THE SWIRL INFLUENCE ON THE VOLUMETRIC IRREVERSIBILITIES OF DIFFUSION FLAMES

Dorin STANCIU, Mircea MARINESCU

UNIVERSITATEA POLITEHNICA, București

Rezumat. Obiectivul lucrării este acela de a analiza influenţa unghiului de turbionare a jetului de oxidant asupra ireversibilităţilor volumice generate de flăcările turbulente difuzive. Baza teoretica a acestei analize o constituie ecuaţia de transfer a exergiei, a cărei formă conservativă permite formularea locală a teoremei Gouy-Stodola. Turbionarea jeturilor reprezintă o metodă uzuală de stabilizare a flăcării difuzive. Utilizând tehnica simulării numerice, această lucrare încearcă să evidenţieze rolul turbionării jetului de oxidant şi a intensităţii turbulenţei atât în intensificarea procesului de ardere cât şi în valoarea disipaţiilor exergetice. Ţinând cont de importanţa tehnică a flăcărilor difuzive, analiza de faţă poate servi la înţelegerea mecanismelor de disipaţie turbulentă şi a relaţiei acestora cu tehnicile de stabilizare a flăcărilor.

INTRODUCTION

In the field of power generation systems the chemical to thermal exergy conversion using the turbulent diffusion hidrocarbonated flames still play a significant rol. The swirling of oxidiser stream is the most common thechnique in stabilising the flame sheet. But the turbulent heat and mass transfer enhancement obtained through this way could lead to the irreversibility growth of exergy conversion process.

There are manny ways in measuring the irreversibilities of diffusion burning processes, but according to the second law of thermodynamics, only the entropy generation rate can reveals the entire mechanisms of exergy dissipations. The entropy generation rate calculus can be performed at a bulk or at continuum level. For the convection heat transfer flows, the both levels of analysis was first formulated by Bejan [1] and successfully used by others authors. In the case of turbulent flows, the continuum level of entropy generation analysis was extended by Stanciu et all. [5], who observed that the turbulent fluctuations induce in the mean flow field theirs specific irreversibility mechanisms, having at least the same order of magnitude as the classical ones, generated by the gradients of mean properties.

The goal of this paper is to investigate, at the continuum level, the liaison between the swirling number of oxidiser stream and the irreversibility values of chemical to thermal exergy conversion, taking into account the turbulent dissipation mechanisms.

MATHEMATICAL MODEL

The mathematical model is split in two parts, one of them referring to the mean flow field and another to the turbulent flow irreversibilities. This happens because the volumetric rate calculus of entropy generation needs some properties of the mean flow field, which can be computed in addition with both, turbulence and turbulence-chemistry interaction models, choosed for closing the multicomponent flow equations.

Mathematical model of diffusion reacting flow

Let consider a turbulent reacting flow of a multicomponent gaseous mixture, chemically rouled by the global single step reaction:

$$\sum_i v_{R,i} A_{R,i} = \sum_j v_{P,j} A_{P,j} \qquad (R1)$$

where subscripts R and P stand for reactants and products. There are many ways in modeling these flows [2],[4]. For this paper we choosed the multi-species approach, which is more appropriate to our goals but more expenseve from computational point of view. It is based on the Favre averaged full Navier-Stokes equations, completed with both, a second order turbulence closure model and a turbulence-chemistry interaction model based on the eddy break-up formulation of volumetric turbulent reaction rate.

The Favre averaged Navier-Stokes system include the continuity, species, momentum and energy balance equations are:

$$\frac{\partial \overline{\rho}}{\partial \tau} + \frac{\partial (\overline{\rho} \tilde{u}_\alpha)}{\partial x_\alpha} = 0 \qquad (1)$$

$$\frac{\partial}{\partial \tau}\left(\overline{\rho}\tilde{Y}_i\right) + \frac{\partial}{\partial x_\alpha}\left[\overline{\rho}\tilde{u}_\alpha \tilde{Y}_i - \overline{\Phi_{i,\alpha}^{(V)}} + \overline{\Phi_{i,\alpha}^{(R)}}\right] = \beta_{M,i}\overline{\rho}\tilde{\omega} \qquad (2)$$

