INCREASING THE SPEED OF COMPUTATIONAL FLUID DYNAMICS PROCEDURE FOR MINIMIZATION THE NITROGEN OXIDE POLUTION FROM THE PREMIXED ATMOSPHERIC GAS BURNER

by

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This article presents innovative method for increasing the speed of procedure which includes complex computational fluid dynamic calculations for finding the distance between flame openings of atmospheric gas burner that lead to minimal NO pollution. The method is based on standard features included in commercial computational fluid dynamic software and shortens computer working time roughly seven times in this particular case.

Key words: *NO_x, atmospheric burner, combustion, computational fluid dynamics, optimization*

Introduction

The necessity of using heating appliance, based on simple atmospheric gas burner, and without electrical equipment is direct consequence of human awareness that there always were and will be the situations when some inhabited regions stay, for shorter or longer period of time, without power. In this kind of situation, this type of heater with two cylinders filed with gaseous fuel can save humans live. On the other side this is the most simple and cheapest heater which serves almost without maintenance. Because of both motives the number of fully autonomic appliances is increasing, and there is necessity to minimize their pollution. The negative influence of air pollution on human health and life quality is well known and for that reason is limited by standards. The established standards are in accordance with the level of implemented technology and are permanently decreasing: by increasing the technology level. In the case of Serbia the effect of pollutant emission on the health risk was studied on the territory of the city of Nis and presented in [1]. For that reason there was a realized project, with broad tasks upon new atmospheric gas burner, aimed to change the old one within existent appliances. The basic burner technical requirements are:

– fully pre-mixed atmospheric gas burner to fit in the combustion chamber of the current appliance (room heater),
– The NO_x emission <50 mg kW/h,
– nominal power 9 kW with turn down ratio 1:2, and
– capable to work with natural gas (which is nominal), propane-butane and biogases.

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In the case of old burner, due to implemented design solution of flame stabilization, there is a connection between operating air coefficient (λ), NO, and CO emissions. When burner operates in primary air-fuel reach regime, combustion is stable, NO pollution high and CO emission low. When burner operates with fuel lean mixture the combustion stars to be unstable, the NO pollution and efficiency are low, and CO high. Today there are new concepts. Low NO_x burner design, like the Ventury low NO_x tends to create stratified flame structure with different sections of the flame operating as fuel rich and fuel lean. Ultra low NO_x burners, like dual rapid mix burner are designed to eliminate fuel reach zones and prompt NO_x [2, 3]. Common deficiency of majority of the new concepts is their price and need for higher power to drive their fuel air mixing systems. Most design procedures within heater producers are based on experimental data and empirical knowledge [4]. Introduction of CFD modeling in burner research and design enables detailed insight on influence of burner's geometry, fuel type, and λ on its characteristics such as: modulation range, temperature effects on structure stress, efficiency, pollution, and noise [5, 6].

This research is concerned with finding the correlation between NO emission and flame to flame opening distance using CFD approach. However it needs huge calculation time and this paper presents one possible method to decrease it. It is based on standard elements: choosing the modeling strategy, reduced chemistry, 3-D CFD modeling, and passing to 2-D CFD model if it is possible. The non-standard, and for this purpose designed element changes the burner shape, using pervious solution as initialization.

Burner geometry and modeling strategy

The form of burner (mantle) is presented in fig. 1. It is the simplex atmospheric premixed gas burner for an individual space heater (appliance). It has punched flame openings which form large surface with small flames. The released heat is well distributed over heat exchanger which transfers the heat to living space by convection. The burner, manufactured from thin (0.6 mm) steel sheet, is partially or fully aerated by energy of gaseous fuel injected through nozzle. Venturi tube is a part of the burner.

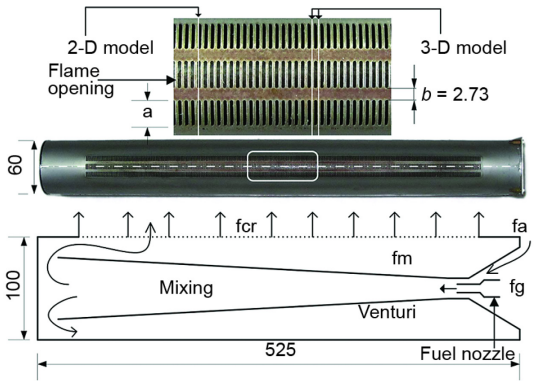

Figure 1. Atmospheric gas burner

As it can be seen (fig. 1), there are many different possibilities for CFD modeling. The first is 3-D model which includes all burner elements. This approach is used in [7] to realize optimal design where target is minimal NO pollution based on quality of air-fuel mixing. In this case, where all implemented chemical reaction zones have to be localized, and mesh adapted in accordance with their dimensions, that approach cannot be accomplished by ordinary PC.

