Chemical and Process Engineering 2012, 33 (3), 397-410
DOI: 10.2478/v10176-012-0035-9

CFD ANALYSIS OF MIXING INTENSITY IN JET STIRRED REACTORS

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The homogeneous stirred reactor designed for kinetic studies of the combustion of hydrocarbons with intensive internal recirculation in high temperature combustion chamber is described. The originality of our reactor lies in its construction which allows to intensively mix fuel and flue gases, measure gas temperature as well as obtain samples which can be used to investigate diffusion flames. The cylindrical construction enables to use the reactor in laboratory cylindrical electrically heated ovens. The CFD analysis of the reactors, the mixing parameters (turbulent Peclet number and mixing level) and the volume average temperature in the reactors were elaborated on the basis of the typical dimensions of classical reactors to kinetics research as well as the own reactor design. The results of the analysis allow to reveal advantages of our construction.

Keywords: jet stirred reactor, kinetic, CFD modelling, reaction design

1. INTRODUCTION

The kinetics of chemical reactions has been researched for many years now. The chemical reaction rate is analysed in appliances working periodically or in constant-flow equipment. In the first case the substrata mix in a reactor and, next, the course of the chemical reaction in the system is observed. In the second, the substrata flow constantly at a defined rate and the course of the reaction is observed only after the steady state is achieved. Reactors used for analysing the kinetics of chemical reactions differ from one another in the operation mode (continuous and batch reactor) and in the type of analysed reactions (homo-and heterogenic reactions). Geometrical parameters, the mixing level of the reagents in the reactor and the manner in which the reagents are fed to the generator should be mentioned among their characteristics. The continuous stirred-tank reactor and jet stirred-tube reactor whose forms approximate to the majority of real reactors, represent the two basic types used in homogenous reactors. The names “continuous stirred-tank reactor” or “jet stirred-tube reactor” are used in an abstract sense. Those reactors do not have to have the shape of a tube or a tank, but in reality they most often do.

A reactor operating continuously in which the mixing in the direction of the main flow is negligible is the jet stirred-tube reactor. If the mixing in the direction of the main flow is intensive then we deal with the continuous stirred-tank reactor. The intensity of mixing in the direction of the main flow defines the type of the reactor. Our own construction presented in the paper was classified as the continuous stirred tank reactor group due to changes observed in concentration along the reactor axis. To this end also the comparative analysis with reactors described in literature was conducted. For the description of intensity of mixing the Peclet number was used (Hill, 1999; Levenspiel, 1977) while the ML (mixing level) was used to describe the mixing level of substrata streams in the reactor. Reactors selected for the analysis had to meet the requirements of the jet-stirred reactor.

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The purpose of the presented study was to determine the possibility of application of a cylindrical reactor to research kinetics of combustion process of gaseous fuels in the diffusion flame as well as assure good mixing of substrata. The construction of our reactor was compared with other constructions including spherical and conical shapes. The Peclet number and mixing level were used to compare mixing intensity in the reactors. Temperature distribution in the reaction zone was estimated in the reactors. It was particularly significant to ensure that the designed construction can be used with cylindrical ovens and at the same time meets the requirements of a high degree of thermal diffusivity necessary in kinetic analyses.

The analyses were based on CFD numerical simulation of our own reactor as well as selected, representative types of reactors quoted in the literature. The flow of substrata streams in the reactor and the reagent mixing intensity were verified using Fluent 6.3 software.

2. OUR CONSTRUCTION

The objective of the present study was to analyse the construction of our reactor for researching kinetics of chemical reactions occurring in homogenous gas phase in high temperatures. The analysed temperature range was between 900 - 1350 K. In order to eliminate the catalytic influence of the reactor walls quartz was used for the construction. Quartz has small thermal diffusivity and thus is highly resistant to quick temperature changes and transmits ultraviolet radiation well. The construction of the reactor was designed to work with laboratory chambers of cylindrical ovens. The construction is supposed to enable to achieve conditions similar to those in the burner area of the heating oven with burner. The designed reactor is schematically presented in Fig. 1.

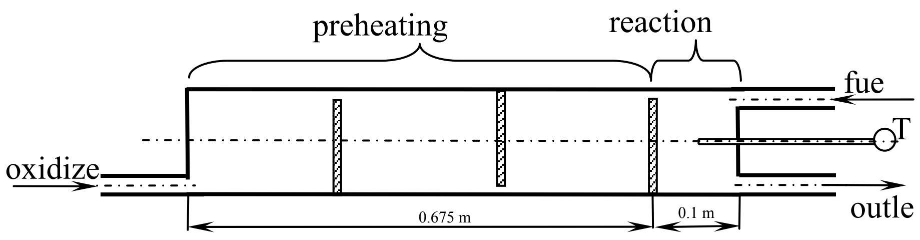

Fig. 1. Scheme of quartz reactor, T - thermocouple

The quartz reactor consists of two parts. The first one is 0.667 m length and it was used to preheat the oxidizer. The second one, 0.1 m in length, is the reaction zone. Internal diameter of the reactor is 0.026 m. The quartz reactor was placed in a cylindrical, electrically heated oven.

This oven is equipped with regulation system which enables to achieve a balanced temperature field with uncertainty of ±5 K. The temperature of the oven can be regulated in the range 870 – 1970 K. The isolated heating chamber of the oven with the dimensions 0.57 m in length and 0.036 m in diameter ensures stable temperature in the oven.