$$\frac{\partial}{\partial \tau}\left(\overline{\rho}\tilde{u}_\beta\right) + \frac{\partial}{\partial x_\alpha}\left[\overline{\rho}\tilde{u}_\alpha \tilde{u}_\beta + \overline{P}\delta_{\alpha\beta} - \overline{\tau_{\beta\alpha}^{(V)}} + \overline{\tau_{\beta\alpha}^{(R)}}\right] = 0 \qquad (3)$$

$$\frac{\partial}{\partial \tau}\left(\overline{\rho}\tilde{h}\right) + \frac{\partial}{\partial x_\alpha}\left[\overline{\rho}\tilde{u}_\alpha \tilde{h} - \overline{q_\alpha^{(V)}} + \overline{q_\alpha^{(R)}}\right] = \frac{\partial \overline{p}}{\partial \tau} \qquad (4)$$

where $i=1$, N denotes the i-specie of gaseous mixture and $\beta_{M,i} = -v_{R,i}M_{R,i}$ for reactants or $\beta_{M,i} = v_{P,i}M_{P,i}$ for products. For the sake of simplicity, in eq. (4) we used the assumption Le=1. In the above equations:

$$\overline{\Phi_{i,\alpha}^{(V)}} = -\overline{\rho}D_{im}\frac{\partial \tilde{Y}_i}{\partial x_\alpha};$$

$$\overline{\tau_{\beta\alpha}^{(V)}} = \mu_V\left(\frac{\partial \tilde{u}_\alpha}{\partial x_\beta} + \frac{\partial \tilde{u}_\beta}{\partial x_\alpha}\right) - \frac{2}{3}\delta_{\alpha\beta}\frac{\partial \tilde{u}_\gamma}{\partial x_\gamma};\qquad(5)$$

$$\overline{q_\alpha^{(V)}} = \frac{\mu_V}{\mathrm{Pr}}\frac{\partial \tilde{h}}{\partial x_\alpha}$$

denote the mass diffusion mean vector, the viscous mean stress tensor and the mean heat flux vector, while:

$$\overline{\tau_{\beta\alpha}^{(R)}} = -\overline{\rho u_\alpha'' u_\beta''};$$

$$\overline{q_\alpha^{(R)}} = -\overline{\rho u_\alpha'' h''};\qquad(6)$$

$$\overline{\Phi_{i,\alpha}^{(V)}} = -\overline{\rho u_\alpha'' Y_i''}$$

represent the corresponding Reynolds quantities. In order to solve the system (1)-(5) a closure turbulence model for expressions (6) and a combustion model for the mean reaction rate $\tilde{\omega}$ must be added.

Although they have been widely criticized, the second order turbulence closure models are very practical for engineering calculation. They relys on the Boussinesq aproximation which states that:

$$\overline{\tau_{\beta\alpha}^{(R)}} = \mu_T\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \frac{2}{3}\delta_{\alpha\beta}\frac{\partial u_\gamma}{\partial x_\gamma}\right) - \frac{2}{3}\delta_{\alpha\beta}\overline{\rho}K \quad(7)$$

where μ_T is the turbulent viscosity.

It is well known that the standard K-ε_K model fails in predicting the separated and swirling flows or the spreading rate of round jet, which are most often used in combustion processes. In order to improve its behavior, some corrections on ε equation, or some modifications of model constants C_μ, $C_{\varepsilon 1}$ and $C_{\varepsilon 2}$ must be added, but they are depending on the flow type. The option we choosed for this work is the improved RNG formulation of two equations K-ε_K model [2], which clearly enhances the prediction accuracy of swirling flows. The model's equations for the high Reynolds number regions of the flows are:

$$\mu_T = \rho C_\mu K^2/\varepsilon_K \qquad(8)$$

$$\frac{\partial \rho K}{\partial \tau} + \frac{\partial}{\partial x_\alpha}\left[\rho K u_\alpha - \alpha_K\left(\mu_V + \mu_T\right)\frac{\partial K}{\partial x_\alpha}\right] = \overline{\tau_{\beta\alpha}^{(R)}}\frac{\partial u_\alpha}{\partial x_\beta} - \rho\varepsilon\,(9)$$

$$\frac{\partial \rho \varepsilon_K}{\partial \tau} + \frac{\partial}{\partial x_\alpha}\left[\rho \varepsilon_K u_\alpha - \alpha_\varepsilon\left(\mu_V + \mu_T\right)\frac{\partial \varepsilon_K}{\partial x_\alpha}\right] =$$
$$= \frac{\varepsilon_K}{K}\left(C_{\varepsilon 1}\overline{\tau_{\beta\alpha}^{(R)}}\frac{\partial u_\alpha}{\partial x_\beta} - \rho C_{\varepsilon 2}^*\right) \qquad(10)$$

where α_K and α_ε represent the model's constants and $C_{\varepsilon 2}^*$ is computed from an algebraic equation involving the strain rate modulus and the K/ε ratio.

