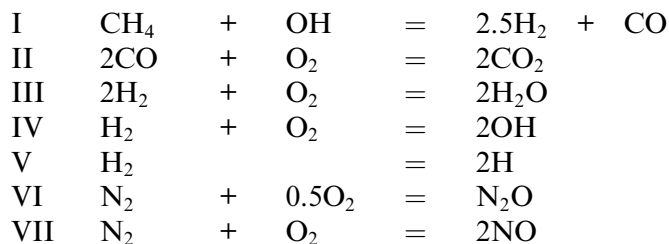## 2. Reduction methodology and mechanism validation

Details of the CSP algorithm [14,15], employed here for the construction of reduced mechanisms, are presented elsewhere [9,10], so only a brief outline of its main features will be given.

The input to the CSP algorithm consists of (i) the detailed mechanism containing N species and E elements, (ii) a numerical solution of the flame structure and (iii) the desired number of global

steps M, in the reduced mechanism. CSP analysis is then performed at each grid point in the computational domain, in order to compute the *local* CSP pointer $D_i(x)$, which is a measure of the degree by which the ith species is locally affected the most by the M fastest chemical time scales. The pointer $D_i(x)$ is integrated across the flame to give a weighted *global* CSP pointer I_i [9,10]. The quantities I_i for each species are ordered and the $N - M$ species with the lowest values, i.e., those globally affected the most by the M fastest chemical time scales, are taken as *major* (or slow) species. The M species with the largest values are identified as *steady-state* (or fast) species. The resulting reduced mechanism consists of $N - M - E$ global steps, the stoichiometry of which involves the major species only and their corresponding global rates involve all, major and steady-state species; the latter calculated from the steady-state algebraic relations with the inner iteration procedure [9].

The detailed chemistry of GRI-3.0 mechanism [13] and its accompanying thermochemistry, incorporating 53 species and 325 reversible reactions, has been used here as the basis for the construction of the reduced mechanisms. The detailed mechanism has been validated over a wide range of pressures and equivalence ratios for methane combustion. Solutions for unstrained, adiabatic, laminar premixed one-dimensional flames with both full detailed and reduced chemistry have been obtained with the code RUN-1DL developed by Rogg [16]. Flames were computed for pressures ranging from 1 to 50 bar, at initial temperatures of 300–900 K and for moisture content of up to 20% by volume. Steam addition was simulated by assuming water to enter the combustor as superheated vapour. It was further assumed that combustion stoichiometry remains constant so that steam does simply act as a diluent.

A seven-step mechanism was constructed on the basis of a detailed solution of the stoichiometric, dry, atmospheric methane-air flame. The global steps for this mechanism are:

$$
\begin{array}{lllllll}
\text{I} & CH_4 & + & OH & = & 2.5H_2 & + & CO \\
\text{II} & 2CO & + & O_2 & = & 2CO_2 \\
\text{III} & 2H_2 & + & O_2 & = & 2H_2O \\
\text{IV} & H_2 & + & O_2 & = & 2OH \\
\text{V} & H_2 & & & = & 2H \\
\text{VI} & N_2 & + & 0.5O_2 & = & N_2O \\
\text{VII} & N_2 & + & O_2 & = & 2NO \\
\end{array}
$$

The mechanism is very similar to that of Massias et al. [9,10] which has been constructed from the GRI-2.11 mechanism based on the same conditions.

