IMPROVEMENT OF CFD MODELS OF TUNNEL FIRE DEVELOPMENT BASED ON EXPERIMENTAL DATA

by

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This paper, dealing with the problems of mathematical description of the tunnel fire development process with the use of experimental data, outlines the procedure of correction of the existing and obtaining of an improved CFD model package. The improved CFD model was developed on the basis of detailed analysis and comparison of experimental and numerical results, through consideration of the physical structure of all processes affecting combustion. During the analysis it was noticed that the existing CFD model in the part covering combustion based on the so-called steady laminar flamelet model, treats the combustion process almost as a direct correlation between the processes of mixing gasses and heat release rate. This potential deficiency has been overcome by correction of the model in the section defining boundary condition for the burning surface and by establishing a direct correlation between the measured value of the fuel mass change rate and the amount of heat released from burning surface. In this way a modification of complex stoichiometric combustion processes was avoided, while providing the model that better describes and predicts the course of events in this type of complex, anisotropic and turbulent flow of gases in the tunnel.

Key words: *tunnel fire, CFD, boundary condition, turbulence, modelling*

Introduction

As a response to great number of fires, catastrophic by their consequences, which occurred at the end of previous and beginning of this century in large traffic tunnels of Europe, a great number of very expensive and extensive scientific research projects was initiated. These projects were supposed to answer questions on reducing fire risks in tunnels, on the possibility of control in case of fire, as well as on the ways of its effective extinguishing and localization, and procedures for quick evacuation of passengers and material goods from the zones affected by the fire. To obtain the answers to most of these questions, it is first necessary to get an insight into physical-chemical essence of combustion processes and phenomena occurring at the initiation and duration of the fire, as well as to establish a mathematical model reflecting dependence on the dynamics of its spread. Faced with a lack of basic data on combustion processes typical for fires in the tunnel, first numerous experimental researches were initiated.

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By processing and statistical analysis of collected experimental data adequate analytical dependences between individual characteristic values were gradually established [1]. However, this traditional approach due to its 1-D could not satisfy the growing demands and needs of researchers [2]. That is why only with the development of CFD and their application has this problem made further qualitative leap compared to the previous approaches. Due to the CFD approach characteristics to allow that, regardless of the complexity of area geometry, boundary spatial and time conditions, very complex fields of velocity, temperature and concentration are relatively easily predicted, it seemed that it would provide *definitive* solution to the problem of fire prediction and analysis. However, it appears that models of turbulent stress developed so far are not able to precisely forecast the development of fire in the case of so-called homogeneous turbulence. The reason for this may certainly be found in the extremely inhomogeneous turbulent flows with large gradients of temperature and pressure fields and strong resulting buoyancy forces during the ignition and spread of fire [3, 4]. In other words, it was shown that the numerical − CFD approach has certain disadvantages and that results obtained by simulations using the *standard* k-ε and k-ω CFD models of turbulent stress are not able to predict fully accurately and to describe the phenomena occurring during the fire [5]. There are several RANS models that have been developed specifically for fire, including JASMINE, KAMELEON, SMARTFIRE, and SOFIE, plus various research and special application codes, which have all been shown to work well for a variety of fire scenarios. While the model developers continue to argue the merits of each technique, the model users should decide for themselves which is more appropriate for their particular applications [6].

These disadvantages, namely still significant deviations between numerical and experimental data on the velocity field, but primarily on temperature and concentration fields, as well as the importance of more accurate predictions of these data, were the reason of entering into the procedure of correction of the existing CFD models package in order to enable it to predict specified fields more accurately. While developing this model, first the causes of incorrect predictions in existing models were located, and then necessary corrections were carried out. The resulting upgraded package of CFD models enables more accurate simulation of fire ignition and hence it can determine fire behavior with greater certainty.

Experimental research

For the verification of data obtained by CFD simulations it is necessary to have good quality experimental data, measured with fully known characteristic (boundary) conditions. Therefore, results of experimental research carried out in the Fire Institute Sachsen-Anhalt (Heyrothsberge, Germany) in the fire tunnel LSA *Idf* were used [7, 8]. This experimental tunnel was 34 m long (with 37 m long porch); its width was 4.5 m and height 3.02 m without the arc (5.22 m with the arc). Its basic geometry and position of the measuring surfaces are shown in the fig. 1.

Research of fire development was carried out within 4 experiments, with two types of fuel, heptane and gasoline. Temperature, velocity, and flow of gases, concentrations of CO, CO_2, and O_2, and fuel mass loss in the pool with fuel were measured in the experiments.

These experiments were selected as representative for numerical simulations, because they were all conducted with natural ventilation and the same amount of fuel, so therefore had approximately same duration (petrol and heptane have not shown significant differences in the behavior during the fire).

