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REDUCTION OF THE REACTION MECHANISM FOR THE “C+H+O+N” REACTING MEDIUM

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Abstract. *The problem of the reaction mechanism reduction in the combustion process is considered. The engagement method developed in previous works is applied for the “C+H+O+N” reacting medium, that is constituted by 209 reactions and 43 species. The formation of reduced mechanism is accomplished in process of calculations about the extinction line, using the model of well stirred reactor. It was obtained a reduced mechanism for set of values of: excess oxidant ratio, temperature and pressure. This mechanism contains the 63 reactions and 31 species and allows to compute the main combustion characteristics without loss of precision, but the pollutant concentrations* NO_x *presents considerable errors.*

Keywords: *combustion, chemical reactions, reduced mechanism, mathematical modeling*

1. INTRODUCTION

The “C+H+O+N” reacting medium is applied in power systems, in technological processes, in automobile engines, etc. The combustion mechanism for this reacting medium is very complex and contains above 200 reactions and 50 species (Foelsche *et al.*, 1994; Jiang and Chin, 1992; Jones and Lindstedt, 1998). The direct application of this mechanism, in bi- or tri-dimensional problems leads to huge computational volumes that can only be accomplished by supercomputers (Blom and Verwer, 2000; Oran and Boris, 1987). At the same time, it is known that most of the reactions and species influence little on the combustion processes and may be excluded.

The numerous works were published about reduction of the reaction mechanisms, using mainly the intuition and experience. But, with increase of complexity of kinetic schemes, this procedure becomes less safe, increasing the probability of errors. Therefore, it were developed different methods for the mechanism reduction: the method of velocity analysis (Peters and Kee, 1987; Glaude *et al.*, 2000; Smooke, 1991); the PCA method (Lam and Goussis, 1994; Tiangfeeng *et al.*, 2001); the “intrinsic low-dimensional manifold method” (Maas and Pope, 1992; Eggels and Goey, 1995), etc.

In Spilimbergo *et al.* (2007) it was proposed the engagement method to form reduced mechanisms in a zone of parameter alteration (α_{ox}, P, T) and was also presented the reduced mechanisms for the “H+O+S+(N)” reaction medium. In the present work, similar researches are developed for the “C+H+O+N” reaction medium.

2. MAIN EQUATIONS AND ENGAGEMENT METHOD

In this work the reduction of complete mechanism (C-mechanism) is accomplished, according to Kalamatianos *et al.* (1998), Peters and Kee (1987) and Tiangfeeng *et al.* (2001) by model of well stirred reactor with P , $\dot{m} = \text{const.}$, ($\dot{m}$ is the flow in reactor), which is described by following equations:

1) The chemical kinetics in the exponential form (Spilimbergo *et al.*, 2005):

$$\frac{d\gamma_i}{d\tau} = -e^{\gamma_i}\left(\sum_j \nu_{ij}\Omega_j + \frac{r_i^+\mu_\Sigma}{\mu^+\tau_p}\right) + \sum_q\sum_j \nu_{qj}\Omega_j + \sum_q \frac{r_q^+\mu_\Sigma}{\mu^+\tau_p} \qquad i, p, q = 1,\dots,\ n_c\,;\ \ \mathrm{j} = 1,\dots,2\,m_c\,; \qquad (1)$$

where: $\Omega_j = k_j\left(\frac{P}{R_0T}\right)^{\overline{m}_j} exp\left(-\sum_p n_{pj}\gamma_p\right)$; $\overline{m}_j = m_j + \sum n_{pj} - 1$; $\gamma_i = -ln\, r_i$;

$\nu_{ij} = \nu''_{is} - \nu'_{is}$; $n_{ij} = \nu'_{is}$; $j = s$; $s = 1,\dots,m_c$;

$\nu_{ij} = \nu'_{is} - \nu''_{is}$; $n_{ij} = \nu''_{is}$; $j = s + m_c$; $s = 1,\dots,m_c$;