In this project 3-D CFD model is realized in parts. The first is nozzle, second Venturi tube, and third internal flow in the burner mantle. The 3-D model with chemical reactions is slice of burner with periodic boundary conditions, fig. 1. The model is presented in the section *3-D CFD model*. The 2-D model (fig. 1), presented in the section *2-D CFD model* is used for finding correlation between NO_x productions and flame to flame distance *b*.

Chemical reactions – reduced chemistry (standard procedure)

In order to enable CFD modeling of flow field flame interaction feasible to PC, a reduced chemical reaction mechanism of CH_4 burning is imperative [7-11]. Even already reduced (12, 13, and 15 step GRI mechanisms) are not operational. After researching other reduced mechanisms (which must have the same flame speed, combustion temperature, main combustion products, *etc.*) the two-step Westbrook-Dryer [10] model has been chosen, tab.1.

Table 1. Reduced chemical reaction mechanism of CH_4 burning [10]

R_1	R_2	R_3
$CH_4 + 3/2O_2 \Rightarrow CO + 2H_2O$	$CO + 1/2O_2 \Rightarrow CO_2$	$CO_2 \Rightarrow CO + 1/2O_2$

Table 2. Chemical reactions forming prompt and thermal NO [12]

R_4 prompt NO	R_5 thermal NO
$CH + N_2 \Leftrightarrow HCN + N$	$N + O_2 \Leftrightarrow NO + O$
$N + O_2 \Leftrightarrow NO + O$	$N + OH \Leftrightarrow NO + H$
$HCN + OH \Leftrightarrow CN + H_2O$	
$CN + O_2 \Leftrightarrow NO + CO$	

In the case of atmospheric burner, and CH_4 as a fuel, forming of NO is not influentially connected with energy and fluid flow. So, after finding solution S, the chemical reactions from tab. 2 are used to calculate NO emission for frozen S (S = *const.*).

The 3-D CFD model

The FLUENT CFD code has been used to investigate the effects of thermal power and burner mantle geometry on combustion and pollutant emissions. The model is steady-state one, for incompressible gas mixture, with buoyancy as main flow driven force. It includes governing equations for conservation of mass and species (1), momentum (2), energy (3), and rate of species production – destruction (4).

$$\nabla(\rho\vec{v}Y_i) = -\nabla J_i + R_i \tag{1}$$

where ρ is the density, v – the velocity, Y_i – the local mass fraction of species i, J_i – the mass diffusion, and R_i – the net rate of production of species i by volumetric finite rate chemical reaction.

$$\nabla(\rho\vec{v}\vec{v}) = -\nabla p + \nabla(\boldsymbol{\tau}) + \rho\vec{g} \tag{2}$$

where p is the static pressure, $\boldsymbol{\tau}$ – the stress tensor, and $\rho\vec{g}$ – the gravitational force.

$$\nabla[\vec{v}(\rho E + p)] = \nabla\left[k_{\text{eff}}\nabla T - \sum_j h_j\vec{J}_j + \left(\boldsymbol{\tau}_{\text{eff}}\vec{v}\right)\right] + S_h \tag{3}$$

where E is the total energy ($h - p/\rho + \vec{v}\,2/2$), k_{eff} – the effective conductivity, defined according to κ-ε turbulence model (to achieve real flow coefficient from flame opening), T – the temperature, and h – the enthalpy. S_h includes the heat of chemical reaction and any other volumetric heat source (used for starting the chemical reaction).

The net rate of production of species i by chemical reaction R_i is computed as the sum of the Arrhenius reaction sources over the N_r reactions:

$$R_i = M_{\mathrm{w},i} \sum_{\mathrm{r}=1}^{Nr} \hat{R}_{i,\mathrm{r}} \tag{4}$$

where $M_{\mathrm{w},i}$ is the molecular weight of species i, and $R_{i,\mathrm{r}}$ – the Arrhenius molar rate of creation/ /destruction of species i in reaction r.