Temperature measurements in the oven chamber were conducted with PtRh10-Pt thermocouple. Measured profiles for two temperatures of the oven chamber are presented in Fig. 2. A balanced profile of the temperatures at the length of 0.38 m (from 0.10 to 0.48 m of the reactor's length) in relation to the left inlet of the oven (Fig.1) was observed. The deviations of the measured temperature across and along did not exceed the measurement error. The reaction zone was placed in that area. At the sections from 0 to 0.10 cm and 0.48 to 0.57 m the temperature fall was 100 and 80 K, respectively.

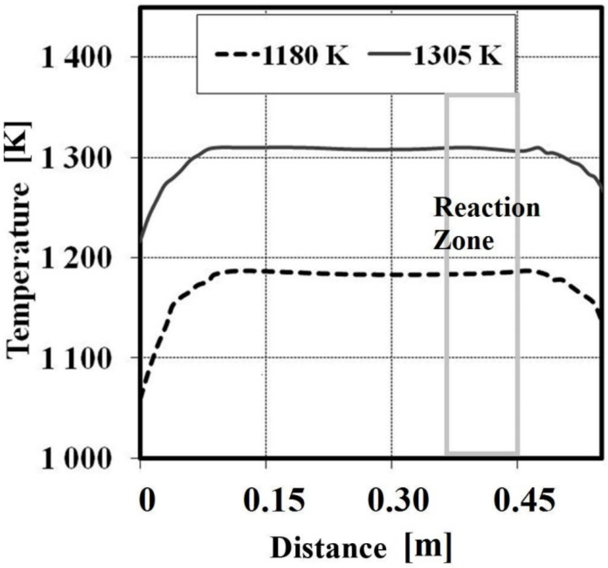

Fig. 2. Profile of temperature oven wall for 2 demand temperature: 1180 K and 1305 K

The reaction zone was placed in the distance of 0.35 m from the inlet to the heating chamber of the oven. In the test runs on methane combustion in air diluted with flue gases, the mixture $CO_2/O_2/N_2$ (with various mole fractions of the respective reagents) was used. In order to reflect the conditions in the burner area, where the hot flue gases contact air for combustion and/or fuel, a mixture of high temperature gases with a composition reflecting typical mixtures participating in the process of natural gas combustion needs to be applied. The heating problem was solved by an adequately long gaseous path for the gas mixture simulating flue gases. Before the gases were introduced into the reactor they had to cover a straight 0.35 m long section in a tube of 0.026 m in diameter. Obstacles mounted before the reaction zone enabled to heat the gas mixture to the required temperature. The temperature in the reactor was measured applying PtRh10-Pt thermocouple. The tube which provided fuel was located on the right side of the reactor at 0.12 m from the outlet from the heating chamber. Such a solution enabled to avoid pyrolysis of the hydrocarbon fuel before its introduction to the reaction zone.

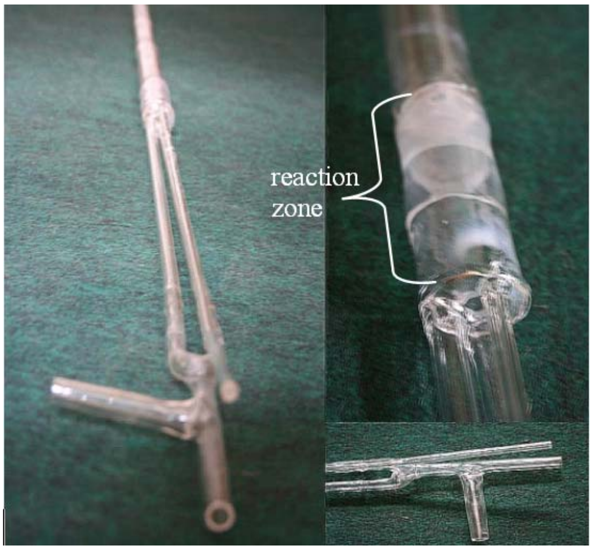

Fig. 3. Reactor A construction

Thus, the conditions in the reactor should reflect the atmosphere of high temperature combustion chambers with intensive gas recirculation. Therefore, the inlets of the flue gases and the fuel are located opposite each other. This solution enables to intensively mix the reagents and ensures adequate circulation of the reagents in the reactor. Photos of the designed reactor are presented in Fig. 3.

The construction of the designed reactor also enables to obtain samples for analysis and "in-situ" temperature measurement during the process. The flow of the substrata streams in the reactor and the intensity of reagent mixing were analysed applying the ANSYS Fluent software.