ν'_{is} , ν''_{is} - stoichiometric coefficients in set of reversible reactions:

$$\sum_i \nu'_{is} B_i \Leftrightarrow \sum_i \nu''_{is} B_i \tag{2}$$

B_i – symbol of *i-th* species; m_j – index of participation of third body M ($m_j = 1$ if particle M participates in *j-th* reaction, otherwise $m_j = 0$); k_j – rate constant of *j-th* reaction; r_i and r_i^+ – molar fractions of *i-th* species in reactor and in input flow (the flow of reagents); n_c e m_c – numbers of species and of reactions in the reacting medium; τ_p – residence time; μ_Σ – average molecular mass in reactor; μ_i – molecular mass of *i-th* specie; R_0 – universal gas constant; μ^+ – average molecular mass of the reagents.

2) The energy equation, in integral form (considering $h = h^+ - Q$):

$$h = \sum_i H_i r_i \Big/ \sum_i \mu_i r_i \qquad i = 1,\ldots,n_c \tag{3}$$

where: h, h^+ – mass specific enthalpies in reactor and in input flow, Q – heat loss per unit of input flow mass; H_i – molar enthalpy of *i-th* specie.

The calculations of the combustion processes in the reactor begin from chemical equilibrium state (with temperature T_0) until establishment of same stationary state (moment τ_f, temperature T_f), with chemical non-equilibrium composition. In the results of the reaction rate analysis of the complete mechanism (C-mechanism) in the stationary state, the engagement method forms a reduced mechanism (S-mechanism) only with the notable reactions. In this method it is used the reduction indicator, which is established by the user and is located in interval $\zeta = 0,\ldots,1$. If the value of $\zeta = 1$, the reduced mechanism is only constituted by reactions with maximum rates. If the value of $\zeta = 0$, the reduced -mechanism is equal to the C-mechanism.

If the reduction is realized for:

- a point in the space { $\alpha_{ox}, P, T_0, \tau_p$ = const.}, then the reduced mechanism is called LS-mechanism;
- a line { α_{ox}, P = const., T_0, τ_p = var.}, then the reduced mechanism is called ST-mechanism;
- a limited zone { $\alpha_{ox}, P, T_0, \tau_p$ = var.}, then the reduced mechanism is called GS-mechanism.

In all calculation variants the initial data are: the reduction indicator ζ, the reagent symbols, the symbols of main combustion products and species interesting for the user.

The additional initial data in LS-mechanism are: α_{ox}, P, T_0 and τ_p. Thus, initially, the LS-mechanism is constituted only by same species (without reactions) and it is formed step by the step using the following algorithm:

P1. For each *i-th* species that is already include in the LS-mechanism, it is considered all reactions with this species.

P2. The maximums for these reactions are obtained:

$$\Omega_{im} = \max\left[\mathrm{abs}\left(\nu_{ij}\Omega_j\right)\right] \qquad j = 1,\ldots,2m_c; \tag{4}$$

$$\Omega_{id} = \max\left[\mathrm{abs}\left(\nu_{is}\left(\Omega_s - \Omega_{s+mc}\right)\right)\right] \qquad s = 1,\ldots,m_c; \tag{5}$$

where Ω_{im} is the maximum value by module among the terms $\nu_{ij}\Omega_j$ of the forward and back directions of reactions with *i-th* species; Ω_{id} is the maximum value by module of differences between the forward and back directions of these reactions.

P3. Among the reactions with *i-th* species are selected those that satisfy one of relations:

$$\mathrm{abs}\left(\nu_{ij}\Omega_j\right) \geq \zeta\,\Omega_{im} \qquad j = 1,\ldots,2m_c; \tag{6}$$

$$\mathrm{abs}\left(\nu_{is}\left(\Omega_s - \Omega_{s+mc}\right)\right) \geq \zeta\,\Omega_{id} \qquad s = 1,\ldots,m_{c.} \tag{7}$$

P4. Each reaction selected by relations (6) and (7) is included in LS-mechanism, if it was not included previously.