Using the same gradient transport model closure, the Reynolds mass diffusion vector $\overline{\Phi_{i,\alpha}^{(R)}}$ is related to the mean mass fraction gradient through the turbulent diffusion coefficient D_T and the Reynolds heat flux vector $\overline{q_\alpha^{(R)}}$ is connected to the mean enthalpy gradient

using the turbulent heat transfer coefficient λ_T. These turbulent quantities are computed with the aid of turbulent Schmidt, Sc_T and Prandtl, Pr_T numbers, whose values result from an algebraic relation.

The turbulence-chemistry interaction models, widely used in the multispecies approach, are mixing controlled combustion techniques that determine the mean volumetric reaction rate $\tilde{\omega}$ as a function of mean mass fraction field, $\tilde{Y}_i$ and the characteristic time of turbulence, ε/K. For this work we selected the well-known eddy-break formulation of Magnussen and Hjertager [3] which set the volumetric rate of reaction ($R1$) as:

$$\tilde{\omega} = \min\left(\tilde{\omega}_1, \tilde{\omega}_2\right) \qquad(11)$$

where:

$$\tilde{\omega}_1 = A\overline{\rho}\frac{\varepsilon}{K}\min_i\left(\frac{Y_{R,i}}{\nu_R' M_{R,i}}\right); \quad \tilde{\omega}_2 = AB\overline{\rho}\frac{\varepsilon}{K}\frac{\sum_j Y_{P,j}}{\sum_j \nu_j'' M_{P,j}}$$

subscripts R and P stands for reactants and products, and $A=2.0$ or $B=0.5$.

Mathematical Model of Flow Irreversibilities

At the continuum level, the mathematical model of turbulent multi-component flow irreversibilities relies on the instantaneous expression of the volumetric entropy generation rate:

$$\dot{S}_{gen}^{(\Omega)} = \left(\dot{S}_{gen}^{(\Omega)}\right)_V + \left(\dot{S}_{gen}^{(\Omega)}\right)_Q + \left(\dot{S}_{gen}^{(\Omega)}\right)_D + \left(\dot{S}_{gen}^{(\Omega)}\right)_{CH} =$$
$$= \frac{\tau_{\beta\alpha}^{(V)}}{T}\frac{\partial u_\beta}{\partial x_\alpha} + \frac{\lambda}{T^2}\frac{\partial T}{\partial x_\alpha}\frac{\partial T}{\partial x_\alpha} - \qquad(12)$$
$$- \frac{1}{T}\sum_{i=1}^N \rho_i \Phi_{i,\alpha}\left(\frac{\partial \mu_i}{\partial x_\alpha}\right)_T + \frac{A\omega}{T}$$

where A represent the chemical affinity. Neglecting the diffusion due to the pressure gradients and dropping the serial decompositions of $T^{-2} = \tilde{T}^{-2}(1 + T''/\tilde{T})^{-2}$ and $Y_i^{-1} = \tilde{Y}_i^{-1}(1 + Y_i''/\tilde{Y}_i)^{-1}$ at the first term, the Favre averaged expression of eq.(10) becomes [5]:

$$\overline{\dot{S}}_{gen}^{(\Omega)} = \left(\overline{\dot{S}}_{gen}^{(\Omega)}\right)_{V,M} + \left(\overline{\dot{S}}_{gen}^{(\Omega)}\right)_{V,T} +$$
$$+ \left(\overline{\dot{S}}_{gen}^{(\Omega)}\right)_{Q,M} + \left(\overline{\dot{S}}_{gen}^{(\Omega)}\right)_{Q,T} + + \qquad(13)$$
$$+ \left(\overline{\dot{S}}_{gen}^{(\Omega)}\right)_{D,M} + \left(\overline{\dot{S}}_{gen}^{(\Omega)}\right)_{D,T} + \left(\overline{\dot{S}}_{gen}^{(\Omega)}\right)_{CH,T}$$

In the above expression, the viscous, thermal and diffusion components of instantaneous volumetric entropy generation rate expression (12) are splitted in two parts, one of them corresponding to the mean flow field exergy dissipations (subscripts M), and another, to the induced exergy dissipations of the fluctuating field at the mean flow level (subscripts T). An exception from this rule is the chemical component, from which only its turbulent part is considered.