Species model include species transport, and volumetric reaction. Combustion is modeled with laminar finite rate chemical reaction. Methane air two step chemical reactions include 6 species (CH_4, O_2, CO_2, CO, H_2O, N_2). Concentration of CO is defined by calculated rate constants for forward and backward reactions $CO + 0.5O_2 \rightleftarrows CO_2$. Model includes inlet diffusion, energy source diffusion, full multi component diffusion, and thermal diffusion.

Turbulence model is standard κ-ε with default vales of constants and full buoyancy effect. It is implemented because it is simple and able to model flame openings turbulent flow. Thermal radiation is not implemented.

Model for NO_x formation have models for thermal and prompt NO implemented in FLUENT. Both are without reduction and turbulent interaction. Thermal model is equilibrium without OH. Prompt fuel carbon number is 1 and equivalence ratio 1.

Fluid is incompressible ideal gas. Constant pressure specific heat, C_p, is calculated on the basis of mixing low. The C_p of every component is the polynomial function of temperature. Thermal conductivity, viscosity, and mass diffusivity have constant values. Thermal diffusion coefficient is calculated on the basis of kinetic theory. Solid material (burner mantle) is special steel. It has density of 7700 kg/m^3, specific heat 0.46 kJ/kg K, and thermal conductivity 26.3 W/mK. Heat transfer through the mantle wall is included.

Solver is pressure based (2-D and 3-D). Operating pressure is 101325 Pa, temperature 288.16 K, and density 1.225 kg/m^3. Solver algorithm is SIMPLE pressure velocity coupling. Discretization is second order upwind.

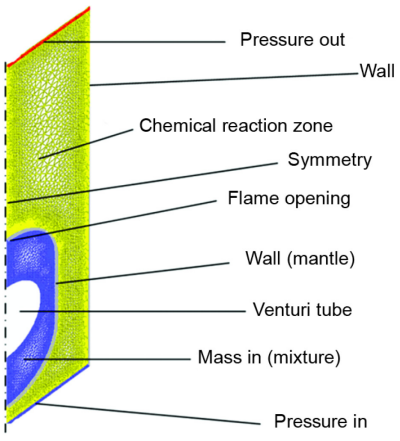

Figure 2. The 3-D burner slice
(*for color image see journal web site*)

The GAMBIT has been used for primary creation of: zones, boundary conditions, and meshes. The mantle wall has structured mesh because of heat transfer, and structural calculations. Further mesh improvements and adaptions have been done by FLUENT in accordance with requirements.

Geometry, boundary conditions, and mesh are presented in fig. 2. Model geometry consist burner slice inserted in fluid (chemical reacted) zone surrounded by boundaries: pressure in, pressure out, wall, and symmetry. Burner slice (fig. 1) has periodic boundary conditions. Wall emulates the appliance flow space. The mixture is supplied from face with the mass in boundary condition.

Mesh is constructed pursuant to forms of solids, flows, chemical reactions, and divided in zones. Basic mesh characteristics and realization problems are:

(1) unstructured tetrahedral (>500000 elements),
(2) adaptation of mesh during calculations (by gradients, values, and visual judgment),
(3) extremely large difference between adjacent elements needs smooth transition, and
(4) every working regime needs particular mesh adaption.

Figure 3 presents part of the burner's wall with two flame openings, and two fluid zones. Burner's wall is solid, and its structural mesh satisfies requirements for getting its temperature field for stress analyses. Fluid zone fm is mixture, and its mesh density rises with approaching to the flame opening. Fluid zone of chemical reactions f_{cr} is made in same manner. Form of its denser place is consequence of its adaption's to capture the chemical reaction R_1.

Some results from 3-D CFD model are presented in figures 4-6.