The variation of burning velocity for dry ($\omega = 0\%$), stoichiometric ($\phi = 1.0$) $CH_4/O_2/N_2$ flames with pressure is shown in Fig. 1. Generally, there is excellent agreement between detailed and reduced mechanisms although the latter tend to slightly under-predict burning velocities for pressures higher than 15 bar. Agreement in the prediction of species profiles, between detailed and reduced mechanisms, is excellent for major species and very satisfactory for steady-state species. This is shown in Fig. 2 for the case of CO_2 in dry ($\omega = 0\%$), stoichiometric ($\phi = 1.0$) $CH_4/O_2/N_2$ flames and for pressures up to 20 bar. A comparison between detailed and reduced computations for NO at high pressures ($p = 20$ bar) as a function of humidity levels is shown in Fig. 3, where the
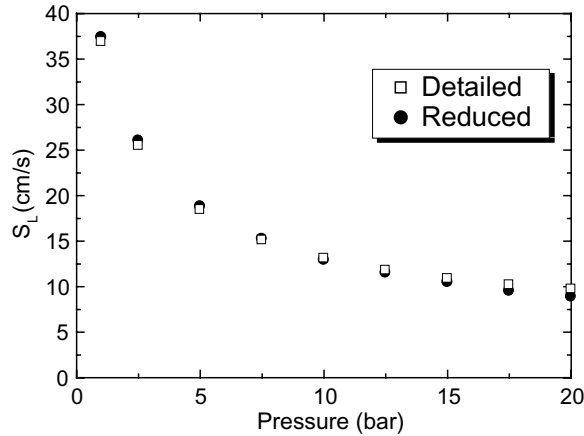
Fig. 1. Computed laminar burning velocities as a function of pressure for dry ($w = 0\%$), stoichiometric ($\phi = 1.0$) CH_4/O_2/N_2 flames.
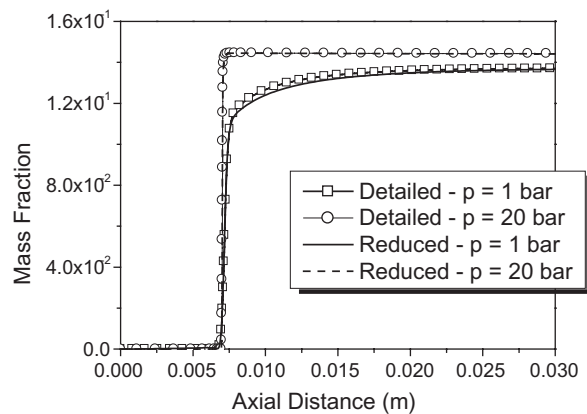

Fig. 2. Computed CO_2 profiles in stoichiometric ($\phi = 1.0$), dry ($w = 0\%$) CH_4/O_2/N_2 flames.

substantial decrease in post-flame ('exhaust') NO levels with increasing water content is clearly outlined. It should be noted that the reduced mechanism tends to slightly over-predict total NO levels in both cases. However, this over-prediction is totally attributed to discrepancies in the flame zone, where the prompt NO mechanism is dominant [2], while in the post-flame zone where the thermal NO mechanism prevails [2] the rate of NO growth is perfectly matched by the reduced mechanism. It can thus be concluded that a reduced mechanism for methane combustion developed for atmospheric conditions may be used to reproduce major flame features of methane flames under high pressure and high humidity conditions, as is further illustrated in Fig. 4. Here the agreement between detailed and reduced computations is excellent for the key H_2 and HO_2 intermediates and at conditions closely resembling realistic MAST combustion.
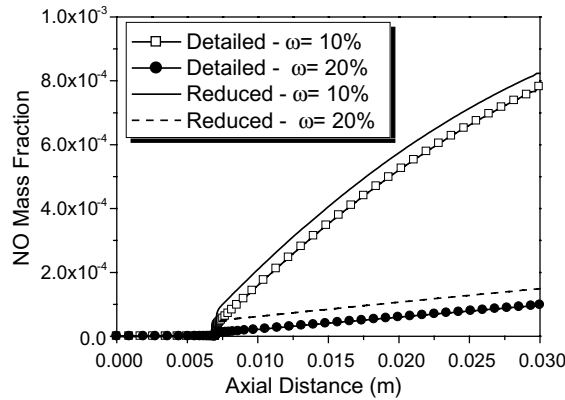
Fig. 3. Computed NO profiles in stoichiometric ($\phi = 1.0$), high pressure ($p = 20$ bar) $CH_4/O_2/N_2$ flames with humidity.
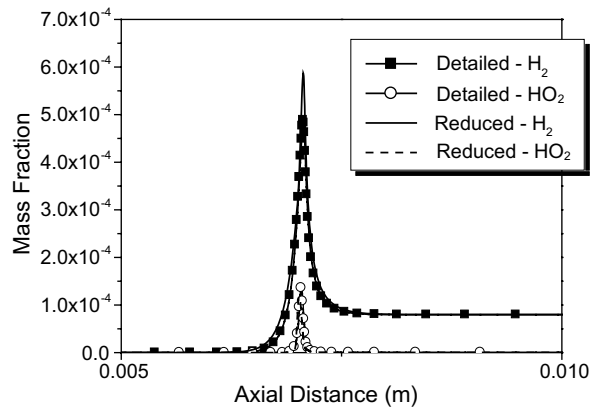