The viscous component expressions are:

$$\left(\dot{\tilde{S}}_{gen}^{(\Omega)}\right)_{VM} \cong \frac{\tilde{\tau}_{\beta\alpha}^{(V)}}{\tilde{T}} \frac{\partial \tilde{u}_\beta}{\partial x_\alpha} \qquad (14)$$

$$\left(\dot{\tilde{S}}_{gen}^{(\Omega)}\right)_{VT} \cong \frac{\overline{\rho}\varepsilon_K}{\tilde{T}}$$

which model the mean viscous irreversibilities, due to the gradients of averaged velocity, and the mean turbulent ones, generated by the dissipation rate:

$$\varepsilon_K = \overline{\tau_{\beta\alpha}^{(V)}\left(\partial u_\beta'' / \partial x_\alpha\right)}/\overline{\rho}$$

of turbulent kinetic energy, $K = \frac{1}{2}\overline{\rho u_\alpha'' u_\alpha''}/\overline{\rho}$.

The mean and turbulent thermal components of volumetric entropy generation rates are expressed by:

$$\left(\dot{\tilde{S}}_{gen}^{(\Omega)}\right)_{QM} \cong \frac{\lambda_V}{\tilde{T}^2} \frac{\partial \tilde{T}}{\partial x_\alpha} \frac{\partial \tilde{T}}{\partial x_\alpha} \qquad (15)$$

$$\left(\dot{\tilde{S}}_{gen}^{(\Omega)}\right)_{QT} \cong \frac{\overline{\rho}c_p}{\tilde{T}^2} \varepsilon_\theta$$

where:

$$\varepsilon_\theta = (\lambda_V / \overline{\rho}c_p) \overline{\rho(\partial T / \partial x_\alpha)(\partial T'' / \partial x_\alpha)}/\overline{\rho}$$

represents the dissipation rate of fluctuating temperature variance $K_\theta = \frac{1}{2}\overline{\rho T''^2}/\overline{\rho}$.

The mean and turbulent diffusion irreversibilities of the flow are modelled by the following two terms:

$$\left(\dot{\tilde{S}}_{gen}^{(\Omega)}\right)_{DM} \cong \sum_{i=1}^N \overline{\rho}D_{im} \frac{R_i}{\tilde{Y}_i} \frac{\partial \tilde{Y}_i}{\partial x_\alpha} \frac{\partial \tilde{Y}_i}{\partial x_\alpha} \qquad (16)$$

$$\left(\dot{\tilde{S}}_{gen}^{(\Omega)}\right)_{DT} \cong \sum_{i=1}^N \frac{R_i}{\tilde{Y}_i} \overline{\rho}\varepsilon_\psi^{(i)}$$

in which:

$$\varepsilon_\psi^{(i)} = D_{im} \overline{(\partial Y_i / \partial x_\alpha)(\partial Y_i / \partial x_\alpha)}$$

is the dissipation rate of fluctuating i-component mass fraction variance $K_\psi^{(i)} = \frac{1}{2}\overline{\rho Y_i''^2}/\overline{\rho}$.

Finaly, the turbulent chemical source of entropy generation rate is approximated by:

$$\left(\dot{\tilde{S}}_{gen}^{(\Omega)}\right)_{CH} \cong \frac{\tilde{\omega}}{\tilde{T}}\left[\sum_i \nu_{R,i}\tilde{\mu}_{M,i} - \sum_j \nu_{P,j}\tilde{\mu}_{M,j}\right] \qquad (17)$$

where the mean chemical molar potential is simply computed like:

$$\tilde{\mu}_{M,i} = \tilde{h}_{M,i} - \tilde{T}s_{M,i}\left(\tilde{T}, \overline{p}, \tilde{X}_i\right) \qquad (18)$$

It must be emphasis that the most rough aproximation appear in the chemical mean component of entropy source because its Favre averaged instantaneous expression including the product between the affinity and the volumetric reaction rate containes many correlation which cannot be modeled with the aid of quantities offered by any turbulence model.

