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A REDUCED KINETIC MECHANISM FOR PROPANE FLAMES

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ABSTRACT

Propane is one of the simplest hydrocarbons that can be a representative of higher hydrocarbons used in many applications. Therefore, this work develops a ten-step reduced kinetic mechanism among 14 reactive species for the propane combustion. The model is based on the solution of the flamelet equations. The equations are discretized using the second-order space finite difference method, using LES (Large-Eddy Simulation). Obtained results compare favorably with data in the literature for a propane jet diffusion flame. The main advantage of this strategy is the decrease of the work needed to solve the system of governing equations.

Keywords: reduced mechanism, diffusion flames, propane

NOMENCLATURE

A frequency factor

c_p specific heat capacity at constant pressure, $J/(kg\ K)$

Ea activation energy, cal/mol

k reaction rate coefficient, $(time)^{-1}$ $(concentration)^{1-n}$, where n is the order of the reaction

L_e Lewis number

Q_k heat of combustion of the reaction k, J/mol

R gas constant, $cal/(mol\ K)$

R_e Reynolds number

S_c Schmidt number

t dimensionless time

T temperature, K

$\widetilde{u}_j$ dimensionless velocity vector

w_k reaction rate of the reaction k, $mol/(cm^3\ s)$

W_i molecular weight of species i, g/mol

x_j dimensionless spatial coordinate

$\widetilde{Y}_i$ mass fraction of the species i

$Y_{C3H8,1}$ mass fraction of fuel in the fuel stream

$Y_{O2,2}$ mass fraction of oxygen in the oxidizer stream

$\widetilde{Z}$ global mixture fraction

$\widetilde{Z}_i$ mixture fraction of each fuel and products important species

Z_{st} stoichiometric mixture fraction

Greek symbols

$\widetilde{\chi}$ dimensionless scalar dissipation rate

β temperature exponent

$\overline{\mu}_T$ dimensionless turbulent viscosity

ν stoichiometric mass ratio

$\nu_{i,k}$ stoichiometric coefficients of the species i in the reaction k

ρ density, g/cm^3

τ dimensionless time defined in the coordinate system attached to the stoichiometric surface

INTRODUCTION

Propane is an important fuel and its high temperature combustion is characterized by the rapid decomposition into smaller C_1-C_3 intermediates (Leung *et al.*, 1993). In combustion and autoignition processes, the propane breaks down first into propene and then into products (Petrova and Williams, 2006). Propane is rapidly consumed on the rich side of the flames to produce a large amount of C_1 and C_2 intermediates, especially at low strain rate conditions. The attack by H and OH radicals are the major consumption paths for propane and the intermediate species, with the exception of the acetylene where the O atom attack is dominant (Leung *et al.*, 1993).

Chemical kinetic modeling has become an important tool for interpreting and understanding the combustion phenomena (Leung and Lindstedt, 1995). A large amount of effort has been devoted to the development of detailed and reduced kinetic mechanisms for hydrocarbon combustion. Detailed kinetic mechanisms describing hydrocarbon combustion are conceptually structured in a hierarchical manner, with H_2 and CO chemistry at the base, supplemented as needed by elementary reactions of larger chemical species (Qin *et al.*, 2000). For the propane, detailed and reduced mechanisms were developed in the works from Leung *et al.* (1993), Leung and Lindstedt (1995), Qin *et al.* (2000), Marazioti and Koutmos (2002), Curran

et al. (2004), Anetor *et al.* (2012), among others. According to Kennel *et al.* (1993), reduced mechanisms for propane premixed flames contains nine, six or four steps, and according to Leung *et al.* (1993), nine or seven steps for propane-air diffusion flames are needed.

In this work, good agreement has been obtained between data from the literature and predictions for the mass fraction of the major species.

OBTAINMENT OF THE REDUCED KINETIC MECHANISM

When detailed kinetic mechanisms are employed to analyze flames, a conservation equation must be solved for each species. Therefore, it is desirable to use simplified kinetic mechanisms that describe the reaction system in terms of few species. In this work is used a set of reactions for the propane combustion given by the references (Leung *et al.*, 1993), (Mehl *et al.*, 2009) and (http://web.eng.ucsd.edu/mae/groups/combustion/mechanism.html, consulted in 21 June 2012).

The reduction of the chemical kinetic mechanism is based on following steps (Peters, 1988):

- Estimate the order of magnitude of the reaction rate coefficients and define the main chain;
- Apply partial equilibrium and steady-state assumptions;
- Identify global reactions and their principal rates;
- Justify the assumptions by asymptotic analysis.