Fig. 4. Computed H_2 and HO_2 profiles in a stoichiometric ($\phi = 1.0$), high pressure ($p = 20$ bar) and high humidity ($\omega = 20\%$) $CH_4/O_2/N_2$ flame with preheat ($T_{in} = 500$ K).

3. Combustion modeling

The turbulent combustion model that is used in the present work is based on RPVs, steady-state and element conservation relations. It is derived analogous to the first combustion model, developed at the University of Twente [17–19], which in turn is based on the work of Janicka and Kollmann [20,21] and Correa [22]. One of the novel features of the present model is the use of CSP to automatically map the chemical mechanism onto RPVs and determine the steady-state and element conservation relations [9]. An outline of this feature is given below.

Non-adiabatic combustion involving N species consisting of E elements is described by N transport equations of the species and one transport equation for the mixture fraction F, which describes the E linear relations for the conservation of the E elements in the stoichiometry.

The number of transport equations is greatly reduced by introducing steady-state relations for some of the species. Thus, use of M steady-state relations leaves $S = N - M - E + 1$ transport

equations to be solved. The CSP method is used here to systematically derive the optimal choice of species assumed to be in steady-state and to determine the RPVs composition, as a linear combination of the species mass fractions. In this way, the S transport equations to be solved are the least stiff possible [9]. The reduced system of equations consists of S species transport equations, one transport equation for mixture fraction, M steady-state relations and E linear relations for the elements conservation. This constitutes a total of N equations, which along with the enthalpy transport equation and the Navier–Stokes equations, describe the combusting flow field.

An advantage of this model over earlier combustion models such as the Bray–Moss–Libby or Eddy Break Up models is, that it incorporates from first principles detailed chemistry in the transport equations for the reduced chemistry system. Either implicitly or explicitly, all specified chemical species and enthalpy are involved in the current model. This is of advantage as opposed to the use of one or a few global reaction steps in BML or EBU models or a phenomenological correlation like the flamelet models. An advantage over the intrinsic-low-dimensional-manifold approach is that the species combination vectors spanning the reduced chemical system space also are specified by the CSP reduction algorithm, ensuring that the resulting system of equations is the least stiff. This is not necessarily the case in the ILDM approach.

4. Transport equation for a reaction progress variable

In this section the transport equations will be described for the case of a turbulent premixed flame, when using the CSP-reaction progress variable modeling approach. The transport equation for the mass fraction of a species Y_i is:

$$\frac{\partial Y_i}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_i) - \nabla \cdot (\rho D \nabla Y_i) = \boldsymbol{\omega}_i \tag{1}$$

where D is the diffusion coefficient, ρ is the density, $\mathbf{u}$ is the velocity vector and $\boldsymbol{\omega}$ is the source term. A linear combination of species mass fraction is defined as

$$\hat{Y}_i = \sum_{j=1}^{N} b_{ij}^{s} Y_j \tag{2}$$

where, b_{ij}^{s} $(i = 1, N - M - E)$ are obtained from CSP, for details see [9]. Using this definition, a RPV can be defined by normalizing $\hat{Y}_i$ with the equilibrium and 'unburnt' or 'frozen' compositions:

$$c_i = \frac{\hat{Y}_i - \hat{Y}_i^{u}}{\hat{Y}_i^{eq} - \hat{Y}_i^{u}} = \frac{\hat{Y}_i - \hat{Y}_i^{u}}{W(f)} \tag{3}$$

where $\hat{Y}_i^{u}$ is the upstream composition and $\hat{Y}_i^{eq}$ is the adiabatic equilibrium composition, both a function of mixture fraction as present in the premixed flame. Under the assumption of equal diffusivity D, a transport equation for a RPV c_i can be created by inserting expression (3) into expression (1) [18]. For use in turbulent combustion simulations, the c_i scalars are Favre-averaged. This is at present done using the presumed shape PDF method (see e.g., [23] for details). Usually, the beta-function or delta-function is employed as probability density function (PDF)

shape. Here, for simplicity, the delta-PDF is used, resulting in transport equations for the mean values of the variables only. Also the combustion is assumed here adiabatic, so that the enthalpy of the system is constant, i.e., $h = h^{in}$. With these assumptions the following equations for the RPVs and the steady-state relations are obtained [18]:

$$\nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{c}_i) - \nabla \cdot \left(\bar{\rho} \left(D + \frac{\mu_T}{Sc_T} \right) \nabla \tilde{c}_i \right) = \tilde{\omega}_{c_i} \tag{4}$$

$$\sum_{j=1}^{N} b_{kj}^{r} \omega_j = 0 \tag{5}$$

where $\tilde{c}_i$ is the Favre-averaged RPV c_i, $i = 1, \ldots, S$, $k = 1, \ldots, M$, the b_{kj}^{r} are obtained from CSP [9].

Note that use of CSP for the algorithmic identification of the M steady-state species and the S RPVs allows the simplification of arbitrary large detailed mechanisms and ensures that the transport equations constructed on the basis of the reduced mechanisms are the most realistic and least stiff; the effects of the fast chemical time scales being absorbed by the steady-state relations [9].

The source terms of the transport equations for the RPVs are calculated a priori and stored in a thermochemical database [18]; this task being performed by a dedicated subroutine. In the problem considered here, i.e., premixed combustion and a presumed delta-PDF, the database needs only to contain the source terms and the mass fraction vector as function of the RPVs.

Solving the transport Eq. (4), the source terms are obtained from the database. In a post-processing step, the mass fractions of the species are regained from the solution, through the definition (3) and the algebraic relations expressing the M steady-state assumptions and the E element conservation.

4.1. Two-step CSP-reduced mechanism

In this section, some database results will be shown for a stoichiometric, atmospheric premixed flame. The database was constructed on the basis of a two-step CSP-reduced mechanism. The calculations were performed using the GRI-3.0 mechanism, consisting of $N = 53$ species and $E = 5$ elements involved in 325 elementary reactions [13]. Since two steps are used to describe the reduced chemistry and the mixture fraction is constant, $S = 2$ and 46 ($= N$–S–E) steady-state relations are needed to close the system. The linear combinations of species mass fraction $\hat{Y}_i$, $i = 1, 2$ defined as in Eq. (2), are displayed on Table 1. Almost all species participate in each scalar, showing that it is impossible to have done this reduction manually. The resulting database took approximately five wall clock minutes to compute on a single CPU of an origin 200 system and consists of 20 points per RPV, 400 points in total.

The database contains the species mass fractions, RPV source terms and density or temperature, as function of $\tilde{c}_1$ and $\tilde{c}_2$. In Fig. 5, where the temperature is plotted, it can be seen that an almost linear behavior is emerging, most likely due to the particular CSP c_1 and c_2 identifications. Indeed, in case a manual reduction is performed (in which case a usual choice for $\hat{Y}_1$ and $\hat{Y}_2$ would be CO_2 and H_2O and the steady-state relations obtained by CSP are still used)