P5. Each species of each reaction selected by step P3 is also included in LS-mechanism, if was not included previously. So a species (initially included) “engages” others reactions and species. For example, analyzing the reactions with species CH_4, was selected in block 4 reaction: $CH_4 + O_2 = CH_2 + H_2O$. Then in LS-mechanism are additionally included the species CH_2 and H_2O (species O_2 is reagent). Therefore, the proposed method is called "engagement" method.

To form a ST-mechanism, the additional initial data are: α_{ox}, P and the temperature interval $[T_0(\max),...,T_0(\min)]$. We remind that stationary temperature T_f depends on the residence time (τ_p) and if the $\tau_p \to \infty$, then value $T_f \to T_0$. Figure 1 shows a line of alteration of the T_f, with the decrease of the τ_p, when T_0 = const. Each value of T_0 corresponds to some value of τ_{ex} (extinction time). If $\tau_p = \tau_{ex}$, then the combustion is extinguished and the temperature T in reactor decreases to the input temperature of reagents. As a result, for different temperatures T_0 is formed the extinction line that separates the extinction zone (B) from the combustion zone (A).

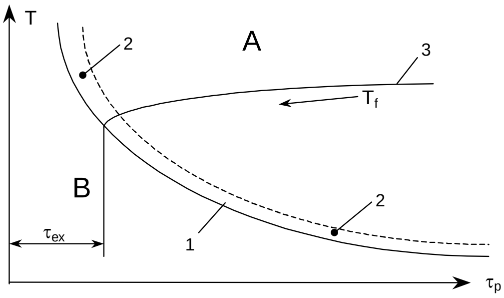

Figure 1. Dependence $T_0 = f(\tau_{ex})$ if T_0 = const. 1 – Extinction line; 2 – boundary zone; 3 – Alteration T_f in zone A with T_0 = const; A – Combustion zone; B – Extinction zone.

Knowing only the character of this line (the dependence $T_0 = f(\tau_{ex})$ is initially unknown) it is possible to propose the following technique of the ST-mechanism formation for interval $[T_0(\max),\ldots,T_0(\min)]$:

a) this interval is divided by n_T parts, with width $\Delta T = (T_0(\max),...,T_0(\min))/n_T$. It is also chosen a step $\delta\tau_p = \tau_{p,i+1}/\tau_{p,i}$ (for example, $\delta\tau_p = 1.1$);

b) it is chosen an initial point $[T_o(\max), \tau_{p,i} < \tau_{ex}]$, inside zone B (Fig. 2) and accomplished a calculation by the C-mechanism to form LS_1-mechanism in this point But LS-mechanism is not formed, because the reacting system is located into extinction zone.

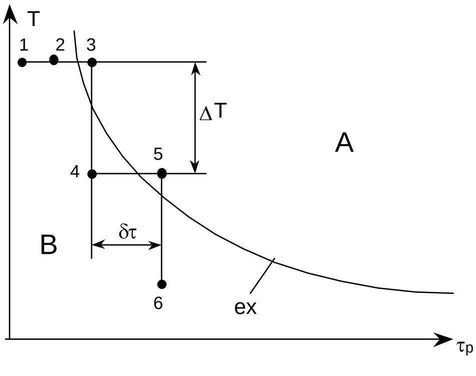

Figure 2. Calculation points for the formation of the ST-mechanism.

c) then residence time is increased ($\tau_{p,2} = \delta\tau_p \cdot \tau_{p,1}$) and the calculation is repeated with the same $T_0(\max)$. If system yet is located in the zone B (point 2 in Fig. 2), then is determined $\tau_{p,3} = \delta\tau_p \cdot \tau_{p,2}$ and again the same calculation is realized for point 3;

d) if this point is located in the combustion zone, then LS_3-mechanism is formed and new value $T_{0,1} = T_0(\max) - \Delta T$ is determined (i.e. system goes to point 4)

