Mathematical Modelling of the Low-reactive Coal Gasification in The Upward Annular Flow

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doi: http://dx.doi.org/10.13005/bbra/2261

(Received: 30 July 2015; accepted: 03 September 2015)

A mathematical model of the low-reactive coal gasification in a vertical upward annular oxidant flow is presented in this work. Air, oxygen or their mixture are used as an oxidizing agent. The developed model is static, one-dimensional with the parameters, distributed along the vertical axis. It is based on differential equations of the energy and mass conservation for a multi-component stationary flow, in which ten chemical reactions occur. In case of the identification of new chemical reactions with the noticeable impact on the results of modelling, it is easy to add them to the existing ones, with all computational processes remaining unchanged. Using the developed model, we composed a computer programme, with which computational experiments were carried out.

Key words: Coal gasification, kinetics, mathematical model, differential equations, matrices, computer programme, stationary flow, computational experiment.

An obvious advantage of the gasification technologies compared with conventional combustion is economic and environmental benefits¹. At the moment, a large number of different gasification methods is developed^{2,3}, nevertheless, the problem of creating new technologies remains relevant. Experimental and theoretical modelling precedes the designing of gasification units and technologies.

In the recent years, the interest to mathematical modelling of different gasification processes increased⁴⁻¹¹. It is due to a need to study the processes before introducing the gasification technologies on an industrial scale. Whereas, we also should note the absence of calculation methods for the gasification of pulverized fuel in an upward jet-vortex flow of the oxidant.

It is a difficult task to create a numerical modelling of coal combustion and gasification processes, taking into account diffusion and chemical kinetics¹²⁻¹⁴. The main issues are the evaluation of the rate constants of homogenous and heterogeneous reactions, which occur during coal gasification, accounting for the impact of diffusion and other chemical factors, aerodynamics of gasification processes. The data of different researches contradicts¹⁵⁻¹⁷.

The presented paper deals with the mathematical modelling results of the solid fuels gasification process in an upward jet-vortex flow in an annular channel. Features of this process and a device for its implementation have been examined in detail previously^{18, 19}.

Method for gasifying solid fuel in the upward annular flow.

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The following types of coal gasification in technical devices are singled out: gasification in a fixed bed, fluidized bed and in a flow. This method of gasification in an upward annular flow refers to the third type. A schematic diagram of the experimental unit with its detailed description was presented in¹⁹. In this unit, pulverized coal is fed into the inner cylinder chamber with a screw feeder, it moves inside this chamber vertically downwards under its own mass (gravity). In the bottom part of the gasifier, pulverized coal meets with a swirling air flow, the rate of which is greater than the hovering rate of solids, and then pulverized coal mixture moves upwards through the annular channel which is formed by the inner and outer cylindrical chambers.

The air is fed to the annular chamber of the gasifier, when heated up to the temperature of 600...900, which is sufficient to start the basic chemical reactions that occur during coal gasification. Water and nanomaterials can be injected into the heated air in front of the gasifier. The air flow is swirled by the axial vane swirler.

The gasification method in an upward flow has the following advantages in comparison with the other gasification method:

- a) With small particle sizes, a large surface is formed, on which the heterogeneous chemical reactions occur;
- b) Large vortex formation intensifies the gasification process;
- c) The bigger the particles in an upward flow, the more time they remain in an annular chamber which has a positive effect on the efficiency of fuel use;
- d) Flow swirling gives additional turbulence to the gas mixture and causes a horizontal sliding in addition to the vertical one between solid and gaseous phases, which intensifies the diffusion in heterogeneous chemical reactions.

Mathematical model

The mathematical model, presented below, describes the processes occurring during coal gasification in the upward annular flow. This model is static and one-dimensional with the parameters distributed along the vertical coordinate. Key assumptions adopted in the development of the mathematical model are presented in ¹⁹. A special feature of this model is vectormatrix representation of the main characteristics of the gasification process. This representation has at least the following advantages:

- a) When identifying a new chemical reaction with a noticeable effect on the modelling result, it is easy to add this reaction to the existing ones, with all the computational processes remaining unchanged;
- b) With the matrix representation it is quite easy to organize checks on different balance ratios, and it was done in the developed computer programme;
- c) Debugging and testing of the programme becomes much easier, as shown by the experience in programming.