3. OTHER CONSTRUCTIONS

For the sake of comparative analysis three reactors, of different geometry, were selected. The first one is a cylindrical reactor designed by the authors of this paper and referred further to as *reactor A*. This reactor is characterised in the section "our own construction" of this paper. The next one is a spherical reactor. From spherical reactors described in the literature: Dagaut et al. (1986); Joannon et al. (2005); Longwell and Weiss (1955), and for further analysis the Dagaut et al. (1986) solution was selected. This reactor was applied directly for the analysis of the kinetics of methane combustion in the atmosphere containing CO_2 and H_2O. The construction of this reactor is based on a quartz sphere 32.8 cm^3 in volume. Substrata after heating go to the pre-mixing section in the reactor where gas-dynamic conditions should hamper chemical reactions. Unfortunately, the authors of the paper (Dagaut et al., 1986) and (Joannon et al., 2005) did not verify in any way whether or not in the pre-mixing zone chemical reactions occur at all. Next, the gas solution from the pre-mixing zone is led through four nozzles to the reaction zone. The nozzles are directed in opposite directions to one another which ensures good mixing in broad time scope. This construction also enables to obtain samples for analysis and temperature measurements during the process. This reactor was used successfully for testing kinetics of combustion reactions of both high and low-calorific value of a fuel in temperature range 900-1200 K. Still, the temperature distribution in the reactor presented by the Dagaut et al. (1986) is not as balanced as in *reactor A* (fig.2). Moreover, using the spherical reactor for laboratory cylindrical heating oven seems problematic. In our analyses the construction proposed by Joannon et al. (2005), was omitted since the volume of their reactor equals 0.1 m^3. Thus, the solution requires a large size heating chamber. Therefore the Dagaut et al. (1986) solution is the most interesting one for application in a laboratory scale. The locations of inlets and outlets are similar in both reactors which decides on their gas dynamic similarity and thus only one of them was selected for analysis. The reactor designed by Dagaut et al. (1986) will be further referred to as *reactor B*.

The last considered geometry is the conical reactor. This reactor was applied by Malte and Pratt (1975). This reactor was cast from calcia-stabilised zirconia. The construction was designed as a 0.956 steradian conical segment of Longwell and Weiss reactor (1955). Substrata are introduced into the reactor through 7 holes located on the top of the tube made of a magnesia-stabilised zirconia. The products are removed from the reactor through 7 holes on the walls and the top surface of the reactor. On the reactor wall a sapphire window cooled with liquid nitrogen is located. In order to eliminate the catalytic impact of the walls and the inlet tube for the sake of the kinetic analysis of the methane combustion it was assumed that the reactor is made of quartz. This reactor will be further called *reactor C*.

The Longwell and Weiss reactor (1955) was not selected for analysis. Although, its construction enables to mix well in the reactor, the material of which it is made can influence the analysed methane combustion in the presence of H_2O and CO_2. The construction of this reactor in quartz is, in turn, complicated. The basic geometric data of the reactors is presented in Table 1.

Table 1. The main parameters of the reactors

Parameters	Type of reactor		
	A	B	C
No. of inlets	2	4	8
No. of outlets	2	1	7
Reactor space geometry	cylindrical	spherical	conical
Reaction space volumes, cm^3	53	32.8	49.5
Inlet diameters, mm	CH_4 – 2 Mixture - 4	1	0.74
Outlet diameters	8	8	9.5
Residence time, ms	160 - 400		
Inlet velocity, m/s	12.6-31.4	62.2-155.0	85.7-214.2

4. NUMERICAL TOOLS

In order to compare the level of reagent mixing in the designed reactor with the reactors described in literature modelling in the ANSYS Fluent reactor was conducted. During modelling the following assumptions were made:

- geometric similarity to the designed reactor,
- equal value of residence time in the reactor,
- the possibility to apply the reactors with the construction described in literature (Dagaut et al., 1986; Joannon et al., 2005; Longwell and Weiss, 1955) for analysis in the process of combustion in air diluted with flue gases.

Table 1 presents the geometrical characteristics of the analysed reactors as well as the range of the analysed flow rates. The value of the residence time of the i-th component was calculated applying

$$\tau = V_r / \dot{V}_i \tag{1}$$

in which V_r is the reactor volume and $\dot{V}_i$ the stream of the i-th component defined for the process temperature. Fig. 4 presents the reactors.

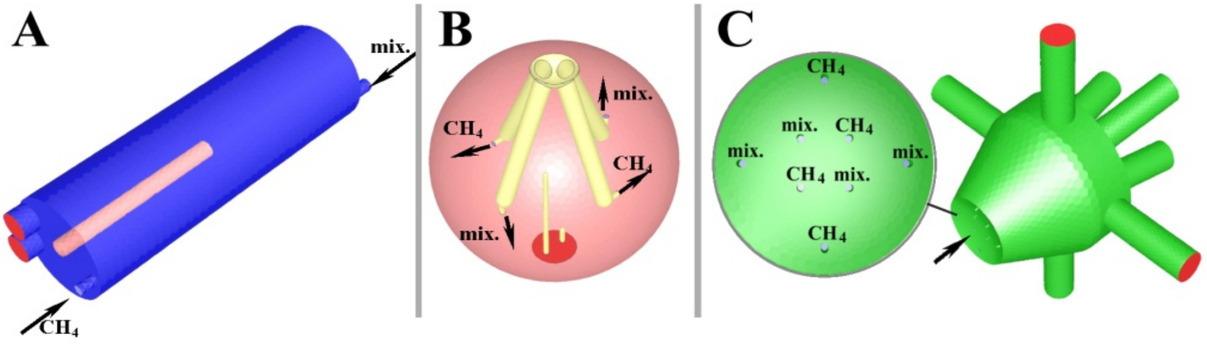

Fig. 4. Reactor geometry; A – cylindrical, B - spherical, C – conical

In order to divide the flow space of the reactors into elementary volumes the GAMBIT mesh generator was applied. The space was divided into tetrahedral elements with the equi-angle-skew factor which was not to exceed the value 0.75. After being input in the ANSYS Fluent the grids were converted to polyhedrons. This procedure enabled to increase the elements of numerical division five to seven times. In order to reduce the impact of the geometry modelling error on the calculation results, several numerical grids with increasing number of division elements were made for each of the geometries presented on Fig. 4. Next, an analysis of the impact of the grid sensitivity on the modelling results was conducted. After initial calculation of the flow fields, for the purpose of further analyses, a grid with the smallest possible amount of elementary volumes and negligible calculation error was selected. The results of the analysis of the impact of distribution of the mesh elements on the obtained calculation results are presented in Table 2.