The first two experiments were conducted with gasoline as a fuel, and the other two with heptane. Duration of experiments was 400 s, and reached temperatures varied within the

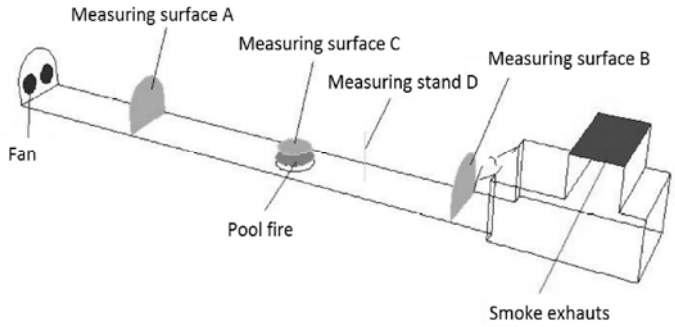

Figure 1. Basic geometry and measuring surfaces in the fire tunnel [7]

range of 275 K to 1241 K (the highest temperature was measured above the measuring surface C), and the measured maximum air velocity was 16.71 m/s (maximum value was measured at the measuring surface B at the tunnel exit). Detailed presentation of all measuring results is given in the paper [8].

Disposition of measuring points at the cross-sections A, B, C and measuring surface D are shown in the figs. 2 and 3.

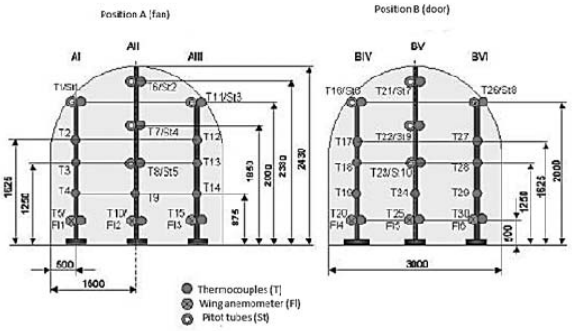

Figure 2. Illustration of measurement points on the measuring surfaces A and B [8]

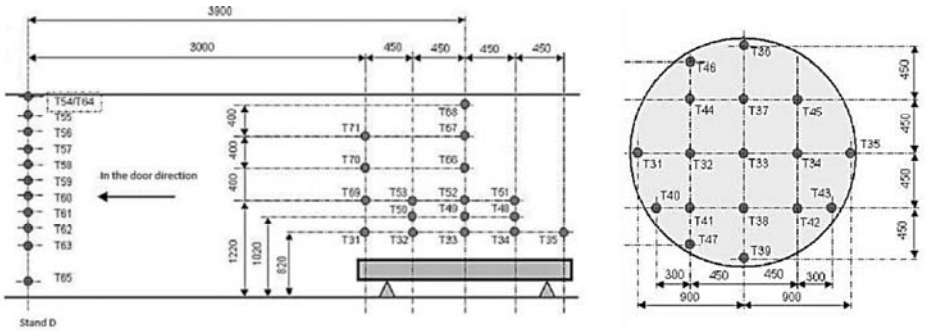

Figure 3. Schematic view of the thermocouples on the measuring surface C, directly above the pool and on the measuring surface D [8]

Numerical simulation (calculation)

For the calculation of flow and temperature fields, *i. e*. smoke concentration fields, the commercial CFD software package FLUENT 13 was used. Model of the 3-D tunnel space is generated in ANSYS Workbench and for formation of control volumes FLUENT network generator ICEM CFD was used, fig. 4. The number of grid planes, *i. e*. number of control volumes was increased in areas where the highest gradients of considered values were expected, such as the space above the pool containing fuel. The total number of control volumes was 96871, control surfaces 13888, while the number of nodes amounted to 31218. With further refinement of mesh there were neither local neither global solution changes.

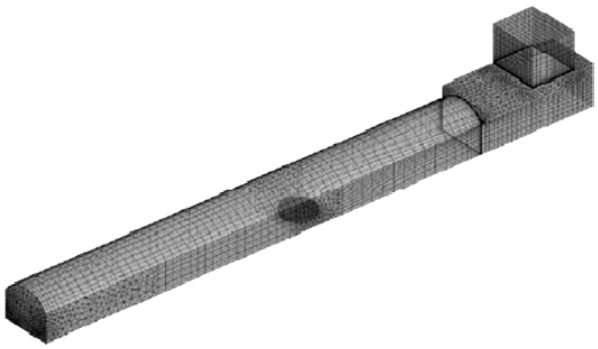

Figure 4. Transparent outer grid of integration domain

Mathematical model

For the mathematical modeling of fire processes in the tunnel, FLUENT basic package was used, where besides k-ε turbulent stress model, thermal radiation model − discrete ordinates and combustion model − so-called steady laminar flamelet model [9] were included.