The reaction rate coefficients, $(time)^{-1}$ $(concentration)^{1-n}$, where n is the order of the reaction, are calculated using the modified Arrhenius equation, for $T = 900K$,

$$k = AT^{\beta} \exp\left(-\frac{Ea}{RT}\right) \qquad (1)$$

where A is the frequency factor, T the temperature, K, β the temperature exponent, Ea the activation energy, *cal/mol*, and R the gas constant, *cal/(mol K)*. The main chain is selected based on the coefficients k of each elementary reaction, and is presented in the Fig. 1.

The reduction strategy is based on the introduction of steady-state and partial equilibrium assumptions. For a homogeneous system, the steady-state hypothesis is valid for those intermediate species that are produced by slow reactions and consumed by fast reactions, such that their concentration remains small (Turns, 2000). The assumption of partial equilibrium may be justified

when the rate coefficients of both the forward and backward steps of a single reaction are much larger than all other rate coefficients (Peters, 1988).
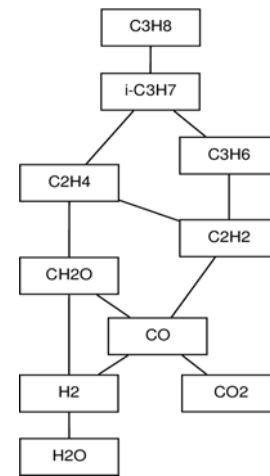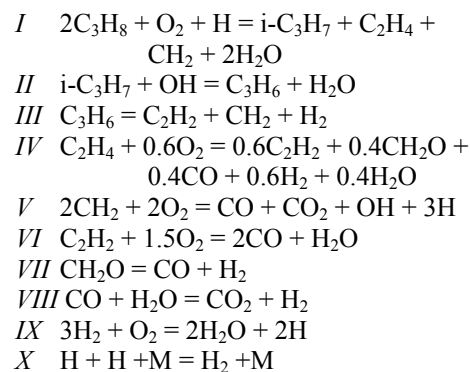

Figure 1. Diagram of the main chain for the propane reduced mechanism.

After applying the hypothesis of partial equilibrium for those reactions with high specific forward and backward rates, it remains the reactions of the Table 1. Considering the steady-state assumption for the species C_2H_3, C_2H, CHCO, CH_3, HCO, HO_2 and O, it results the following ten-step mechanism among 14 species for the propane

$$
\begin{array}{ll}
I & 2C_3H_8 + O_2 + H = i\text{-}C_3H_7 + C_2H_4 + \\
& \qquad CH_2 + 2H_2O \\
II & i\text{-}C_3H_7 + OH = C_3H_6 + H_2O \\
III & C_3H_6 = C_2H_2 + CH_2 + H_2 \\
IV & C_2H_4 + 0.6O_2 = 0.6C_2H_2 + 0.4CH_2O + \\
& \qquad 0.4CO + 0.6H_2 + 0.4H_2O \\
V & 2CH_2 + 2O_2 = CO + CO_2 + OH + 3H \\
VI & C_2H_2 + 1.5O_2 = 2CO + H_2O \\
VII & CH_2O = CO + H_2 \\
VIII & CO + H_2O = CO_2 + H_2 \\
IX & 3H_2 + O_2 = 2H_2O + 2H \\
X & H + H + M = H_2 + M
\end{array}
$$

where M is an inert needed to remove the bond energy that is liberated during recombination.

Table1. Propane mechanism rate coefficients[1].

Reactions	A	β	Ea
1. $O_2 + H = OH + O$*	2.00E+14	0.00	70.3
2. $H_2 + O = OH + H$*	5.06E+04	2.67	26.3
3. $H_2 + OH = H_2O + H$*	1.00E+08	1.60	13.8
4. $H + H_2O = H_2 + OH$***	2.29E+09	1.40	18320
5. $H_2 + M = H + H + M$***	4.58E+19	-1.40	104400

[1] Units are *mol*, cm^3, *s*, *K* and *kJ/mol* for *Leung *et al.* (1993), **http://web.eng.ucsd.edu/mae/groups/combustion/mechanism.html, consulted in 21 June 2012, and *mol*, cm^3, *s*, *K* and *cal/mol* for ***Mehl *et al.* (2009).