In Table 2, three types of grids were selected and the temperature calculations for an average gas mixture at the outlet are presented and the concentration of the gas components are compared with the average values at the outlet of the reactors which were obtained on the basis of substantial and energy balances. The sensitivity analysis the results of which are presented in Table 2 was conducted for the residence time of 160 ms.

Table 2. Results of the grid sensitivity analysis

Parameter		grid 1	grid 2	grid 3
Grid cells	Reactor A	33000	67000	120000
	Reactor B	17500	35000	70000
	Reactor C	12000	23000	50000
		Absolute uncertainty %		
Outlet average temperature, K	Reactor A	1.1	0.5	0.25
	Reactor B	1.5	0.7	0.28
	Reactor C	3.0	0.7	0.22
Outlet mole fraction of selected components	Reactor A			
	CH_4	2.7	0.8	0.7
	N_2	7.4	4.0	1.4
	Reactor B			
	CH_4	3.1	0.7	0.5
	N_2	8.8	3.6	2.1
	Reactor C			
	CH_4	4.1	0.5	0.3
	N_2	7.7	5.1	1.8

Numerical calculations were based on the following assumptions:

- the reactors are in the balanced temperature areas of the oven ($T \approx 1300$ K),
- in each case the CH_4 stream provided through nozzle has the temperature of 873 K (in practice, above this temperature value thermal decomposition of methane would occur),
- the scope of inlet velocities results from the assumed values of theoretical residence times provided in Table 1,
- the proper thermal value, thermal conductivity and viscosity of the respective components were estimated on the basis of molecular theory of gases.

The mentioned parameters in the respective calculation cells were estimated on the basis of the additivity principle. All the thermo-chemical data of the gas components in the reactor were described using the data from tables NIST-Janaf (1998). The basic numerical calculation parameters are presented in Table 3.

Table 3. Boundary conditions and the main simulation parameters

Parameter	Value
Outlet boundary	Operating pressure, outlet hydraulic diameter, turbulence intensity - 8 %
Inlet boundary	Velocity, inlet hydraulic diameter, turbulence intensity - 8 %
Wall boundary	No slip conditions, wall temperature -1300 K, emissivity - 0.9
Discretization	
Pressure	Simple
Momentum	Second order upwind
Turbulence kinetic energy	Second order upwind
Turbulence dissipation rate	Second order upwind
Under relaxation factors	
Pressure	0.3
Density	0.5
Body forces	0.5
Momentum	0.3
Turbulence kinetic energy k	0.5
Turbulence dissipation rate ε	0.5
Turbulent viscosity	0.4
Minimum mesh volume, m^3	$4 \cdot 10^{-8}$

Mathematical modelling includes coupled problems conditioned by the balance of substance, momentum and energy together with proper initial and boundary conditions. To solve the problem, the Fluent (User Guide, 2006) software with implemented continuity equations was used. These equations take the form of a coupled problem, and for the stationary state they can be formulated as the mass balance equation

$$\nabla \cdot (\rho \mathbf{w}) = 0 \tag{2}$$

momentum equation

$$\nabla \cdot (\rho \mathbf{w} \otimes \mathbf{w}) + \nabla p = \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g} \tag{3}$$

energy balance with source element S_r describing the radiation factor

$$\nabla \cdot (\rho \mathbf{w} h) = \nabla \cdot \left(\frac{\lambda_z}{c_p} \nabla h \right) + S_r \tag{4}$$

In order to estimate the S_r element, the P1 (Sazhin et al., 1996; Siegel et al., 1992) model was used. The energy stream emitted by the gas volume according to P1 model takes the following shape

$$\dot{q}_r = -\frac{1}{3(a + \sigma_s) - C\sigma_s} \nabla G \tag{5}$$

In the model, chemical reactions were not included in order to analyse the mixing process, thus Equation (4) lacks the source element describing the chemical reactions. Turbulence mixing was described with the equations of the Laudner-Spalding (1972) *k*-*ε* model in the form of Equations (6), (7) describing the kinetic energy of turbulence *k* and its dissipation *ε*.

$$\frac{\partial}{\partial t}(\rho k)+\nabla\cdot(\rho k w)=\nabla\cdot\left[\left(\eta+\frac{\eta_T}{\sigma_K}\right)\nabla k\right]+G_k+G_b+\rho\varepsilon-2\rho\varepsilon\frac{k^{0.5}}{a} \tag{6}$$

$$\frac{\partial}{\partial t}(\rho\varepsilon)+\nabla\cdot(\rho\varepsilon w)=\nabla\cdot\left[\left(\eta+\frac{\eta_T}{\sigma_\varepsilon}\right)\nabla\varepsilon\right]+C_1\left(G_k+C_3G_b\right)-\frac{C_2\rho\varepsilon^2}{k} \tag{7}$$

RANS (Reynolds averaged Navier –Stockes) equations were used to describe mixing intensity. Favre averaging was used to consider temperature influence on physical quantities (e.g. density, viscosity) (Fluent User Guide, 2006).