Table 1
CSP definition of RPVs, two-step mechanism, GRI-3.0 mechanism

| Y^1				
H_2	$-1.5*H$	$-O$	$-0.5*OH$	$-1.5*HO_2$
$-H_2O_2$	$-3*C$	$-2.5*CH$	$-2*CH_2$	$-2*CH_2(S)$
$-1.5*CH_3$	$-CH_4$	$-1.5*HCO$	$-CH_2O$	$-2.5*CH_2OH$
$-2.5*CH_3O$	$-2*CH_3OH$	$+0.5*C_2H$	$+ C_2H_2$	$-0.5*C_2H_3$
$-1.5*C_2H_5$	$-3*C_2H_6$	$-0.5*HCCO$	$+2*CH_2CO$	$+2*HCCOH$
$-2*N$	$-1.5*NH$	$-3*NH_2$	$-2.5*NH_3$	$-1.5*NNH$
$-NO$	$-N_2O$	$-0.5*HNO$	$-CN$	$-0.5*HCN$
$-2*H_2CN$	$-2.5*HCNN$	$-1.5*HCNO$	$+0.5*HOCN$	$-1.5*HNCO$
$-1.5*C_3H_7$	$-3*C_3H_8$	$+0.5*CH_2CHO$		$-CH_3CHO$
Y^2				
H_2	$+0.5*H$	$-O$	$-2*O_2$	$-0.5*OH$
$-1.5*HO_2$	$-H_2O_2$	$+C$	$+1.5*CH$	$+2*CH_2$
$+2*CH_2(S)$	$+2.5*CH_3$	$+3*CH_4$	$+0.5*HCO$	$+CH_2O$
$+1.5*CH_2OH$	$+1.5*CH_3O$	$+2*CH_3OH$	$+2.5*C_2H$	$+3*C_2H_2$
$+3.5*C_2H_3$	$+4*C_2H_4$	$+4.5*C_2H_5$	$+5*C_2H_6$	$+1.5*HCCO$
$+2*CH_2CO$	$+2*HCCOH$	$+0.5*NH$	$+NH_2$	$+1.5*NH_3$
$+0.5*NNH$	$-NO$	$-2*NO_2$	$-N_2O$	$-0.5*HNO$
$+CN$	$+1.5*HCN$	$+2*H_2CN$	$+1.5*HCNN$	$+0.5*HCNO$
$+0.5*HOCN$	$+0.5*HNCO$	$+6.5*C_3H_7$	$+7*C_3H_8$	$+2.5*CH_2CHO$
$+3*CH3CHO$				
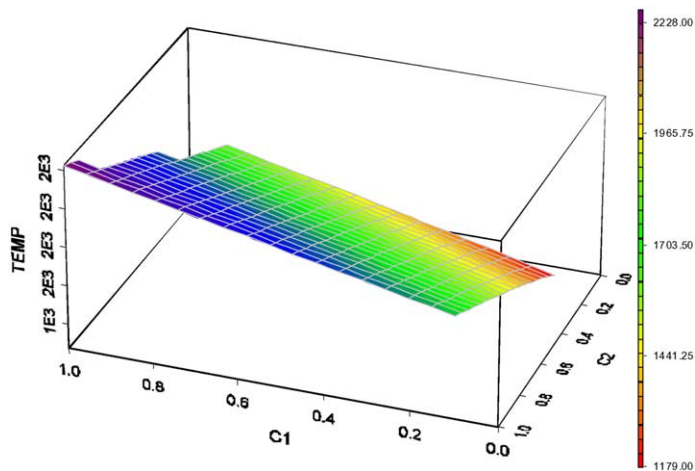
Fig. 5. Temperature as function of RPV values.