Visual verification of CFD model is presented on fig. 4 by comparing photographed real zone R_1 (from working burner) with modeled one. Fluid path lines presented on fig. 5 are

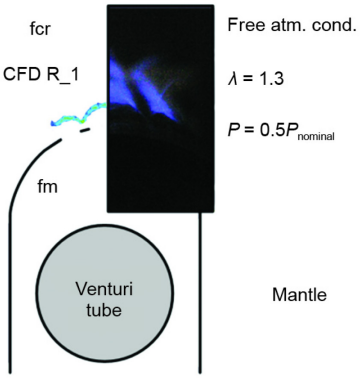

Figure 4. The R_1 from CFD and photo
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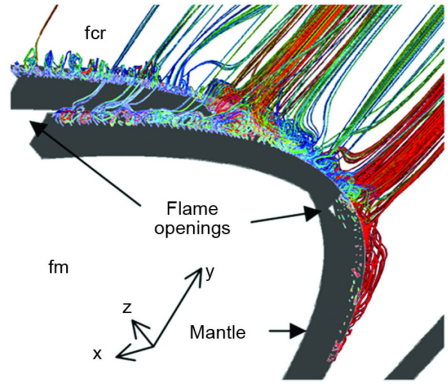

Figure 5. Fluid path lines
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colored by its resident time calculated from the departed flame opening exit. The CFD results indicate that flame to flame distance, fig.1(b) have important role in micro vortices zones between them, and that have influence on local reactant residual time. It is known [3] that this time is connected with NO generation (R_4 in fig. 6). This is additional motivation for CFD research of correlation between NO emission and flame to flame distance, for this particular burner, in order to minimize its NO emission.

During finding the solution it is extremely difficult to make continual end effective adaptation of mesh according R_1

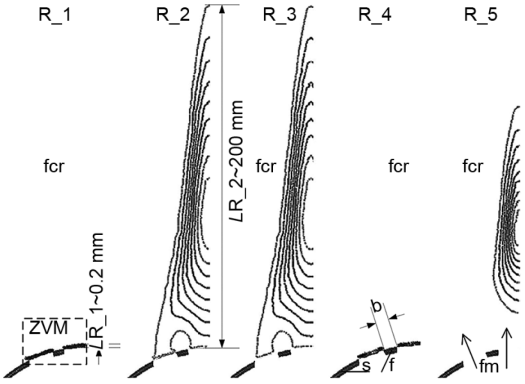

Figure 6. Shapes, positions and dimensions of various chemical reaction zones

reaction zone because its position is variable, with thickness of about 0.2 mm. From fig. 6 is plainly visible connection between R_1 and R_4 (forming of prompt NO).

The 2-D CFD model (passing from 3-D to 2-D model – standard procedure)

Because of complexity of 3-D CFD model, the 2-D case is done with same physical model.

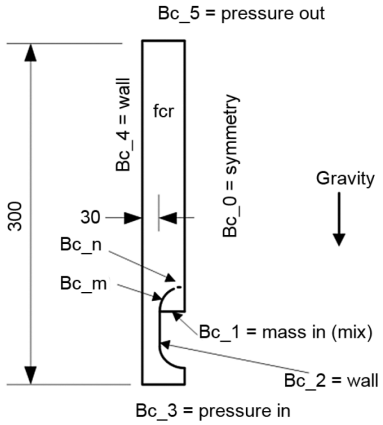

Figure 7. 2-D geometry and outline boundary conditions (Bc)

Geometry of 2-D CFD model is presented in fig. 7. It is based on burners' cross-section in the plane of flame opening symmetry (fig. 1). This geometry cannot predict longitudinal flame to flame interaction, but can model their transversal interaction which geometrically includes distance *b*. Due to passing from 3-D to 2-D model term transversal is equivalent to radial (flame openings are on cylindrical surface).

Most of boundary conditions are the same as in 3-D model, except in the regions in which it is physically impossible to keep similarity. All Bc = *wall* are with no slip conditions.

First region is the mixture entrance, fig. 7. The mixture may have only planar velocity, and for that reason boundary edge Bc_1 defined as (mixture) *mass in* is used. In real situation, temperature of mixture depends of longitudinal plane position. On the Venturi exit the temperature is the same as temperature of surrounding atmosphere. On the opposite side the temperature is higher due to the heat transfer from the combustion zone. In the presented case the temperature is same as the temperature of surrounding atmosphere.

Second region includes boundaries Bc_m and Bc_n. Those boundaries are *interior*, which permits to change them in accordance to needs. Some of them are walls, some interior, some fluid (mesh), and some solid (mesh). When flame to flame distance has to be changed it is provided by changing of their type.

Boundary Bc_3 is also boundary which changes its type. On the beginning of iteration, in the state of initialization Bc_3 = *velocity in*. This is because only driven force of flow is buoyancy, and on the beginning of iteration it is so small that solver tends to find wrong solution. For that reason Bc_3 has the task to form the flow-field similar to real, and after that it takes its natural type *pressure in*.