Residence time described by Equation (1) is a theoretical measure, in reality the construction of the flow space and the distribution of the inlet nozzles condition the level of mixing in the appliance. The assessment of the gas-dynamic properties of the reactors was done on the basis of the dispersion of the reagents such as the Peclet number of mixing occurring along the main flow axis, in the analyses the main axis was the axis of the outlets. This dispersion is defined in the form (Levenspiel, 1977)

$$Pe_l=\frac{wl}{D_T} \tag{8}$$

In Equation (8) *w* is the local velocity value defined in the main direction i.e. in the axis of *A* and *B reactor* outlets as well as *reactor C* symmetry axis. Thus, together with the increase of the mixing intensity the local value of the Peclet number decreases.

5. RESULTS AND DISCUSSION

The Figs. 5-7 present gradient maps for mixing in the reactors. Black arrows indicate the main gas flow directions.

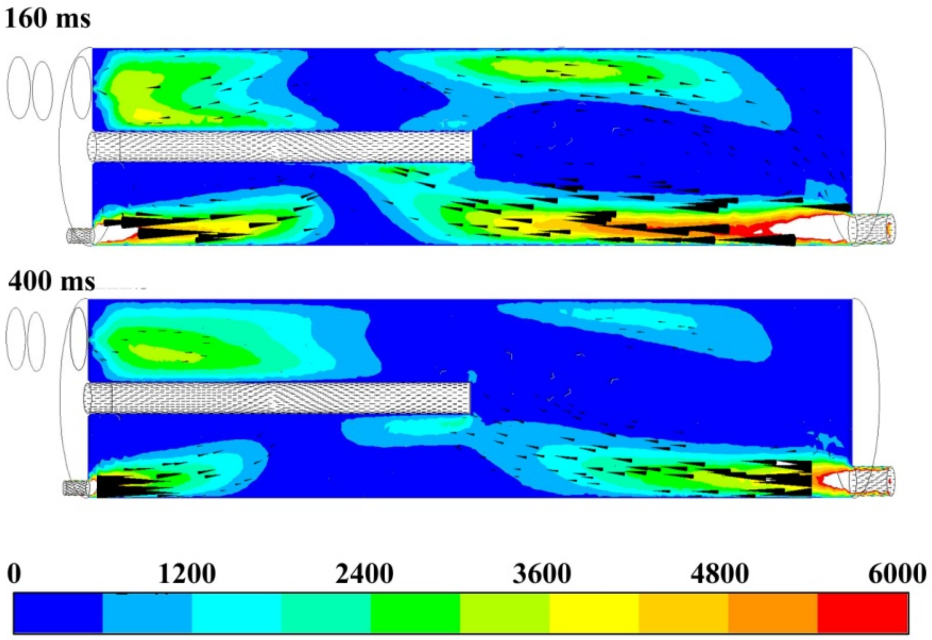

Fig. 5. Peclet number gradient maps for *reactor A*

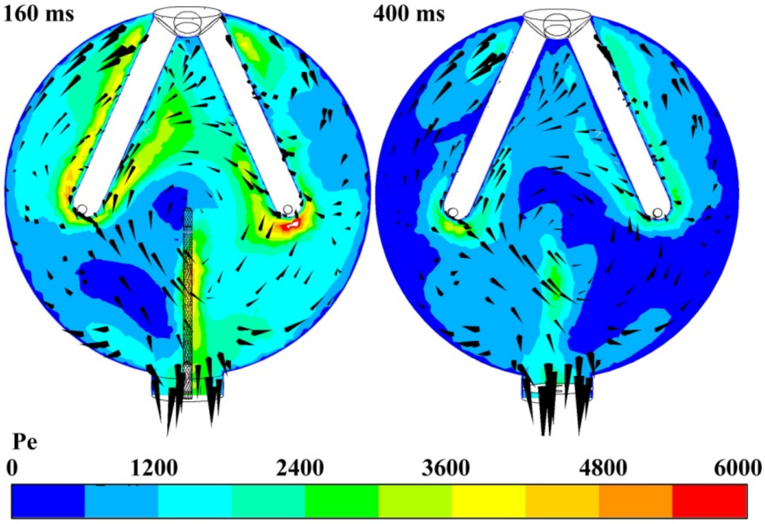

Fig. 6. Peclet number gradient maps for B type reactor

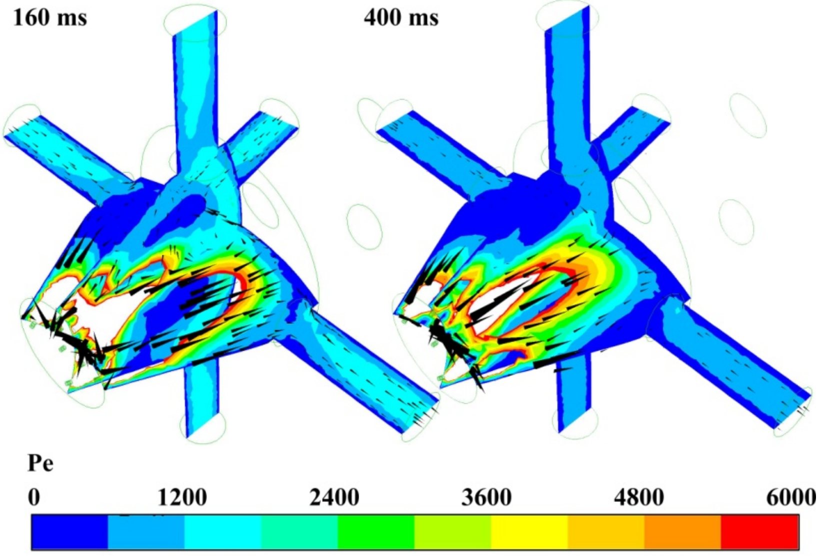

Fig. 7. Peclet number gradient maps for reactor C

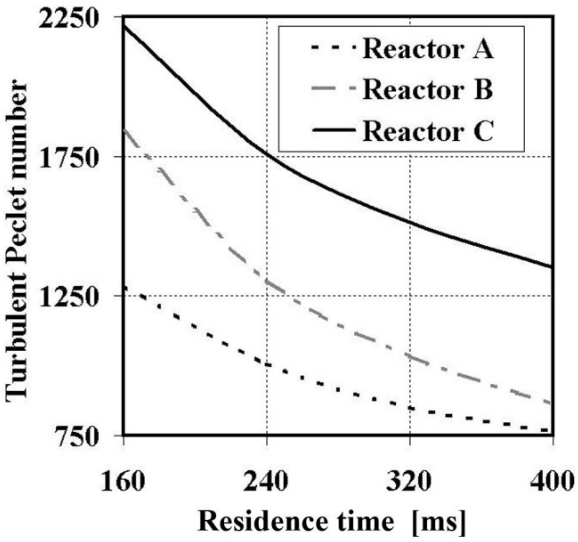

Fig. 8. Volume average Peclet number inside the reactors for different residence times

Fig. 8 presents the values of the Peclet number for various residence times. From the results presented in this figure (Fig. 8) it follows that the construction of *reactor A* ensures the lowest Peclet number values. For short residence times the number takes the value of *Pe* ≈ 1250 and with the prolonged residence time the Pe number value decreases. The largest change of the Pe number with residence time was observed for *reactor B*. For *reactor C* however the Peclet number took the highest values. From the distribution of the Pe number in the function of residence time for the analysed *reactors A, B* and *C* it follows that the construction of *reactor A* ensures the most intensive mixing and the construction of *reactor C* the least intensive one.

Another significant parameter which conditions the application of the reactor for analysing the kinetics of chemical reactions is the temperature field. The balance of temperature in the reactors is significant for a correct analysis of the kinetic mechanism of the occurring reactions. In the frames of the numerical calculations the temperature field of the mixing in the reactor was determined from which the average temperature values in the modelled space were defined. The closer the average temperature to the value of nominal temperature of the oven (e.g. $T = 1300$ K) the better technical parameters of a given reactor. Figs. 9-11 present gradient temperature maps for different theoretical residence times. As can be incurred from the figures *reactor A* has the best temperature distribution in the whole scope of residence time.