the temperature profile is heavily non-linear in c_1 and c_2. The source terms themselves, shown in Figs. 6 and 7, are not linear in c_1 and c_2. However, it can be seen that both are described by smooth surfaces, an obviously desired outcome. The same is true for the NO mass fraction, shown in Fig. 8.
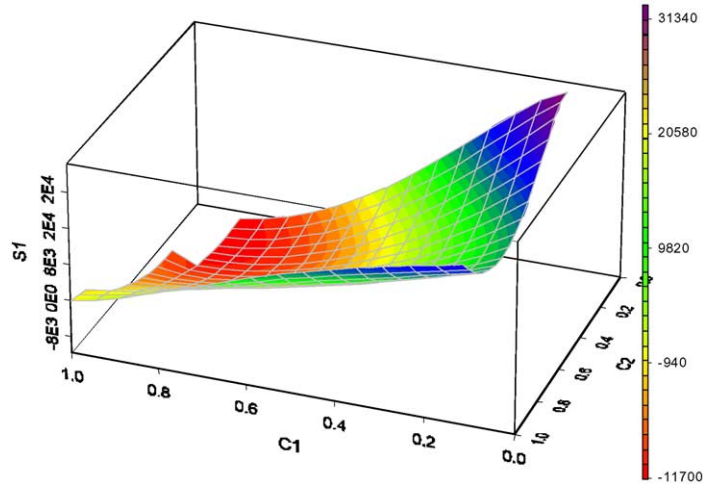
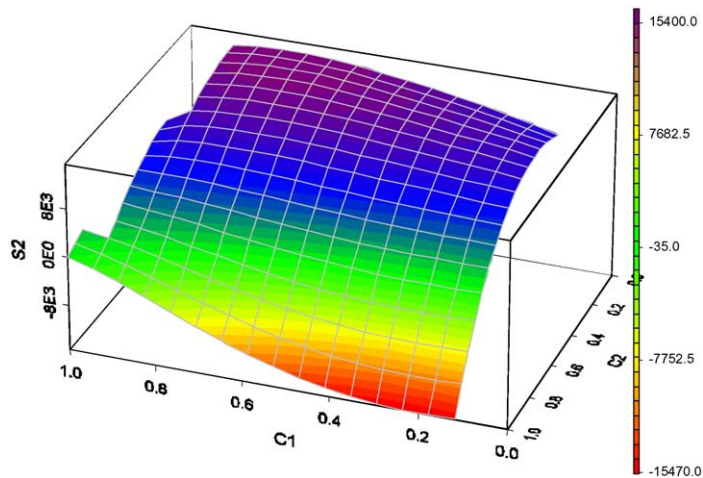Fig. 6. Source term of RPV1 as function of RPV values.

Fig. 7. Source term RPV2 as function of RPV values.

5. Conclusions

It was shown that, with the use of CSP, an accurate seven-step reduced mechanism was developed for methane combustion valid for high pressure and high humidity conditions. Using the same methodology, a two-step mechanism was constructed, for use in turbulent calculations. The generated thermochemical databases were shown to be smooth with respect to the dependent variables, thus very suitable for use in turbulent combustion simulations of methane or natural gas. In the future, these databases will be used to perform numerical simulations of MAST combustion chambers to assess their performance and to propose design guidelines.
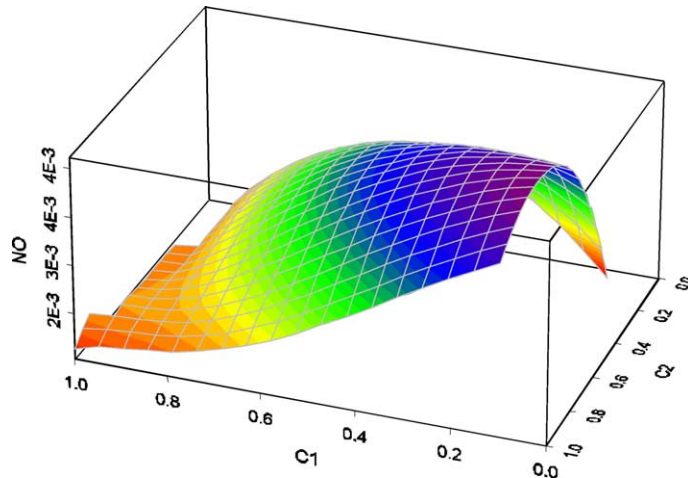
Fig. 8. NO mass fraction as function of RPV values.

Acknowledgement

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