Basic equations which describe used model are averaged continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho U_i) = 0 \tag{1}$$

Modelled Reynolds vector equation:

$$\frac{\partial}{\partial t}(\rho U_i) + \frac{\partial}{\partial x_j}(\rho U_i U_j) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left[(\mu_\mathrm{f} + \mu_t) S_{ij} - \frac{2}{3}\rho k \delta_{ij}\right] + \rho F_i \tag{2}$$

Modelled averaged equation of energy balance:

$$\frac{\partial}{\partial t}(\rho H) + \frac{\partial}{\partial x_j}(\rho U_j H) = U_i \frac{\partial P}{\partial x_i} + 2\mu_\mathrm{t} S_{ij} S_{ij} + \frac{\partial}{\partial x_i}\left[\left(\rho a_\mathrm{f} + \frac{\mu_t}{Pr_h}\right)\frac{\partial H}{\partial x_i}\right] + S_\mathrm{rad} + S_\mathrm{comb} \tag{3}$$

then two transport equations of k-ε model [10, 11], *i. e*. equation of transport of the kinetic energy of turbulence k:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial}{\partial x_i}(\rho U_i k) = P_k + \frac{\partial}{\partial x_i}\left[\left(\mu_\mathrm{f} + \frac{\mu_\mathrm{t}}{Pr_k}\right)\frac{\partial k}{\partial x_i}\right] - \rho\frac{\mu_\mathrm{t} g_i}{\sigma_h}\frac{\partial \rho}{\partial x_i} - \rho\varepsilon \tag{4}$$

and equations of transport dissipation of the kinetic energy of turbulence ε:

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \frac{\partial}{\partial x_i}(\rho U_i \varepsilon) = C_{\varepsilon 1}\frac{\varepsilon}{k}P_k - C_{\varepsilon 2}\rho\frac{\varepsilon^2}{k} + C_{\varepsilon 3}\rho\frac{\mu_\mathrm{t} g_i}{Pr_t}\frac{\partial \rho}{\partial x_i} + \frac{\partial}{\partial x_i}\left[\left(\mu_\mathrm{f} + \frac{\mu_\mathrm{t}}{Pr_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right] \tag{5}$$

The values of empirical constants in this model, as well as the values of the Prandtl's number, are given in literature [9].

Since both fluids – air and smoke – can be considered as ideal gases, *i. e*. their mixture, regardless of fractions of particular components, could be treated as an ideal gas, for determining flow and temperature fields and smoke concentration fields, the so-called scalar variable marking method was used.

For (molecular) air viscosity square thermodynamic temperature dependency was assumed: $\mu_f = -4.9468\cdot10^{-6} + 4.5839\cdot10^{-8}T + 8.0974\cdot10^{-11}T^2$ [m^2/s], and for the specific thermal capacity of air at constant pressure, *i. e*. its thermal conductivity, it was assumed that they have constant values, $c_p = 1004$ Jkg^{-1}K^{-1}, $\lambda_f = 2.63\cdot10^{-2}$ Wm^{-1}K^{-1}.

Due to high temperature of combustion products generated in the analyzed combustion process, and in order to increase the accuracy of numerical calculation, in addition to the usual modeling of convective heat transfer, numerical analysis also covered a phenomenon of heat exchange by radiation. Basic transfer equation for description of heat transfer by radiation for the fluid − processes of absorption, emission and reflection of the position defined by position vector $\vec{r}$ in the direction $\vec{s}$ is as follows:

$$\frac{\mathrm{d}I(\vec{r},\vec{s})}{\mathrm{d}s} + (a+\sigma_s)I(\vec{r},\vec{s}) = an^2\frac{\sigma T^2}{\pi} + \frac{\sigma_s}{4\pi}\int_0^{4\pi} I(\vec{r},\vec{s}')\Phi(\vec{s}\cdot\vec{s}')\mathrm{d}\Omega' \tag{6}$$

Numerical calculation was carried out assuming that the absorption coefficient a and the reflection coefficient σ_s are constant. According to the recommendation, it is assumed that the values of these coefficients are $a = 0.92$ and $\sigma_s = 0.85$ [9].