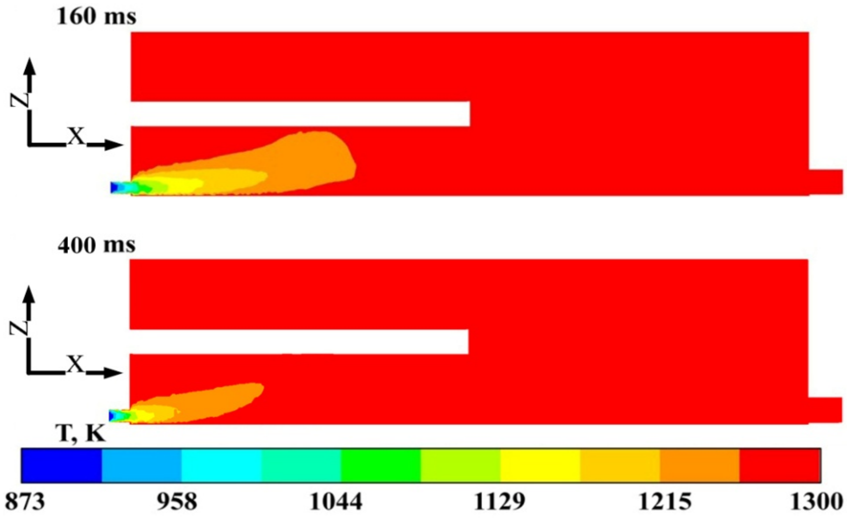

Fig. 9. Temperature gradient maps for reactor A

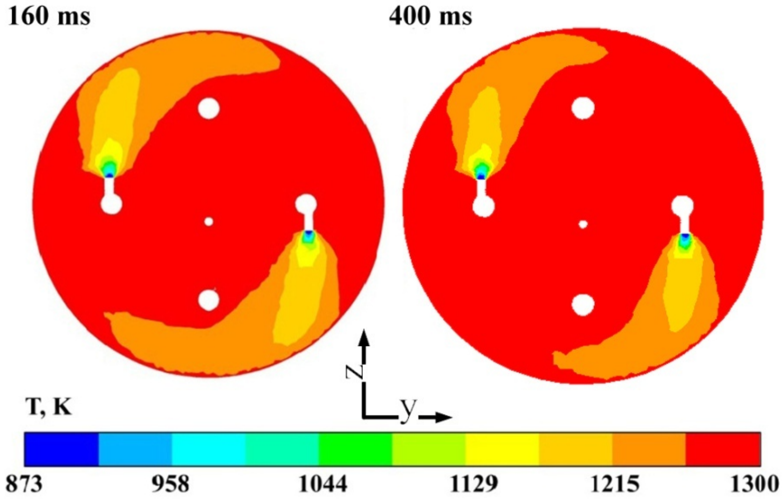

Fig. 10. Temperature gradient maps for reactor B

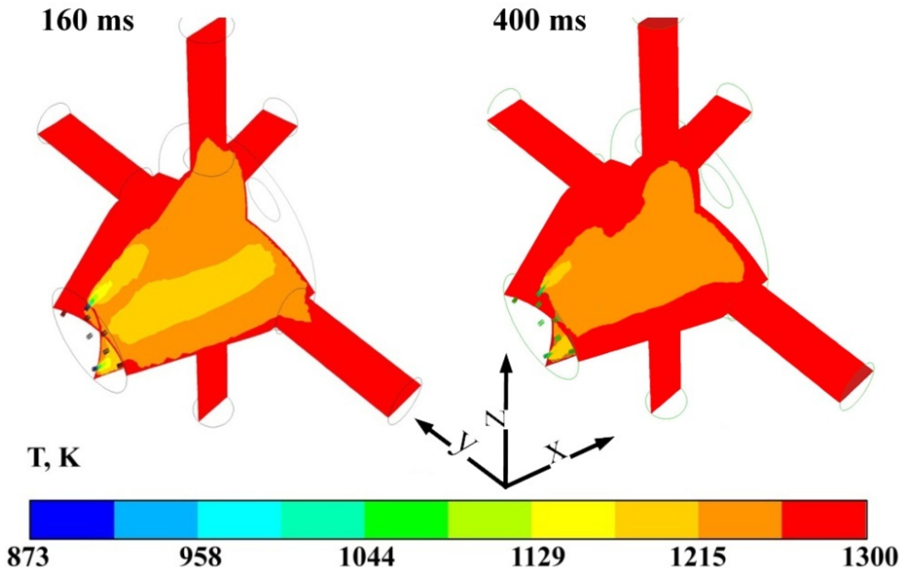

Fig. 11. Temperature gradient maps for reactor C

In Fig. 12. a comparison of the average gas temperature for different residence time values, is presented. The temperature profile in the *reactor* A is the nearest to the demanded temperature ($T = 1305$ K) in the whole range of the residence time.

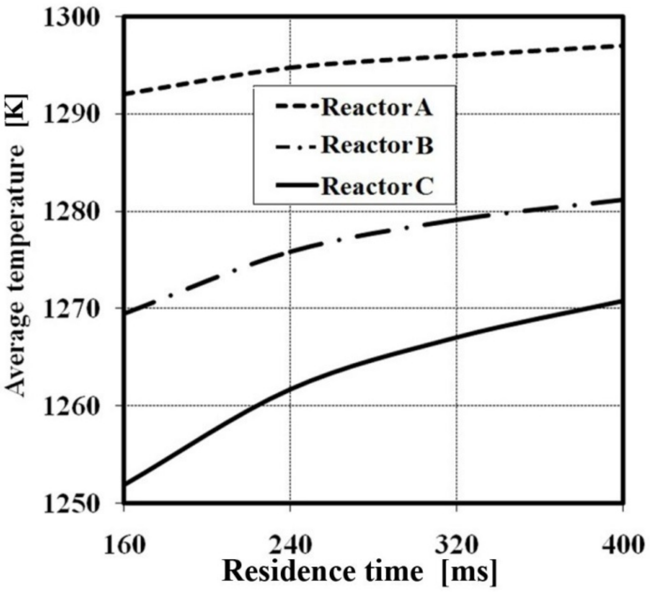

Fig. 12. Volume average temperature inside the reactors for different residence times for the temperature wall equal 1305 K

In the next step the mixing level (ML) in the reactors was defined by

$$ML = 1 - \frac{\sqrt{\left(z_{co_2} - \bar{z}_{co_2}\right)^2}}{\bar{z}_{co_2}} \tag{9}$$

The computation results were presented in Fig. 13. Ideal mixing jet stirred reactors have a ML value of 1. The best ML was observed for *reactor B*, the worst in *reactor A*. However, the mixing level in *reactor* A increases for longer residence time but decreases for *reactor* B.