6. $O_2 + M = O + O + M$***	4.42E+17	-0.63	118900
7. $O + O + M = O_2 + M$***	6.17E+15	-0.50	0
8. $O + H + M = OH + M$***	4.71E+18	-1.00	0
9. $HO_2 + H = H_2O + O$*	3.00E+13	0.00	7.2
10. $HO_2 + M = H + O_2 + M$***	3.09E+12	0.52	48870
11. $HO_2 + H = H_2 + O_2$***	1.66E+13	0.00	823
12. $HO_2 + OH = H_2O + O_2$***	1.97E+10	0.96	-328.4
13. $H + H + M = H_2 + M$*	1.80E+18	-1.00	0
14. $CO + OH = CO_2 + H$*	4.40E+06	1.50	-3.1
15. $HCO + O_2 = CO + HO_2$***	7.58E+12	0.00	410
16. $CH_2O + H = HCO + H_2$***	5.74E+07	1.90	2740
17. $CH_2 + O_2 = CO + OH + H$*	6.50E+12	0.00	6.3
18. $CH_2 + O_2 = CO_2 + H + H$*	6.50E+12	0.00	6.3
19. $CH_3 + H = CH_2 + H_2$*	1.80E+14	0.00	63
20. $CH_3 + O_2 = CH_2O + OH$*	3.40E+11	0.00	37.4
21. $CHCO + O = CO + CO + H$*	1.00E+14	0.00	0
22. $C_2H + O_2 = CHCO + O$*	5.00E+13	0.00	3.6
23. $C_2H_2 + OH = C_2H + H_2O$*	1.00E+13	0.00	29.3
24. $C_2H_3 = C_2H_2 + H$*	2.00E+14	0.00	166.29
25. $C_2H_4 + O = CH_3 + CO + H$*	1.60E+09	1.20	3.1
26. $C_2H_4 + OH = C_2H_3 + H_2O$*	3.00E+13	0.00	12.6
27. $C_2H_4 + H = C_2H_3 + H_2$***	5.07E+07	1.93	12950
28. $C_2H_4 + O = CH_3 + HCO$***	8.56E+06	1.88	183
29. $C_3H_6 = C_2H_3 + CH_3$***	2.73E+62	-13.3	123200
30. $i-C_3H_7 = C_2H_4 + CH_3$*	6.30E+13	0.00	154.5
31. $i-C_3H_7 + O_2 = C_3H_6 + HO_2$*	1.00E+12	0.00	20.9
32. $C_3H_8 + O_2 = i-C_3H_7 + HO_2$**	4.00E+13	0.00	199
33. $C_3H_8 + OH = i-C_3H_7 + H_2O$***	1.05E+10	0.97	1586

The obtained reduced mechanism can be justified by an asymptotic analysis. For the set of elementary reactions shown in the Table 1, the balance equations can be written as

$$w_{O2} = - w_1 - w_6 + w_7 + w_{10} + w_{11} + w_{12} - w_{15} - w_{17}$$
$$- w_{18} - w_{20} - w_{22} - w_{31} - w_{32}$$
$$w_{H2} = - w_2 - w_3 + w_4 - w_5 + w_{11} + w_{13} + w_{16} + w_{19}$$
$$+ w_{27}$$
$$w_{H2O} = + w_3 - w_4 + w_9 + w_{12} + w_{23} + w_{26} + w_{33}$$
$$w_{OH} = + w_1 + w_2 - w_3 + w_4 + w_8 - w_{12} - w_{14} + w_{17}$$
$$+ w_{20} - w_{23} - w_{26} - w_{33}$$
$$w_{HO2} = - w_9 - w_{10} - w_{11} - w_{12} + w_{15} + w_{31} + w_{32}$$
$$w_H = - w_1 + w_2 + w_3 - w_4 + 2w_5 - w_8 - w_9 + w_{10}$$
$$- w_{11} - 2w_{13} + w_{14} - w_{16} + w_{17} + 2w_{18} - w_{19}$$
$$+ w_{21} + w_{24} + w_{25} - w_{27}$$
$$w_O = + w_1 - w_2 + 2w_6 - 2w_7 - w_8 + w_9 - w_{21} + w_{22}$$
$$- w_{25} - w_{28}$$
$$w_{C3H8} = - w_{32} - w_{33}$$
$$w_{i-C3H7} = - w_{30} - w_{31} + w_{32} + w_{33}$$
$$w_{C3H6} = - w_{29} + w_{31}$$
$$w_{C2H4} = - w_{25} - w_{26} - w_{27} - w_{28} + w_{30}$$
$$w_{C2H3} = - w_{24} + w_{26} + w_{27} + w_{29}$$
$$w_{C2H2} = - w_{23} + w_{24}$$
$$w_{C2H} = - w_{22} + w_{23}$$