Boundary Bc_4 = *wall*, and imitates burner working conditions in the appliance.

The modeled chemical reactions of CH_4 combustion are based on Arrhenius law, and because of that it is necessary to *patch* high (2000 K) temperature field over flame openings.

Figure 8 presents solved flow field near the flame openings by fluid path lines. They show dimensions and position of the existing recirculation zones which are so powerful (compared with buoyancy) that mainly shapes the flow field, velocities, and chemical reaction zones. Because those recirculation zones depends of *b*, and NO_x production should depend on them.

Mesh of this 2-D model has 38861 mixed cells.

The maximum absolute value of difference in calculated (prompt + thermal) NO emission, for same conditions, between 3-D and 2-D model, for burner thermal powers: 5, 8 and 10 kW is 5.3 %. This fact signifies that 2-D CFD model may be used in procedure for NO minimization.

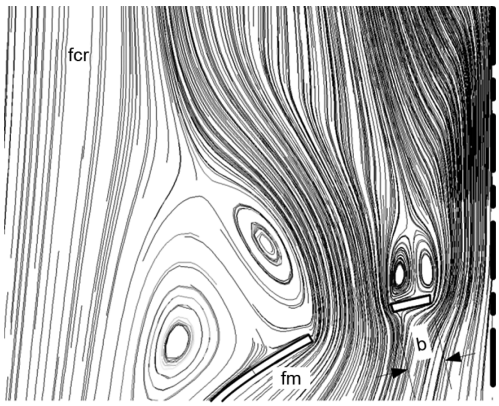

Figure 8. 2-D fluid path lines

Changing the shape and using previous solution as initialization (non-standard procedure)

It has to be pointed that getting solution *S*, from beginning (initialization), PC needs about 70 working hours. For three different regimes and eight different flame ports, the distances PC need about 1680 hours which is 70 days. Bearing in mind that solution procedure needs manual modifying ZVM, the task is almost impossible (in defined schedule). Because of that the new procedure is developed in which starting point for every new flame distance is previous solution *S*. Physical region cowered with this procedure is the area of boundaries Bc_m, Bc_n, and their neighborhood, fig. 8.

Whole procedure is based on interior edge which has fluid cells on both sides but not require any boundary conditions to be set. When that edge has its own zone it can be separately changed into another type of boundary conditions (fan, radiator, porous-jump or wall).

Enlarged pictures end explanations are given in figs. 9-11. First step is finding the CFD solution S_0 from $S = S_{in}$ ($b = b_0$, length of left flame opening a, and specified burner power). Solution includes calculation of NO emission. Next step is moving flame opening a left for incremental value d. Part of its right sided fluid zone f must be converted in to the solid zone s keeping the form of mantle. This is done by extending solid zone SR for length d to the left and converting covered fluid zone to solid s. Constant a requires changing (shortening) of SL for incremental value d. The forlorn solid zone must be converted in to the fluid

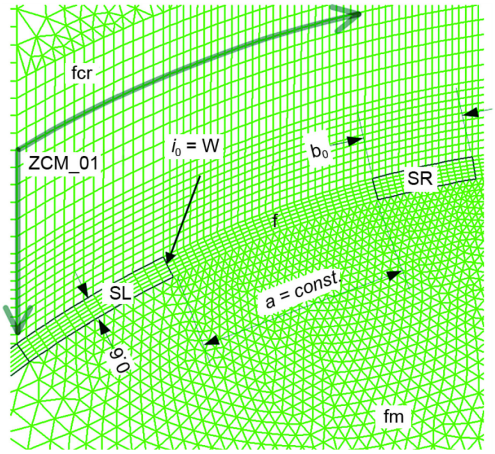

Figure 9. Initial mesh when $b = b_0$
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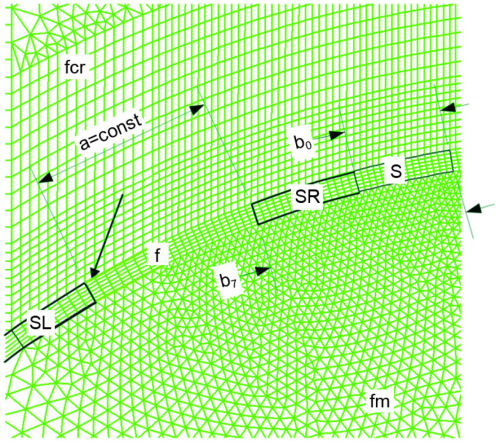

Figure 10. Mesh when $b = b_7$
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zone. In this phase there is a new configuration heaving small geometrical changes comparing to the old one. The old CFD solution S_0 is very close to new one, and for that reason the time needed for finding new solution S_1 is about 30 minutes. The seventh geometry configuration is presented on fig.10. Procedure ends when $b = b_{max}$. Finding of another correlation for another specified burner power starts from the beginning, where $S = S_{in}$.