With the aim of solving the radiation transfer equation (12) so-called discrete ordinate radiation model was used. With this model, the eq. (6) is converted to transfer equation for the radiation intensity $I(\vec{r},\vec{s})$ for the spatial coordinates (x,y,z).

$$\frac{\partial}{\partial x_i}\left(I(\vec{r},\vec{s})\vec{s}\right) + (a+\sigma_s)I(\vec{r},\vec{s}) = an^2\frac{\sigma T^2}{\pi} + \frac{\sigma_s}{4\pi}\int_0^{4\pi} I(\vec{r},\vec{s}')\Phi(\vec{s}\cdot\vec{s}')\mathrm{d}\Omega' \tag{7}$$

Use of this model has enabled numerical procedure of solving transfer equations for description of heat transfer by radiation, eq. (7), to be identical to the one used for solving of all other transfer equations.

As the principle intention of solving the radiation transfer equation is not to compute the intensity distribution in the considered domain but a source term S_{rad} for the energy conservation eq. (3):

$$S_{rad} = a\int_0^{4\pi} I(\vec{r},\vec{s})\,\mathrm{d}\Omega - 4\sigma T^4 \tag{8}$$

which results from integrating the radiation transfer equation over all solid angles $\mathrm{d}\Omega$ [12].

In order to define the boundary condition, which would include the impact of the combustion process on velocity and temperature field, first the approach offered by FLUENT 13 software package was used. In case of combustion of previously non-mixed fuel and oxidant, which includes the so-called pool fires, all three models offered by this software package were used: − combustion model in case the process takes place in a chemical equilibrium, then if it is *close* to the chemical equilibrium − steady laminar flamelet model, or if it differs significantly from the chemical balance − unsteady laminar flamelet model.

The common feature of all of these models is that the analytics of the combustion process comes down to solving the transfer equations of passive scalar size f_i, so-called the instantaneous mixture fraction is mass fraction of the *i*-the fraction of fuel in the mixture:

$$\frac{\partial}{\partial t}(\rho \overline{f}_i) + \frac{\partial}{\partial x_j}(\rho U_j \overline{f}_i) = + \frac{\partial}{\partial x_k}\left(\frac{\mu_f + \mu_t}{\mu_t} \frac{\partial \overline{f}_i}{\partial x_k} \right) + S_m + S_{\text{user}} \tag{9}$$

The mixture fraction can be written in terms of the atomic mass fraction as:

$$f_i = \frac{Z_i - Z_{i,\text{ox}}}{Z_{i,\text{fuel}} - Z_{i,\text{ox}}} \tag{10}$$

where Z_i is the element mass fraction for element, *i*. The subscript *ox* denotes the value at the oxidizer.

The modeled transfer equations of the average square value of its fluctuation $\overline{f_i'^2}$ [13]:

$$\frac{\partial}{\partial t}(\rho \overline{f_i'^2}) + \frac{\partial}{\partial x_j}(\rho U_j \overline{f_i'^2}) = \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_t} \frac{\partial \overline{f_i'^2}}{\partial x_i} \right) + C_g \mu_t \left(\overline{f}_i \right)^2 - C_d \rho \frac{\varepsilon}{k} \overline{f_i'^2} \tag{11}$$

where relation between the mean mixture fraction $\overline{f}$ and its variance f' and is $f' = f - \overline{f}$ is the sum of the default values of the constants defined by the model are $\sigma_t = 0.85 C_g = 2.86$, $C_d = 2.00$. Also, in accordance with those models the combustion source term S_{comb} in the energy conservation eq. (3) is defined as:

$$S_{\text{comb}} = \rho S_{\text{c}} H_{\text{comb}} Y_{\text{fuel}} \tag{12}$$

where S_{c} is normalized average rate of product formation, H_{comb} is heat of combustion for burning 1 kg of fuel, Y_{fuel} is fuel mass fraction of unburnt mixture [13].

Also, the common feature of these models, which potentially represents both their main advantage and their main disadvantage, is that the stoichiometry of chemical reactions or thermochemical consequences of the combustion process is determined for each type of fuel by using tabular data in the preprocessing section. In this way, the problem of combustion is simplified and reduced to the problem of mixing, and the difficulties associated with the closure of nonlinear components of reaction rate are completely overcome [5].

Boundary (spatial and time) conditions

Based on the assumed geometry of the integration domain, problem unsteadiness and the elliptical nature of transmission equations, boundary conditions at the surface of: the entrance of the fluid flow (air) in to the domain of integration (tunnel entrance), then at the surface of fluid contact with the tunnel walls (along the surface of the solid body), on surfaces of locations where fluids (combustion products) leave the domain of integration (tunnel exit), have been set in accordance with the measured experimental values and the common numerical practice [9]. As a boundary condition for the pool fires area for the purposes of numerical simulation was assumed constant heat flow called *fixed power*. The value of *fixed power* for each simulation were determined from experimental data on the duration of the combustion process and the totally combusted fuel.