$$w_{CHCO} = - w_{21} + w_{22}$$
$$w_{CH3} = - w_{19} - w_{20} + w_{25} + w_{28} + w_{29} + w_{30}$$
$$w_{CH2} = - w_{17} - w_{18} + w_{19}$$
$$w_{CH2O} = - w_{16} + w_{20}$$
$$w_{HCO} = - w_{15} + w_{16} + w_{28}$$
$$w_{CO} = - w_{14} + w_{15} + w_{17} + 2w_{21} + w_{25}$$
$$w_{CO2} = + w_{14} + w_{18}$$

where w_k represents the reaction rate of the reaction k, $mol/(cm^3\ s)$. The positive sign refers to the species which appears as products in the elementary reaction, while the negative sign refers to the species that appear as reactants. For example, in the reaction 1: $O_2 + H = OH + O$, $w_{O2} = -w_1$ and $w_{OH} = +w_1$, repeating this procedure for all other species and reactions of the mechanism.

The application of the steady-state hypothesis for the species C_2H_3, C_2H, $CHCO$, CH_3, HCO, HO_2 and O, leads to 8 algebraic equations among the reaction rates w_k:

$$w_8 = + w_1 - w_2 + 2w_6 - 2w_7 + w_9 - w_{25} - w_{28}$$
$$w_{12} = - w_9 - w_{10} - w_{11} + w_{16} + w_{31} + w_{32} + w_{28}$$
$$w_{15} = + w_{16} + w_{28}$$
$$w_{18} = + 4w_1 - 2w_3 + 2w_4 + 4w_6 - 4w_7 + 4w_9$$
$$+ 2w_{10} + 2w_{11} - 2w_{14} - 2w_{16} + w_{17} + w_{20}$$
$$- 2w_{23} - w_{25} - 2w_{26} - 3w_{28} + 2w_{30} - 3w_{32} - 3w_{33}$$
$$w_{19} = - w_{20} + w_{25} + w_{28} + w_{29} + w_{30}$$
$$w_{21} = + w_{23}$$
$$w_{22} = + w_{23}$$
$$w_{24} = + w_{26} + w_{27} + w_{29}$$

Thus, the balance equations can be rewritten as

$$w_{O2} = - 5w_1 + 2w_3 - 2w_4 - 5w_6 + 5w_7 - 5w_9 - 2w_{10}$$
$$- 2w_{11} + 2w_{14} + 2w_{16} - 2w_{17} - 2w_{20} + w_{23}$$
$$+ w_{25} + 2w_{26} + 3w_{28} - 2w_{30} + 3w_{32} + 3w_{33}$$
$$w_{H2} = - w_2 - w_3 + w_4 - w_5 + w_{11} + w_{13} + w_{16} - w_{20}$$
$$+ w_{25} + w_{27} + w_{28} + w_{29} + w_{30}$$
$$w_{H2O} = + w_3 - w_4 - w_{10} - w_{11} + w_{16} + w_{23} + w_{26}$$
$$+ w_{28} + w_{31} + w_{32} + w_{33}$$
$$w_{OH} = + 2w_1 - w_3 + w_4 + 2w_6 - 2w_7 + 2w_9 + w_{10}$$
$$+ w_{11} - w_{14} - w_{16} - w_{17} + w_{20} - w_{23} - w_{25} - w_{26}$$
$$- 2w_{28} - w_{31} - w_{32} - w_{33}$$
$$w_H = + 6w_1 + 2w_2 - 3w_3 + 3w_4 + 2w_5 + 6w_6 - 6w_7$$
$$+ 6w_9 + 5w_{10} + 3w_{11} - 2w_{13} - 3w_{14} - 5w_{16}$$
$$+ 3w_{17} + 3w_{20} - 3w_{23} - w_{25} - 3w_{26} - 6w_{28}$$
$$+ 3w_{30} - 6w_{32} - 6w_{33}$$
$$w_{C3H8} = - w_{32} - w_{33}$$
$$w_{i-C3H7} = - w_{30} - w_{31} + w_{32} + w_{33}$$
$$w_{C3H6} = - w_{29} + w_{31}$$
$$w_{C2H4} = - w_{25} - w_{26} - w_{27} - w_{28} + w_{30}$$
$$w_{C2H2} = - w_{23} + w_{26} + w_{27} + w_{29}$$
$$w_{CH2} = - 4w_1 + 2w_3 - 2w_4 - 4w_6 + 4w_7 - 4w_9$$
$$- 2w_{10} - 2w_{11} + 2w_{14} + 2w_{16} - 2w_{17}$$
$$- 2w_{20} + 2w_{23} + 2w_{25} + 2w_{26} + 4w_{28} + w_{29}$$
$$- w_{30} + 3w_{32} + 3w_{33}$$
$$w_{CH2O} = - w_{16} + w_{20}$$
$$w_{CO} = - w_{14} + w_{16} + w_{17} + 2w_{23} + w_{25} + w_{28}$$
$$w_{CO2} = + 4w_1 - 2w_3 + 2w_4 + 4w_6 - 4w_7 + 4w_9$$