Stage 0 fig. 11 (a):

$S = S_{in}$ (initialization state)

$b = b_0$

$i_0 = w$ (defining boundary conditions) [12]

calculation – 70 hours

$S = S_0$

Stage 1 fig. 11 (b):

$S = S_0$

$b_1 = b_0 + d$

$i_0 = i$ (changing boundary conditions) [12]

$i_1 = w$ (changing boundary conditions) [12]

calculation – 30 minutes

$S = S_1$

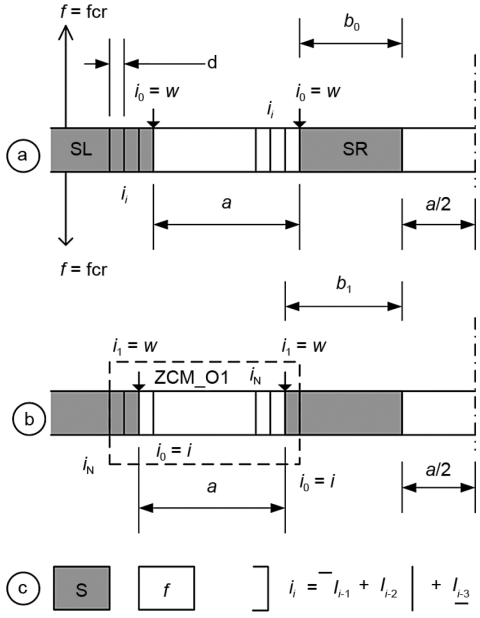

Figure 11. Elements of adopted procedure

Zone of constant mesh, ZCM,_01 is another key element of procedure. It has to be done in accordance with planned solid shape changes, heat conduction and temperature field through wall, fluid flow, and chemical reaction.

The following algorithm plainly describes procedure and computer consumed time.

Research results

Due to the implemented procedure (paragraph 6) the research was realized within 10 days, which is seven time less than realization of the same research without this procedure.

The obtained result of radial flame to flame distance b influence on NO emission (fig. 12) confirms initial hypothesis. From fig. 12 it can be clearly observed that optimal relative radial distances are in the regions of 0.7 and 1.4. Experimental data from dedicated produced burners, with relative flame to flame distances 0.7 and 1.4 are presented in fig.13. They confirm the predicted way in which NO emission depends of power, similar as CFD obtained correlation between flame distance and NO emission.

The experimental set-up for testing the atmospheric gas burner, B, is schematically shown in fig. 14. The nozzle was removed from the burner and replaced by direct premixed mixture supplier. In this way the performance of the burner mantle pattern (different b) can be studied independently of the air entrainment system in which λ depends of working power. In this set-up for the whole range of studied burner thermal power (5-10 kW) λ has constant (1.3) value.

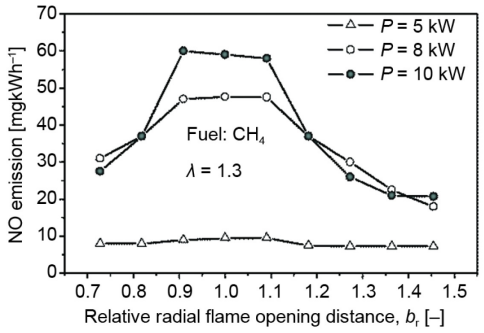

Figure 12. Calculated correlation between NO emission and flame port distance

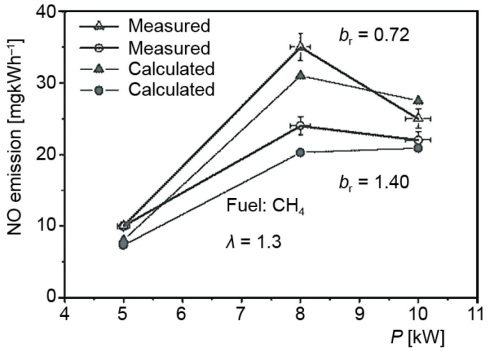

Figure 13. Measured and calculated data of NO emission of two burners

Experiment set-up

Probe of gas sampler S has form of triangular prism with 10 mm distance between parallel walls. The probe is on the burner's half length. When real burners works, near the blow out (~12 kW) regime, the mixture flow inside burner starts to produce non-uniform flow on the flame ports surface and the flame on the burners ends start to rise up and be unstable. This appearance is the lowest on the burner's half length.