Reference experimental data from [8] are presented in fig. 5. The analysis showed that acceptable good results were provided only by the steady laminar flamelet model. However, even in the case of conducting simulation with steady laminar flamelet model, the results of numerical simulation showed significant deviations from the experimental results. The largest deviations were observed in the plane immediately above the pool with fuel (measuring surface C), as well as in the area of the tunnel behind the flame (position D and surface B) in the period after initial fire development, so-called the first period of fire stagnation, *i. e*. in the period from 40 to 120 seconds from the initial moment of the combustion process.

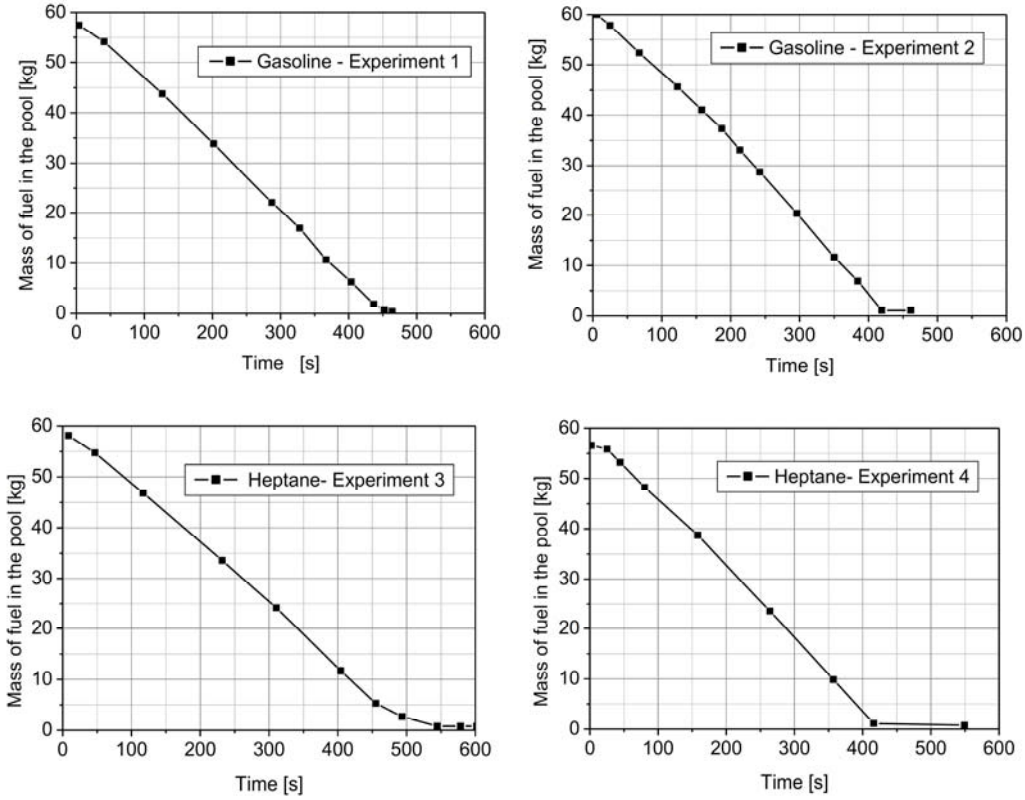

Figure 5. Changes of the fuel mass in the pool during the experiment [8]

The analysis of experimental data found that in the so-called period of first fire stagnation there is a drop of temperature in the flame zone. Considering the physical essence of this process it was concluded that during this period, in the area around the flame and downstream, there is a local lack of oxygen and local drop of gas pressure. At the same time with the drop of gas pressure on one side, and the increase of temperature on the other side, an intensive mixing of gases and increased turbulence occurs in the zone. As one of the consequences of this phenomenon, there also appears accelerated movement of air which with its macroscopic motion, starts to remove by convection more and more heat released in the com-

bustion process. This phenomenon, mainly due to the local lack of oxygen, leads to the local drop of the temperature of gases, which represents a kind of anomaly within this type of combustion process.

For these results to be used, it was necessary to prepare a proper subroutine of experimentally obtained speed of decreasing of the fuel mass in the pool and transposed into the main software.

After the simulation performed with corrected and upgraded model of combustion, and subsequent comparison of obtained numerical results with experimental results and establishing of the degree of model improvement by means of conducted χ^2 tests, it was shown that the applied modification gives better results than the previously used steady laminar flamelet model.