$+ 2w_{10} + 2w_{11} - w_{14} - 2w_{16} + w_{17} + w_{20} - 2w_{23}$
$- w_{25} - 2w_{26} - 3w_{28} + 2w_{30} - 3w_{32} - 3w_{33}$

resulting in the mechanism *I-X*. From the reactions *I-X*, it is observed that the production rates of the 14 species, which appear explicitly in the reduced mechanism, can be expressed in terms of 10 global rates as:

$w_{O2} = - w_I - 0.6w_{IV} - 2w_V - 1.5w_{VI} - w_{IX}$
$w_{H2} = w_{III} + 0.6w_{IV} + w_{VII} + w_{VIII} - 3w_{IX} + w_X$
$w_{H2O} = 2w_I + w_{II} + 0.4w_{IV} + w_{VI} - w_{VIII} + 2w_{IX}$
$w_{OH} = - w_{II} + w_V$
$w_H = - w_I + 3w_V + 2w_{IX} - 2w_X$
$w_{C3H8} = - 2w_I$
$w_{i-C3H7} = w_I - w_{II}$
$w_{C3H6} = w_{II} - w_{III}$
$w_{C2H4} = w_I - w_{IV}$
$w_{C2H2} = w_{III} + 0.6w_{IV} - w_{VI}$
$w_{CH2} = w_I + w_{III} - 2w_V$
$w_{CH2O} = 0.4w_{IV} - w_{VII}$
$w_{CO} = 0.4w_{IV} + w_V + 2w_{VI} + w_{VII} - w_{VIII}$
$w_{CO2} = w_V + w_{VIII}$

where

$w_I = 0.5(w_{32} + w_{33})$
$w_{II} = w_{30} + w_{31} - 0.5(w_{32} + w_{33})$
$w_{III} = w_{29} + w_{30} - 0.5(w_{32} + w_{33})$
$w_{IV} = w_{25} + w_{26} + w_{27} + w_{28} - w_{30}$
$\quad + 0.5(w_{32} + w_{33})$
$w_V = 2w_1 - w_3 + w_4 + 2w_6 - 2w_7 + 2w_9 + w_{10}$
$\quad + w_{11} - w_{14} - w_{16} + w_{17} + w_{20} - w_{23} - w_{25} - w_{26}$
$\quad - 2w_{28} + w_{30} - 1.5(w_{32} + w_{33})$
$w_{VI} = w_{23} + 0.6w_{25} - 0.4w_{26} - 0.4w_{27} + 0.6w_{28}$
$\quad + 0.4w_{30} - 0.2(w_{32} + w_{33})$
$w_{VII} = w_{16} - w_{20} + 0.4(w_{25} + w_{26} + w_{27} + w_{28}$
$\quad - w_{30}) + 0.2(w_{32} + w_{33})$
$w_{VIII} = 2w_1 - w_3 + w_4 + 2w_6 - 2w_7 + 2w_9 + w_{10}$
$\quad + w_{11} - w_{16} - w_{23} - w_{26} - w_{28} + w_{30}$
$\quad - 1.5(w_{32} + w_{33})$
$w_{IX} = w_1 + w_6 - w_7 + w_9 - 0.5(w_{23} + w_{25} + w_{28}$
$\quad + w_{32} + w_{33})$
$w_X = w_1 - w_2 - w_5 + w_6 - w_7 + w_9 - w_{10} + w_{13}$
$\quad + w_{16} - 0.5w_{23} - 1.5w_{25} - 0.5w_{28}$

NUMERICAL PROCEDURE

To validate the reduced mechanism developed for the propane, consider the simulation of a jet diffusion flame. For the combustion process, the set of equations for the chemistry includes the temperature, mixture fraction and species mass fraction equations. Favre filtering, or density weighted Favre filtering, becomes convenient when writing the governing equations for turbulent flows. The variables are Favre averaged or density weighted by $\tilde{f} = \overline{\rho f} / \overline{\rho}$, where the bar denotes the standard LES (Large-Eddy Simulation) filtering (Qin *et al.*, 2000), (Steiner and Bushe, 1998), and ρ is the

density, g/cm^3. In these results it is employed the Lagrangian flamelet model for the chemistry, which allows to decouple the fluid flow from the chemistry problem. As combustion occurs in a thin layer of the flame, where the local mixture fraction gradient is sufficiently high, we introduce an orthogonal coordinate system attached to the surface of the stoichiometric mixture. The equations in nondimensionalised form can be derived by applying a spatial, density-weighted filter, resulting in for the:

- Mixture fraction

$$\frac{\partial\left(\overline{\rho}\tilde{Z}\right)}{\partial t} + \frac{\partial\left(\overline{\rho}\tilde{u}_j\tilde{Z}\right)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\overline{\mu}_T}{R_e S_c}\frac{\partial\tilde{Z}}{\partial x_j}\right) \quad (2)$$

- Temperature

$$\frac{\partial\tilde{T}}{\partial\tau} - \frac{a\tilde{\chi}}{2}\frac{\partial^2\tilde{T}}{\partial\tilde{Z}^2} = \tilde{w}_T \quad (3)$$

- Species mass fractions

$$\frac{\partial\tilde{Y}_i}{\partial\tau} - \frac{a\tilde{\chi}}{2L_e}\frac{\partial^2\tilde{Y}_i}{\partial\tilde{Z}^2} = \pm\tilde{w}_i \quad (4)$$

where '~' denotes the Favre averaged variables; $\tilde{Z} = \sum_{i=1}^{n}\tilde{Z}_i$ is the global mixture fraction, $\tilde{Z}_i$ the mixture fraction of each fuel and products important species (C_3H_8, i-C_3H_7, C_3H_6, C_2H_4, C_2H_2, CH_2O, CH_2, CO, CO_2, H_2 and H_2O), $\tilde{Y}_i$ the mass fraction of the species i, t the time, $\tilde{u}_j$ the velocity vector, x_j the spatial coordinate, $\overline{\mu}_T$ the turbulent viscosity, τ the time defined in the coordinate system attached to the stoichiometric surface, $a = \Delta Z Z_{st}\left(1 - Z_{st}\right)$, $\Delta Z \approx 2Z_{st}$, $\tilde{\chi}$ is the scalar dissipation rate, $\tilde{w}_T = \left(\sum_{k=1}^{r}Q_k\tilde{w}_k\right)/c_p$, $\tilde{w}_i = W_i\sum_{k=1}^{r}\nu_{i,k}\tilde{w}_k$ the reaction rate of the species i, Q_k the heat of combustion of the reaction k, J/mol, c_p the specific heat capacity at constant pressure, $J/(kg\ K)$, W_i the molecular weight of species i, g/mol, $\nu_{i,k}$ the stoichiometric coefficients of the species i in the reaction k, and $\tilde{w}_k$ the reaction rate of the reaction k, R_e the Reynolds, S_c the Schmidt, and L_e the Lewis numbers.

The stoichiometric mixture fraction is obtained considering the global mechanism for propane combustion,

$$C_3H_8 + 5O_2 = 3CO_2 + 4H_2O \quad (5)$$
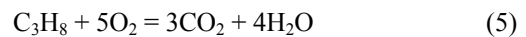
through the expression

$$Z_{st} = \left(1 + \frac{\nu Y_{C3H8,1}}{Y_{O2,2}}\right)^{-1} \quad (6)$$

where ν is the stoichiometric mass ratio, $Y_{C3H8,1}$ the mass fraction of fuel in the fuel stream ($Y_{C3H8,1} = 1$), and $Y_{O2,2}$ the mass fraction of oxygen in the oxidizer stream ($Y_{O2,2} = 0.21$).

The differential equations are discretized based on the central second order finite difference scheme. To check the reduced mechanism two approaches were adopted. First, the mechanism was implemented in the solver DASSL (Differential/Algebraic Systems Solver) (Petzold, 1982). After, the flamelet equations were implemented.

SOLVER DASSL

This solver implements the Backward Differentiation Formulas of orders one through five to solve implicit differential equations for initial values of y and y_0. These values must be consistent, that is, if t_0, y_0 and y_0' are the given initial values, they must satisfy $f(t_0; y_0; y_0') = 0$ (Brenan *et al.*, 1996). The resulting nonlinear system at each time-step is solved by Newton's method.

The subroutine solves the system from t_0 to t_{out} (final time of integration). It also allows to continue the solution to get results at additional t_{out}. This is the interval mode of operation. Intermediate results can also be obtained easily by using the intermediate-output capability. The linear systems are solved using routines from the LINPACK subroutine package (Dongarra *et al.*, 1979). Error handling is accomplished using routines from the SLATEC common mathematical library package. This code performs well for stiff ordinary differential equations (ODE) and for differential/algebraic equations (DAE) of moderate size, where it is appropriate to treat the Jacobian matrix with dense or banded direct LU decomposition. For large-scale stiff ODE and DAE problems, it should be consider to employ the DASPK. For ODE or DAE problems which must stop at the root of a given function of the solution, the user should consider DASKR. Moreover, the code includes an extensive amount of documentation (see Petzold (1982)).