e) calculation in point 4 is carried; if the stationary state is not reached, then it increases the residence time $\tau_4 = \delta\tau_p \cdot \tau_{p,3}$ and the system goes to point 5. If the stationary state is reached, then the LS_5-mechanism are formed and a new version of the mechanisms ST = $LS_3 + LS_5$; it is also determined the value $T_{0,2} = T_{0,1} - \Delta T$;

f) calculation for point 6 is carried out and so forth to reached the temperature $T_0(\min)$ with the corresponding increase of τ_p. When the reacting system enters in a point of the combustion zone, ST-mechanism is completed by the LS-mechanism formed in that point. As a result, for the prescribed values α_{ox}, P, ζ and for the temperature interval $[T_0(\max),...,T_0(\min)]$ the ST(α_{ox}, P, ζ)-mechanism is formed and the extinction line is also determined.

To form a GS-mechanism, the additional initial data are: the intervals of temperature $[T_0(\max),...,T_0(\min)]$, of coefficient $[\alpha_{ox}(\max),...,\alpha_{ox}(\min)]$ and of pressure $[P(\max),...,P(\min)]$. In this case it is necessary to choose different values $\alpha_{\mathrm{ox},m}$ and P_j and to carry out the calculations (each time in interval $[T_0(\max),...,T_0(\min)]$ generating the ST-mechanisms for each point ($\alpha_{\mathrm{ox},m}$ P_j) and then, to obtain the GS(ζ)-mechanism, joining all ST-mechanisms.

3. THE CHOICE OF C-MECHANISM FOR THE "C+H+O+N" MEDIUM

The "C+H+O+N" reacting medium is important for the practice because the carbohydrate fuels are very used. The reaction mechanisms for this medium are presented in numerous publications (Foelsche *et al.*, 1994; Glaude *et al.*, 2000; Jiang and Chin, 1992; Jones and Lindstedt, 1998; etc.). In this work, the complete combustion mechanism (C-mechanism) was formed using the thermodynamic properties of species (molar enthalpy H_i and entropy S_i^o) of the base LEED's (2004) and the reactions (with rate constants) were taken mainly from Glarborg *et al.* (1986). The resulting C-mechanism contains 43 species and 209 reactions. This reacting medium, from a point of view to form the reduced mechanisms, presents a larger complexity than the "S+H+O+(N)" medium (Spilimbergo *et al.*, 2007) because:

- almost half of the reactions ("C+H+O" sub-medium) describes the energetic aspect and these reactions have high rates W_i^{CHO} which form the main combustion products $\mathrm{H_2O}$, $\mathrm{CO_2}$ and the pollutants CO and $\mathrm{C_nH_m}$);
- the other half of the mechanism is responsible for the formation of pollutant $\mathrm{NO_x}$ in the "N+H+O" and "C+N+O" sub-mediums This pollutant has little concentration (≈ 100ppm) and its formation happen with low rates $W_i^{\mathrm{NO}} \approx 10^{-4} W_i^{\mathrm{CHO}}$.

It is expected that the engagement method will encounter some difficulties, reducing this mechanism with such different rates. But, initially it is necessary to verify the mathematical model and the C-mechanism with data of others authors. The corresponding calculations were accomplished for the conditions (theoretical and experimental) presented of Glarborg *et al.* (1986): "$\mathrm{CH_4}$ + air (oxidizer)", $\alpha_{ox} = 0.6,\ldots,1.5$; $P = 1\,\mathrm{atm}$; $T^+ = 464\,\mathrm{K}$; $\tau_p = 2\,\mathrm{ms}$; (where T^+ is the temperature of reagents). The results of comparison are presented in Fig. 3 and 4. It is observed that the data for T_f and r_{NO}^f are matched and the discrepancies may be explained by the differences in thermodynamic properties used in LEED's (2004) and in Glarborg *et al.* (1986).