For all four experiments, the most significant improvement was achieved in the prediction of temperature field, especially in the space above the fuel pool (measuring surface C),

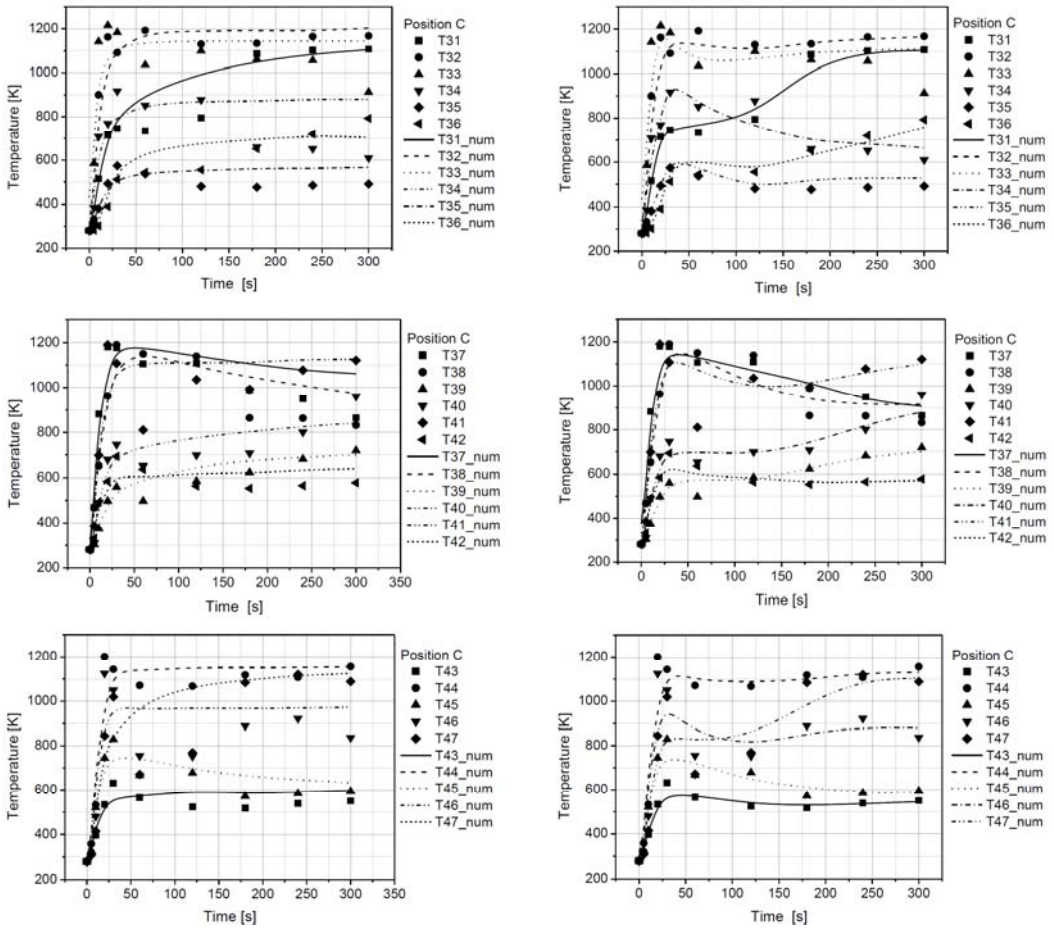

Figure 6. Comparison of experimental results and results of numerical simulations of air temperature changes along the tunnel axis at the measuring surface C, using the basic and corrected model for the first experiment

as well as in the area of the tunnel behind the flame (position D and surface B) in the so-called first period of fire stagnation (period from 40 to 120 seconds), which occurs in the area around the flame due to a local lack of oxygen. In order to provide for a quality illustration of the achieved improvement the fig. 6 shows the results of predicting changes in the temperature field at the measuring surface C and D, in the first experiment.

Empirical comparisons of the numerical and experimental results of temperature field for the first experiment are shown in fig. 7. Comparisons of the difference between numerical and experimental results of temperature field and gas velocity field for all four experiments are shown in figs. 8 and 9. Comparison was carried out through the presentation of the sum of deviation values χ^2 at measuring points in cases of basic and improved numerical models. The analysis of results shown in fig. 7 clearly shows a significant quantitative improvement in prediction of gas temperature fields, which is obtained using the newly proposed model.