Although DASSL is a code written for problems of index ≤ 1, it can handle some of the higher index problems by adjusting the error control.

The results produced for the principal mass fractions of chemical species of the reduced mechanism are presented in the Table 2. Satisfactory results were obtained compared to the results given by Leung *et al.* (1993) (Table 2).

Table 2. Results from Solver DASSL.

Mass fraction	Results from DASSL	Data (Leung *et al.*, 1993)
Y_{C3H8}	0.000000000000000E+00	0.0000
Y_{O2}	0.000000000000000E+00	0.0000
Y_{H2O}	0.154535365116772E+00	0.1420

Y_{CO2}	0.793807529862030E-01	0.0802
Y_{CO}	0.598568131360495E-01	0.0607
Y_{H2}	0.331286126648532E-01	0.0340

Figure 2 presents the mass fractions for the C_3H_8, O_2 and H_2O along the time. The results from solver DASSL shows the decreasing of the fuel and oxidant, and the increasing of the product H_2O during the burn.
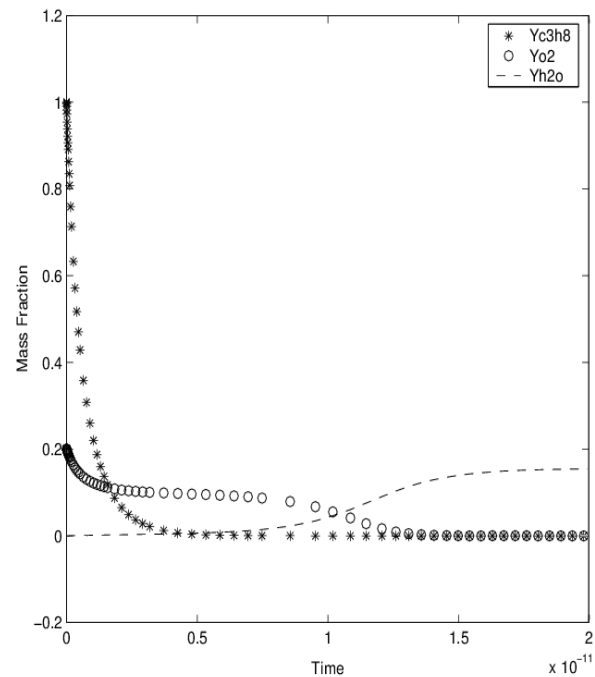

Figure 2. Numerical results for the mass fraction of fuel, oxidant and water vapor, along the time obtained via DASSL (for the reduced kinetic mechanism).

NUMERICAL RESULTS

Now, it is presented the numerical results for the Eqs. (2)-(4). The numerical results are compared with the skeletal chemical mechanism of 87-step for the propane (Leung *et al.*, 1993). In the figures, numerical results are indicated with "num".

Figure 3 shows the comparison for the propane mass fraction along the mixture fraction space. The mixture fraction measures the reactants mixing and is mainly related to the large scale motions of the flow. The solution indicates the decreasing behavior of the propane mass fraction.

The behavior of the oxidizer O_2 is given in the Fig. 4. For the reduced mechanism proposed, the mass fraction of O_2 decreases more slowly.