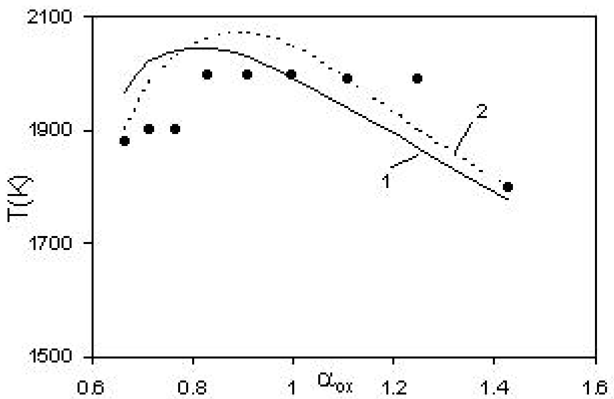

Figure 3. Alteration of temperature T_f in function of α_{ox}; $P = 1\mathrm{atm}$, $\tau_p = 2\,\mathrm{ms}$; $T^+ = 464\,\mathrm{K}$; 1 – our calculations; 2 – theoretical results, ● – experimental results (Glarborg *et al.*, 1986).

The first calculations to form the S-mechanism, were accomplished for the following conditions: reagents: "$\mathrm{CH_4}$ + air"; $\alpha_{ox} = 1$; $P = 1\,\mathrm{atm}$; $T_0 = 1400,...,2000\,\mathrm{K}$; with the objective of determining the convenient reduction indicator (in the interval $\zeta = 0.1,...,0.4$). These calculations (i.e., the generation of reduced mechanisms) were accomplished around of the extinction line (Fig. 2) according to technique of formation of ST-mechanisms. In result, the ST-mechanism (with indicator $\zeta = 0.3$) was obtained, and it includes 25 species (C, H, O, N, N_2, NO, NH, NH_2, NH_3, HNO, N_2O, N_2H, O_2, OH, H_2, H_2O, HCO, HNCO, CO, CO_2, CH, CH_2, CH_3, CH_4, CH_2O) and 45 reactions. It is observed that C-mechanism was reduced more than in 4 times and the S-mechanism contains 23 "energetic" reactions and 22 reactions of formation of NO_{ox}.

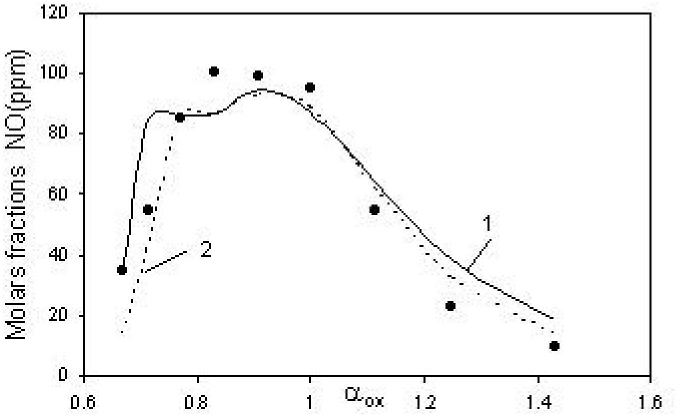

Figure 4. Alteration of r_{NO} in the stationary state of reactor in function of α_{ox}, $P = 1$ atm, $\tau_p = 2$ ms, $T^+ = 464$K ; 1 – our calculations; 2 – theoretical results, ● – experimental results (Glarborg *et al.*, 1986).