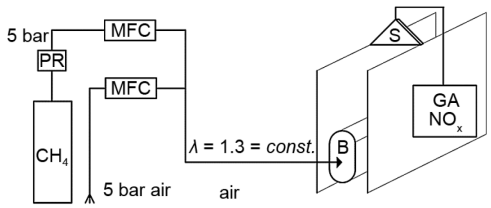

Figure 14. Scheme of experimental set-up; PR – pressure regulator, MFC – mass flow controller, B – burner, S – gas sampler, GA – gas analyzer

The flows of gases (methane and air) were controlled using Dwyers MFC. The GA is TESTO 350. Accuracy, ε, of measured values is calculated as highest probability random propagation error [13]. The values are: $\varepsilon\lambda$ = ±2.1%, εP = ±2.1%, and εNO_x production = = ±5.28%.

Conclusions

The introduced procedure substantially decreases computer working time. The procedure is not universal and may be applied only in similar situations. On the other hand it may initialize new ideas in rapid growing branch of CFD-optimization [14-16]. The procedure can similarly be implemented for 3-D cases.

The next advantage of this procedure is that there is no need for mesh adaption, except during finding the first solution S_0 for particular power. After that, finding the successive solutions for all discrete changes of flame distances can be done with the same mesh.

The method can be improved by implementing automatic mesh adaption of chemical reaction zones. In general, the problem is not so simple because the model may have much more zones with different shapes and positions depended on burner working regime (power).

It has to be noticed that elements presented in fig. 11 are flat although the burner is of round cross-section shape; this type of presentation is clearer without losing any element of the idea of the mentioned procedure.

There are two main requests which must be satisfied for using this procedure: changing of R_1 dimensions and form must be small enough so that solution S_i is close to so-

lution S_{i+1}. In this case for constant power and small d the request is satisfied, the form of mantle should permit this kind of procedure.

Although this procedure of NO emission minimization is, from optimization point of view, simple and is in fact correlation, from the engineering point of view the procedure is full of constrains. There are a lot of implicit constrains in it. The minimum distance between flames is dictated by technological constrains which include production tools and mantle material constrains. On the contrary the maximum value is determined by flame to flame interaction. When distance is too large every flame is stand-alone and overall burner blow out limit falls on the level of separate individual flame. This can be simulated with this type of CFD model.

Next stages of the development of the presented method have to be in the direction of automatic mesh generation, automatic switching of boundary's (internal, fluid, and solid). These *differentially* small boundaries may be realized as a part of the large edges, faces, and volumes. In that case the presented method my serve as the large scale correlation method.

Nomenclature

a – length of flame port, [mm]
b – distance between flame ports, [mm]
b_0 – initial b, [mm]
b_r – b relative (= b_0/b), [–]
d – length increment of b, [mm]
L – length, [mm]
P – power, [W]

Greek symbols

λ – air-fuel ratio (= $m_{air}/m_{air\ Stoichiometric}$)

Subscripts

0 – initial value (step, state)
i – any value (step, state)
N – final value (step, state)
r – relative value

Abbreviations

f – fluid zone
fa – atmospheric air zone
fcr – chemical reaction zone
fm – mixture (CH_4 and air) zone
fg – gaseous fuel CH_4 zone
i – interior [12]
Bc_ – boundary conditions
R_1 – energy release (chemical reaction zone)
R_2 – CO oxidation (chemical reaction zone)
R_3 – CO_2 reduction (chemical reaction zone)
R_4 – prompt NO formation (ch. reac. zone)
R_5 – thermal NO formation (ch. reac. zone)
s – solid zone
S – field state (CFD solution)
w – wall boundary condition
ZCM – zone of constant mesh
ZVM – zone of variable (adaptable) mesh
ZCM_01 – zone of const. mesh (flame opening)

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