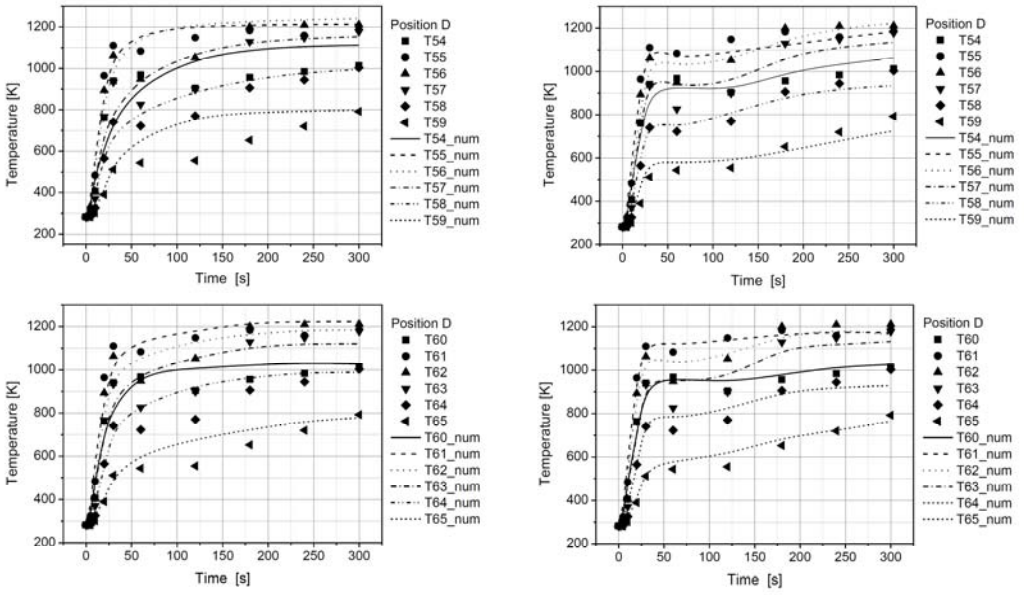

Figure 7. Comparison of experimental results and results of numerical simulations of air temperature changes in the tunnel axis at the measuring position D, using the basic and corrected model for the first experiment

Conclusions

Through detailed analysis and comparison of the experimental and numerical results, through consideration of the physical essence of all processes that affect combustion, it was noticed that the basic package of CFD models simply reduces the numerical combustion process to the mixing process, but without being able to cover the appearance of a local lack of oxygen, *i. e*. it models an almost direct correlation between the process of mixing gases and the heat rate released in the combustion process. Therefore, assuming the boundary condition for the pool fires area as *fixed power* boundary conditions can lead to significant errors in the CFD predictions.

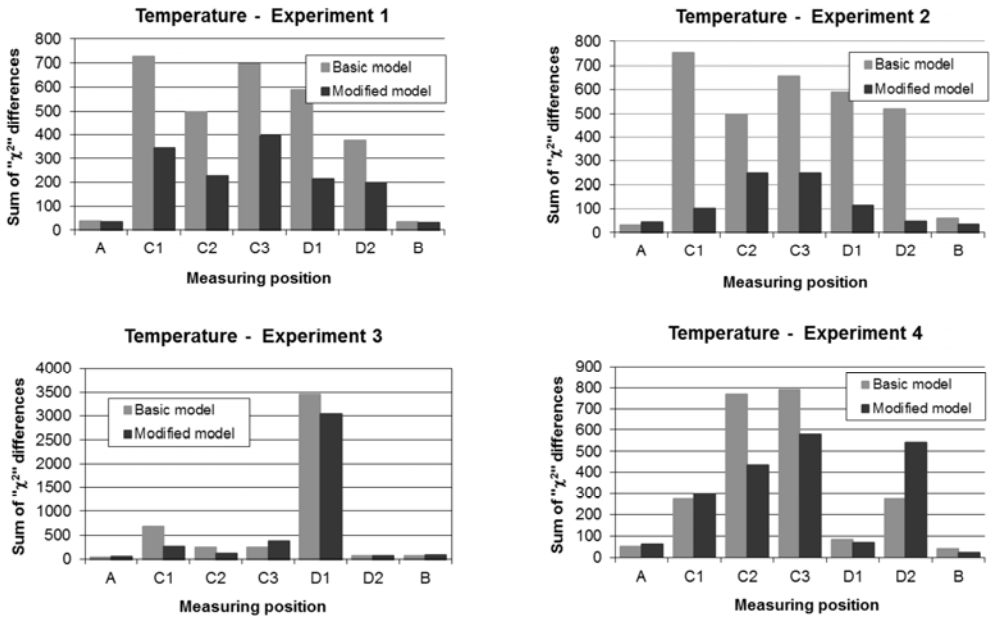

Figure 8. Comparison of deviation of experimental results from all 4 experiments for gas temperature values, with the results obtained by numerical simulation with the basic and corrected packages of CFD models, through the display of the value of the sum of χ^2 differences