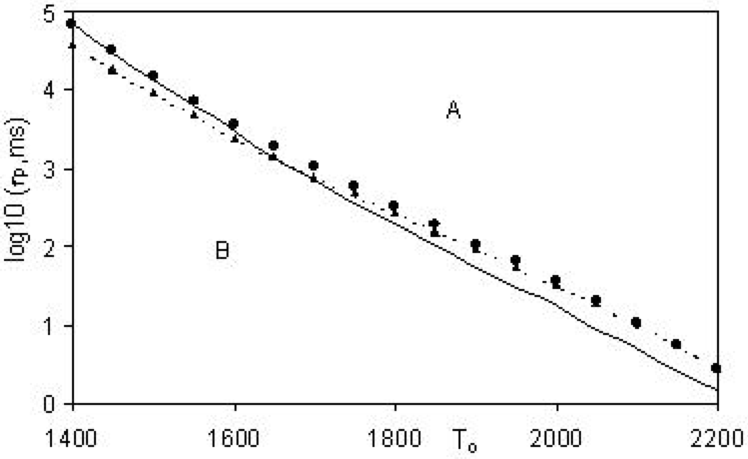

Figure 5. Extinction lines for different mechanisms: — C-mechanism; ▲ - S-mechanism (ζ = 0.2) ● - S-mechanism (ζ = 0.3) --- S-mechanism (ζ = 0.4); A – combustion zone; B – extinction zone.

The same calculations, carried out with other values of indicator ζ, show: a) S-mechanism with $\zeta = 0.4$ contains the 39 reactions and 25 species; b) S-mechanism with $\zeta = 0.2$ contains the 73 reactions and 35 species. The reduced mechanisms were verified, comparing the extinction lines obtained by the C-mechanism and by the reduced mechanisms (Fig. 5). It is observed that the extinction lines are matched sufficiently. Therefore it is possible to conclude that the reduced mechanisms describe correctly the "C+H+O+N" reacting medium and can be applied to predict the combustion processes in this medium, but only in the restricted zone ($\alpha_{ox} = 1$; $P = 1$ atm; $T_0 = 1400,...,2000$ K).

4. FORMATION AND ANALYSIS OF GS-MECHANISM

Basing on the results of the previous item were established: the value $\zeta = 0.4$ and the zone $\alpha_{ox} = 1,...,1.5$, $P = 1,...,16$ atm; $T_0 = 1400,...,2400$ K to form the GS-mechanism. To generate the ST-mechanisms, inside this zone were chosen the values: $\alpha_{ox,m} = 1.0$, 1.11, 1.25, 1.42 and $P_j =$ 1atm, 4atm, 16 atm. Accomplishing the calculations for each point $\lfloor \alpha_{ox,m},\ P_j \rfloor$ in the interval $T_o = 1400,...,2400\ \mathrm{K}$ with step $\Delta T_o = 50\,\mathrm{K}$, were generated the 12 ST-mechanisms. Joining these was obtained the GS-mechanism:

$$GS(\zeta = 0.4) = \bigcup_{m,j} ST(\alpha_{ox,m};\ P_j;\ \zeta = 0.4) \tag{8}$$