The gap between models

Correlating the irreversibility and the flow mathematical models in can be seen that the turbulent thermal and turbulent dissusion components of entropy source (11) cannot be computed. This is happening because the mathematical flow model relys on the classical Pr_T=const. and Sc_T=const. hypothesis instead of using another two equations models like K_θ-ε_θ and K_ψ-ε_ψ for determining λ_T and $D_{im,T}$. In this case, the equilibrium turbulence feature can be invoked, for which the productions terms and the dissipation rates appearing in K_θ and $K_\psi^{(i)}$ balance equations are equals so that:

$$\left(\dot{\tilde{S}}_{gem}^{(\Omega)}\right)_{QT} \cong \frac{\rho c_p \alpha_T}{\tilde{T}^2} \frac{\partial \overline{T}}{\partial x_j} \frac{\partial \overline{T}}{\partial x_j} = \frac{\lambda_T}{\tilde{T}^2} \frac{\partial \overline{T}}{\partial x_j} \frac{\partial \overline{T}}{\partial x_j} \qquad (19)$$

$$\left(\dot{\tilde{S}}_{gen}^{(\Omega)}\right)_{DT} \cong \overline{\rho}D_{im,T} \sum_{i=1}^N \frac{R_i}{\tilde{Y}_i} \frac{\partial \tilde{Y}_i}{\partial x_\alpha} \frac{\partial \tilde{Y}_i}{\partial x_\alpha} \qquad (20)$$

There are another important aproximations, which are obvious induced by the flow turbulence model. Instead of using the Pr_T concept, the two equations K_θ-ε_θ model of Sommer [6] could be used, but its ε_θ equation seems to be numerically unstable. Beyond that, no K_ψ-ε_ψ model is available at this time, so that the aproximations (17) and (18) represent the only choice for computing the turbulent thermal and turbulent difusion components of volumetric entropy generation rates.

RESULTS AND DISCUTIONS

For the numerical analysis we choosed an axial-simetrical geometry presented in *fig. 1*. The original combustible gas mixture had the following volumetric composition: 27% CH_4, 55%H_2, 4%CO, 2%C_2H_6, 8%CO_2 and 4%N_2. In order to reduce the number of solved equations, this gas mixture was replaced with an equivalent mixture having the mass fraction composition of 0.6068 $C_{0.397}H_{2.612}O_{0.0463}$, 0.298 CO_2 and 0.0952 N_2. Then, the resulting stoichiometric chemical equation was:
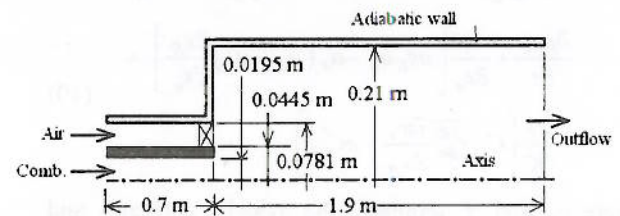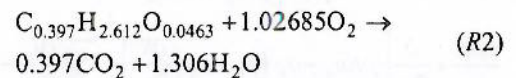
$$C_{0.397}H_{2.612}O_{0.0463} + 1.02685O_2 \rightarrow$$
$$0.397CO_2 + 1.306H_2O \qquad (R2)$$

Fig. 1 The geometry of numerical simulation.

The numerical simulation was made whith the solver FLUENT 6.0.12 for the flow Reynolds number:

$$Re = \frac{4\left(\dot{m}_{fuel} + \dot{m}_{air}\right)}{\pi \mu D} = 20520 \qquad (21)$$

where $D=0.21$m represents the furnance diameter, and $\mu=1.78 \times 10^{-5}$ Pa.s is the dynamic viscosity of the oxidant. The fuel/air mass fraction was $\dot{m}_{fuel}/\dot{m}_{air}=0.0652$ from which the reactant and oxidizer mass flow rates were computed and were imposed at the inlet air and inlet combustible streams. Beyond that, on the dividing boundary between furnace and oxidizer stream domains, the swirl component of air velocity was added. This component was determined with the aid of swirl angle α, which is defined as the angle between the velocity vector and the axial flow direction. In accordance with eq. (8), the standard wall function boundary condition was selected for all the solid frontiers.