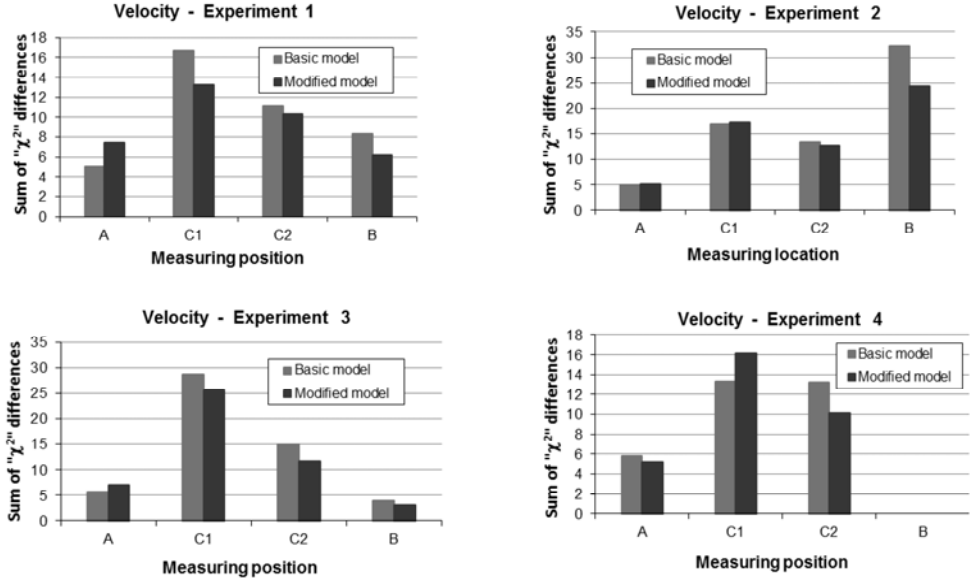

Figure 9. Comparison of deviation of experimental results from all 4 experiments for gas velocity values, with the results obtained by numerical simulation with basic and corrected package of CFD models, through the display of value of the sum of χ^2 differences

By model correction in the part of defining the boundary conditions for the burning surface, establishing a direct correlation between measured values of fuel mass change rate and the amount of heat released from the burning surface, enabled us not only to avoid entering into complex stoichiometric combustion process, but also to avoid a potential deficiency within the basic CFD model.

By direct comparison of experimental and numerical data on the changes in gas temperature at measuring positions upstream and downstream of the flame, but also by comparing deviations of these data at all measuring positions by using χ^2 test, qualitatively significant improvement was observed in predictions that are obtained by using experimentally determined boundary conditions for the pool fires area, compared to by assigning *fixed power* boundary conditions regardless of the type and complexity of the combustion model. Also, it was noticed that the gas temperature changes in the corrected model, not only expressed in numerical values, but also by the character of the curve, gives a better prediction than the basic model and therefore allows more accurate simulation of the startup and development of the fire.

Nomenclature

a – absorption coefficient of the air, [m^{-1}]
a_f – thermal diffusivity, [m^2s^{-1}]
f' – variance of mean mixture fraction, [–]
$\overline{f}$ – mean mixture fraction, [–]
F_i – body force per unit mass, [N kg^{-1}]
g_i – gravity force per unit mass, [N kg^{-1}]
H – specific mean enthalpy, [J kg^{-1}]
I – radiation intensity, [W sr^{-1}]
k – turbulent kinetic energy, [m^2s^{-2}]
P – mean static pressure, [Pa]
P_k – Production of k, [kg $m^{-1}s^{-3}$]
Pr_h – Prandtl number for entalpy, [–]
Pr_k – Prandtl number for k, [–]
Pr_ε – Prandtl number for ε, [–]
$\vec{r}$ – position vector, [m]
s – scattering coefficient of air, [m^{-1}]
x – direction vector, [m]
$\vec{s}'$ – scattering direction vector, [m]
S_{ij} – mean strain-rate tensor, [s^{-1}]
S_{rad} – source term for radiation, [Wm^{-3}]
S_{com} – source term for combustion, [Wm^{-3}]
T – time, [s]
T – local temperature, [K]
U_i – mean velocity vector, [ms^{-1}]
Z_i – element mass frac. for element i, [–]
x_i – position vector in tensor notation, [m]

Greek symbols

δ_{ij} – Kronecker delta, [–]
ε – dissipation of k, [m^2s^{-3}]
μ_f – molecular viscosity, [Pas]
μ_t – turbulent viscosity, [Pas]
ρ – mass density, [kg m^{-3}]
σ – Stefan-Boltzmann constant, [$Wm^{-2}K^{-4}$]
σ_s – scattering coefficient, [m^{-1}]
Φ – phase function, [–]
Ω – solid angle, [sr]

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