Table 1. GS-mechanism of the "C+H+O+N" reacting medium with ζ = 0.4

R1	$H+O_2=O+OH$	R22	$CH+H=C+H_2$	R43	$NO_2+H=NO+OH$
R2	$H_2+OH=H_2O+H$	R23	$CH+O_2=HCO+O$	R44	$HNO+M=H+NO+M$
R3	$OH+OH=H_2O+O$	R24	$CH+CO_2=HCO+CO$	R45	$HNO+OH=NO+H_2O$
R4	$H+O_2+M=HO_2+M$	R25	$C+OH=CO+H$	R46	$HCN+O=NCO+H$
R5	$HO_2+H=OH+OH$	R26	$C+O_2=CO+O$	R47	$HCN+OH=CN+H_2O$
R6	$HO_2+OH=H_2O+O_2$	R27	$N_2H+M=N_2+H+M$	R48	$HCN+OH=HOCN+H$
R7	$CO+OH=CO_2+H$	R28	$N_2H+H=N_2+H_2$	R49	$CN+OH=NCO+H$
R8	$CH_4+H=CH_3+H_2$	R29	$NH_3+M=NH_2+H+M$	R50	$CN+H_2=HCN+H$
R9	$CH_4+OH=CH_3+H_2O$	R30	$NH_3+H=NH_2+H_2$	R51	$CN+O_2=NCO+O$
R10	$CH_3+H=CH_2+H_2$	R31	$NH_3+OH=NH_2+H_2O$	R52	$NCO+H=NH+CO$
R11	$CH_3+O=CH_2O+H$	R32	$NH_2+H=NH+H_2$	R53	$NCO+O=NO+CO$
R12	$CH_3+O=CH_2+OH$	R33	$NH_2+OH=NH+H_2O$	R54	$NCO+OH=NO+HCO$
R13	$CH_3+OH=CH_2+H_2O$	R34	$NH+H=N+H_2$	R55	$HOCN+H=HNCO+H$
R14	$CH_3+OH=CH_2O+H_2$	R35	$NH+OH=HNO+H$	R56	$HNCO+H=NH_2+CO$
R15	$CH_2O+H=HCO+H_2$	R36	$NH+OH=N+H_2O$	R57	$C+NO=CN+O$
R16	$CH_2O+OH=HCO+H_2O$	R37	$N+O_2=NO+O$	R58	$CH+NO=HCN+O$
R17	$HCO+M=CO+H+M$	R38	$N+OH=NO+H$	R59	$CH_2+NO=HNCO+H$
R18	$CH_2+H=CH+H_2$	R39	$N+NO=N_2+O$	R60	$CH+N_2=HCN+N$
R19	$CH_2+O=CO+H+H$	R40	$N+CO_2=NO+CO$	R61	$NH+NO=N_2O+H$
R20	$CH_2+OH=CH_2O+H$	R41	$NO+HO_2=NO_2+OH$	R62	$N_2O+M=N_2+O+M$
R21	$CH_2+OH=CH+H_2O$	R42	$NO_2+M=NO+O+M$	R63	$N_2O+H=N_2+OH$

This GS-mechanism is constituted by 31 species: C, H, O, N, N_2, NO, NO_2,NO, NH, NH_2, NH_3, HNO, N_2O, N_2H, NCO, O_2, OH, H_2, H_2O, HO_2, HCO, HOCN, HNCO, HCN, CO, CO_2, CH, CH_2, CH_3, CH_4, CH_2O, CN and by 63 reactions, presented in the Table 1. The "C+H+O" sub-medium (energetic part) contains 26 reactions and 15 species and the "nitrogen" sub-medium, - 37 reactions and 16 species. So, the C-mechanism is reduced in $(209/63) \approx 3$ times in relation to the reactions and in $(43/31) \approx 1{,}3$ in times in relation to the species.

The verification of the GS-mechanism was accomplished, comparing of the data obtained by this mechanism and by the C-mechanism in the points $\lfloor \alpha_{ox,m},\ P_j \rfloor$ where *m* = 1,…,4; and *j* = 1,…,3. Some results of this comparison are presented in Fig. 6 and 7.

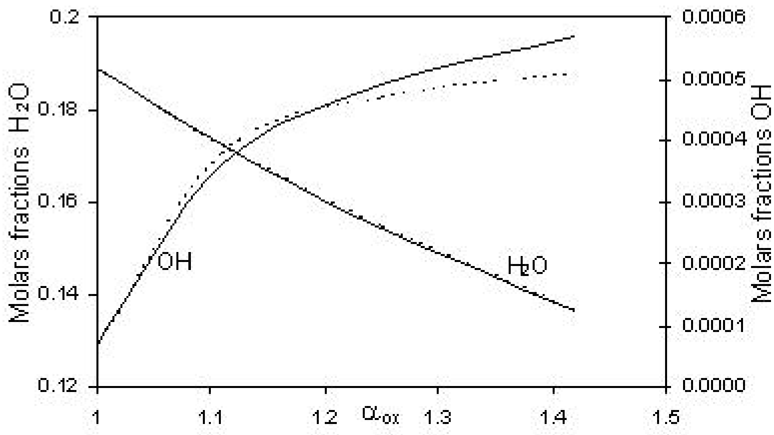

Figure 6. Alteration of r_{H_2O}, r_{OH} in function of α_{ox}; T_o = 1600 K; *P* = 16 atm.

— C-mechanism; - - - - GS-mechanism.