Figure 5 shows the mass fractions for the major species, H_2O and CO_2. The H_2O species was well predicted. The carbon dioxide mass fraction was reasonably well predicted.
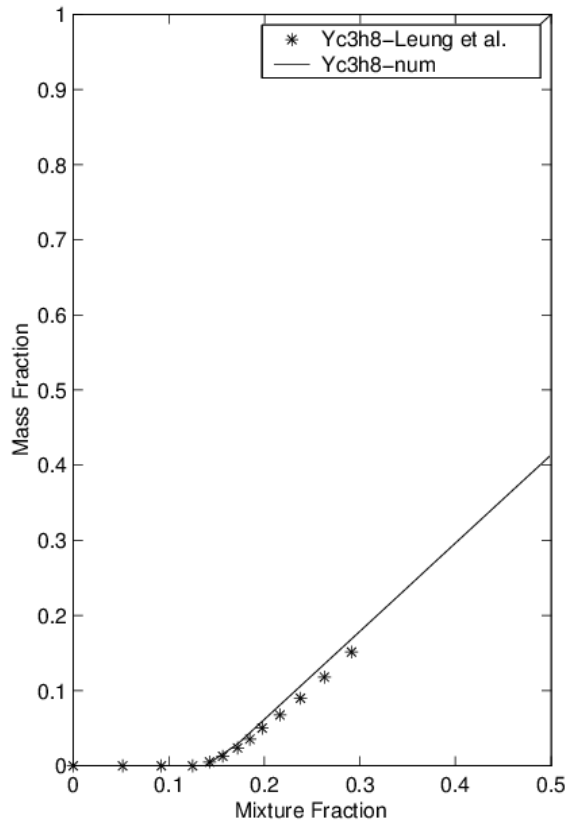
Figure 3. Numerical results for the mass fraction of
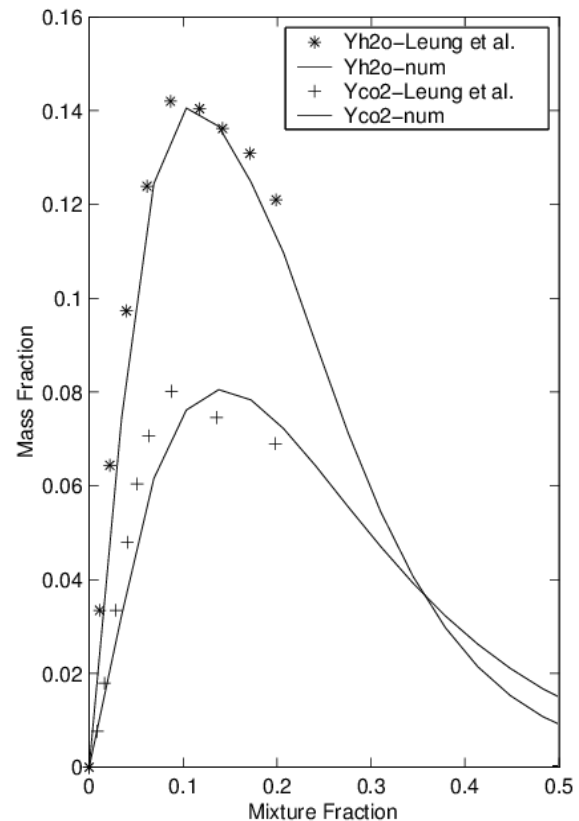fuel along the mixture fraction space.

Figure 5. Numerical results for the mass fraction of
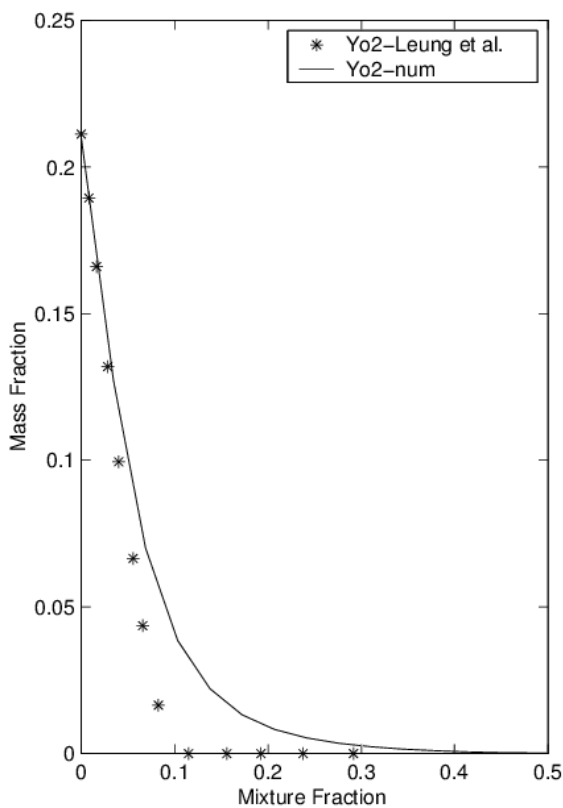H_2O and CO_2 along the mixture fraction space.

CONCLUSIONS

In this work we have developed a method to obtain a reduced kinetic mechanism for propane diffusion flames, considering steady-state and partial equilibrium assumptions. Good agreement has been obtained between predictions and measurements for the major species H_2O and CO_2. The main advantage of the strategy is the decrease of the work needed to solve the resultant system of chemical equations. Such reduction is proportional to the number of reactions of the complete mechanism, i. e., a decrease of one order of magnitude compared to the skeletal mechanism of 87-step for methane (Leung *et al.*, 1993).

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Figure 4. Numerical results for the mass fraction of
O_2 along the mixture fraction space.

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