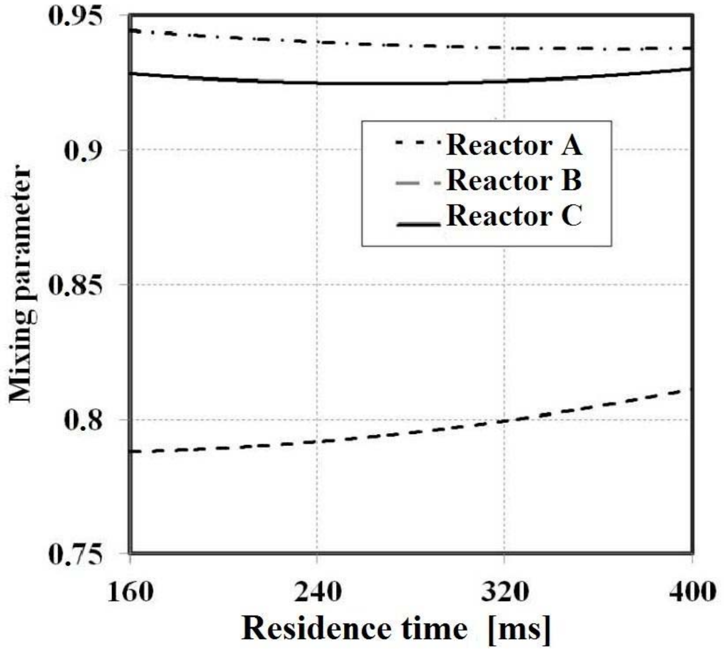

Fig. 13. Mixing level in the reactor for different residence times for the temperature wall equal 1305 K

6. CONCLUSIONS

The proposed construction of *reactor A* can be applied for analysing the kinetics of combustion of hydrocarbon gas fuels in diffusion flames in broad scope of temperatures and flow rates. Nevertheless, reactors B and C can not be used to investigate diffusion flames since their mixing levels are almost 1. Therefore, they are used only to analyse the kinetics of flames.

A measurable advantage of *reactor A* is its shape. The construction is not only easy to make but also can be easily used in cylindrical laboratory heating ovens. Cylindrical heating ovens with good thermal characteristics allow to conduct tests in a constant temperature which is crucial for kinetic analyses.

A comparative analysis of mixing intensity in the reactor using the no-dimensional Peclet number indicates the construction of *reactor A* as the one ensuring most intensive mixing of the reagents. The observed mixing along the reactor axis enables to qualify the reactor as a continuous stirred-tank reactor.

The studies conducted so far on methane combustion in the air diluted with CO_2 were carried out in the following conditions:

- pressure range from 1 to 1.5 atm,
- temperature range from 850 to 1350 K,
- residence time from 80 to 400 ms,
- the excess air ratio from 0.1 to 5,
- carrier gas – nitrogen,
- the initial mole fraction of hydrocarbons from 0.078 to 0.1327 (in volume).

The experimental results were compared with those of numerical calculations (Gil et al., 2008; Gil, 2009; Gil, 2010). The reaction scheme used for the calculations was taken from the publications by Miller and Bowman (1989). Experiments and modelling on methane combustion in the air diluted with flue gases is the object of further analyses.

SYMBOLS

a	gas absorption coefficient, m^{-1}
a_s	speed of sound, ms^{-1}
c_p	heat capacity at constant pressure, $Jkg^{-1}K^{-1}$
C	linear anisotropic phase function coefficient
C_1, C_2, C_3	constants for k-ε turbulence model,
D_T	turbulent diffusion coefficient, m^2s^{-1}
i	specific enthalpy, $J\cdot kg^{-1}$
G	incident radiation, Wm^{-2}
G_k	production of turbulence energy, $kgm^{-1}s^{-3}$
G_b	production of turbulence due to buoyancy, $kgm^{-1}s^{-3}$
h	sensible enthalpy, Jkg^{-1}
h_j	j'th species sensible enthalpy, Jkg^{-1}
J_j	diffusion flux of j'th species, $kg\cdot m^{-2}\cdot s^{-1}$
k	turbulence kinetic energy, m^2s^{-2}
l	reactor length, m
ML	mixing level
p	pressure, Pa
$Pe_l = \frac{w \cdot L}{D_T}$	the Peclet number,
$\dot{q}_r$	radiation flux, Wm^{-2}
S_r	radiation source term, Wm^{-3}
T	gas local temperature, K
V_r	reactor volume, m^3
$\dot{V}_i$	volume stream of the i'th component, $m^3\cdot s^{-1}$
$\mathbf{w}$	velocity vector, $m\cdot s^{-1}$
w	velocity in the main direction, $m\cdot s^{-1}$
Y_M	dilatation dissipation term
z_{CO2}	mole fraction of CO_2
$\bar{z}_{co_2}$	average mole fraction of CO_2

Greek symbols

ε	turbulent dissipation rate, m^2s^{-3}
λ_z	equivalent heat transfer coefficient, $W\cdot m^{-1}\cdot K^{-1}$
μ	dynamic coefficient of viscosity, $kgm^{-1}s^{-1}$
μ_T	dynamic coefficient of turbulent viscosity, $kgm^{-1}s^{-1}$
ρ	density, $kg\cdot m^{-3}$
σ_e	turbulent Prandtl number for ε,
σ_k	turbulent Prandtl number for k,
σ_s	scattering coefficient, m^{-1}
$\boldsymbol{\tau}$	stress tensor, Pa
τ	theoretical residence time, s

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Received 19 October 2011
Received in revised form 05 July 2012
Accepted 08 July 2012