It is observed that the GS-mechanism shows small errors for the species of the "C+H+O" sub-medium that is confirmed by the comparison of concentrations H_2O, OH and CO. But for the "nitrogen" species with small concentrations presented by species NO (Fig. 7) the comparison shows considerable errors. In order to reduce them, it is necessary (according to Spilimbergo *et al.*, (2007)) to diminish the indicator to $\zeta = 0.2;...;0.3$ and to generate new GS-mechanism. In this case need to consider that with the decrease of the indicator ζ, the volume of the GS-mechanism grows. But the mechanism GS ($\zeta = 0.4$) is already great (Table 1).

This circumstance is explained by imperfection of automatic generation of the reduced mechanisms, which is based only on the analysis of the reaction rates (non-considering the species concentrations and the "closed" reactions). Particularly, the reactions R29, R30 and R31 were included in the GS-mechanism because they have considerable rates W_i^{NO}. But the concentrations of NH_3 are small $\left(r_{\mathrm{NH_3}} < 10^{-7}\right)$ in every researched zone and besides, the reaction R29, R30 and R31 are "closed", i.e. the species NH_3 is only formed through the species NH_2, and it no participates in the other reactions. Therefore, these reactions (with the substance NH_3) can be excluded of the GS-mechanism.

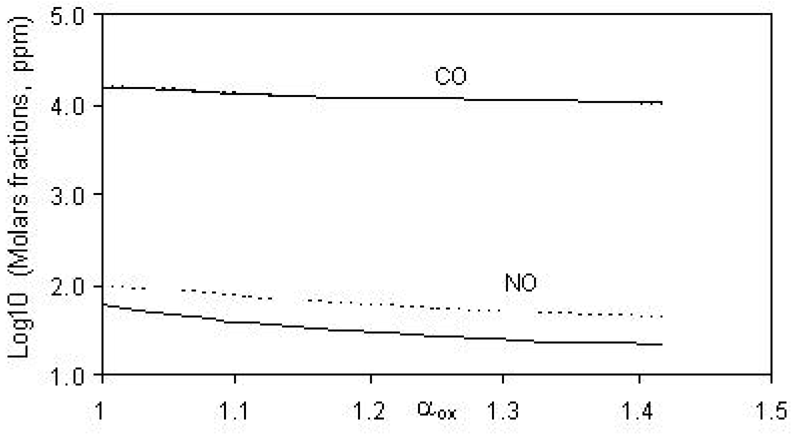

Figure 7. Alteration of r_{NO}, r_{CO} in function of α_{ox}; $T_0 = 2000$K; $P = 1$atm.
— C-mechanism; - - - - GS-mechanism.

The species N_2H (with the reactions R27 and R28) and NO_2 (with the reactions R41, R42 and R43) present the same peculiarities. Then, using the similar analysis, the 3 species and 8 reaction can be excluded from the mechanism GS($\zeta = 0.4$). Applying this technique and the researcher's experience, it is possible to reduce even more the GS-mechanism. For example, in Alzueta *et al.* (2001) the C-mechanism was reduced from 82 reactions to 23 reactions, but this result was obtained "manually" and in restricted zone.

5. CONCLUSIONS

1. The engagement method (Spilimbergo *et al.*, 2007) it was applied for the "C+H+O+N" reacting medium to generate the reduced mechanisms of chemical reactions.
2. The numeric simulations were accomplished for the "CH_4 + air" mixture in the zone $\alpha_{ox} = 1,...,1.5$; $P = 1,...,16$atm; $T_0 = 1400,...,2000$K with the reduction indicator $\zeta = 0.4$. The complete C-mechanism was reduced: in relation to the reactions in 3 times and in relation to the species in 1.3 times.
3. This mechanism allows the computing of the main combustion characteristics (temperature, concentrations CO_2, H_2O and CO) with insignificant errors. But considerable errors were observed in the prediction of pollutant NO.
4. The GS-mechanism can still be reduced, excluding the "closed" reactions with the participation of the species NH_3, N_2H and NO_2.

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