The volumetric irreversibility components, defined by the eq. (14)-(17), were computed from the numerical solutions, obtained after reducing the flow equations residuals with at least five orders of magnitude. Among them, those generated by the turbulent heat transfer, turbulent diffusion and turbulent chemical reaction strongly prevail [5]. These irreversibilities are located near the flame sheet and around the recirculation zone. Then, the distribution of the total volumetric entropy generation rate (13) generally keeps their shapes, but it is affected by the air swirl intensity. Fig. 2 presents the volumetric entropy generation rates distributions for two values of air swirl angle. In order to assure the correct comparison of irreversibility maps, the graphic representation is realized between the same minimum and maximum values of volumetric entropy generation rates. As expected, the irreversibility affected volume increases with the swirl angle, whose growth spatially spread the mixing process and reduce the flame length. In these conditions, the integral values of irreversibility will depend not only on theirs volumetric maximal values but also on the affected volume.
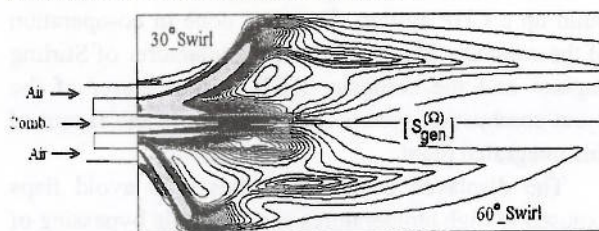

Fig. 2. Volumetric entropy generation rate distributions for two different values of swirl angle.

The entropy generation rate components were determined by integrating theirs volumetric rate on the entire flow domain:

$$\left(\bar{S}_{gen}\right)_{VM,VT,DM,DT,CH} = \frac{1}{V}\int_V \left(\bar{S}_{gen}^{(\Omega)}\right)_{VM,VT,DM,DT,CH} dV \tag{22}$$

All the mean components are negligible comparing with the turbulent ones. So, the *fig. 3* presents the dependence of all turbulent components and entropy generation rates with the swirl angle. It can be seen that

the swirl angle growing determines the entropy generation rate diminution, because the acting volume of irreversibilities decreases. This rule is imposed by the chemical component and partially by the thermal one, while the diffusion component seems to by nearly constant. On the other side, fig. 3 suggests that, for an imposed geometry of combustion chamber, there is an optimal swirling angle which minimizes the exergetic losses. This is happen because the growth of the swirl beyond a certain value will approach the flame sheet to the outer wall that will obvious cause the growth of the irreversibility affected volume.
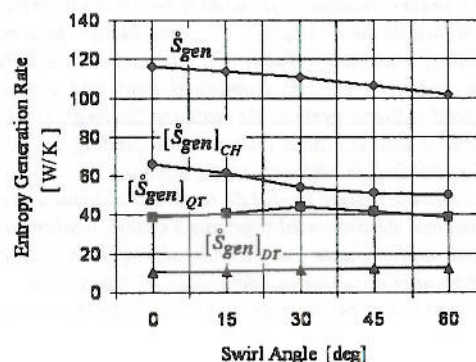

Fig. 3. Entropy generation rate variation with swirl angle.

CONCLUSION

The goal of this work was to investigate the swirl angle influence on the turbulent diffusion flame irreversibilities. In accordance with the second law of thermodynamics, these irreversibilities were measured by the rate of entropy generation, whose components are born by both, the mean and the turbulent flow field. The numerical simulations revealed that only the turbulent components affect the reacting flow irreversibilities, which are decreasing when the swirl angle is growing, as long as theirs affected volume is rising. From the exergetic losses point of view, our numerical simulations suggest that it is better to spread the irreversibilities in a greater volume.

BIBLYOGRAPHY

[1] BEJAN, A., *Entropy generation through fluid flow and heat transfer*, John Wiley&Sons, 1983.

[2] Fluent Inc., *User's Guide*, vol II.

[3] MAGNUSEN, B.F., HJERTAGER, B.H., *On the Mathematical Model of Turbulent Combustion, with Special Emphasis on Soot Formation and Combustion* 16th Symp. On Combustion (The combustion Institute), 1976.

[4] WILCOX D.C., *Turbulent Modeling for CFD*, DCW Industries, 1993.

[5] STANCIU, D., ISVORANU, D., MARINESCU, M., *Entropy generation rates diffusion flames*, Int. J. of Applied Thermodynamics, 2001, 4, pp 1-18.

[6] SOMMER T. P., So R. M.C., LAY Y. G., *A near-wall two equations model for turbulent heat fluxes*, Int. J.Heat Mass Trans, 12, pp. 3375–384, 1997.