The following indices are the basis for the matrix representation of parameters: i – number of a chemical reaction, j – number of a component, which is involved in the energy and material balance in the gasification process. Information on chemical reactions and component, used in the presented variant of the mathematical model are presented in Table 1.

The value N_{ij} in Table 1 shows the number of moles of the *j*-th component, which reacted in the *i*-th reaction (N_{ij} – negative value) and which are the products of the *i*-th reaction (N_{ij} – positive value).

Kinetic equations, which determine the rates of heterogeneous and homogeneous reactions are the basis for mathematical models. To ensure uniformity, in this study the rate of heterogeneous reaction has the same dimension as the rate of homogeneous chemical reactions: kmol/m³s.

For heterogeneous reactions we can write down:

$$W_i = \frac{k_i \mu_i f \mu_0}{M_j} I_i \qquad \dots (1)$$

where W_i - rate of the *i*-th chemical reaction, kmol/m³s; k_i - constant of the chemical reaction rate, m/s; μ_j - concentration of the *j*-th component, kg/m³; *f*-specific contact area of coke particles with gases, m²/kg; μ_0 - carbon concentration (*j*=0, Table 1), kg/m³; M_j-molar mass of the *j*-th component, kg/kmol; I_i - indicator of the *i*-th reaction, if $I_i = 0$, the reaction is excluded from this process, $I_i=1$ - reaction is present.

The I indicator, which is introduced for research purposes, allows analysing the contribution of any reaction to the results of the solid fuels gasification processes.

Connection between the *i* reaction and the j component depending on (1) is presented in Table 2.

For homogeneous reaction (i=6...9) we wrote down the dependences, similar to the formula (1).

Using the above parameters N_{ii} and W_i, we can write:

$$\left(M_{\mathcal{V}}^{km}\right)_{jj} = N_{jj} \cdot W_{i}, i=0...i_{max}, j=0...j_{max}, \dots (2)$$

where $\left(M_{V}^{km}\right)_{i}$ – power of mole source, kmol/m³s, i_{max} – maximal number of a chemical reaction (in this model i_{max} =9); j_{max} – maximal number

of the component (in this model j_{max} =8).

The $(M_{r}^{s})_{r}$ power of mole source shows how many moles of the *j*-th component is used $((M_{r}^{lm}))_{r}$ – negative value) or formed $((M_{r}^{lm}))_{r}$ – positive) in the *i*-th reaction.

Entry in the right part of the dependence (2) means multiplication element wise, i.å. the *i*, *j*-th element of the matrix (M =), is obtained by multiplying the i, j -th element of the N_{ii} matrix by the i-th element of the W_i vector.

Then, using the same multiplication element by element, we pass from the amount of substance in moles (2) to its mass in kilograms:

$$\left(M_{\nu} \right)_{\mu} = \left(M_{\nu}^{\text{loc}} \right)_{\mu} \cdot M_{\nu}, i=0...i_{max}, j=0...j_{max}, \dots (3)$$

where $(M_{\nu})_{\mu}$ – power of a component mass source, kg/m³s.

For the material balance it is necessary to know the mass of each component, which is formed or used in all chemical reactions:

$$(M_{\nu}^{\Sigma})_{j} = \sum_{i=0}^{i_{max}} (M_{\nu})_{ij}, j=0...j_{max},$$
 ...(4)

where $\left(M_{*}^{\mathtt{L}}\right)_{j}$ – total power of the mass source of the *j*-th component, kg/m^3s .

For the energy balance it is necessary to know heat radiation in a volume unit:

$$Q_i^v = -\left(M_v^{km}\right)_{ij} \cdot Q_i, \qquad \dots (5)$$

where Q_{i}^{v} – amount of heat, which is

generated in a volume unit per unit of time as a result of the *i*-th chemical reaction, kJ/m³s,Q_i-heat effect of the *i*-th reaction, kJ/kmol; for the reactions i=0...5 – kmol of carbon; for the reactions i=6...7 – kmol of *CO*; for $i=8 - \text{kmol of } \hat{I}_2$; for i=9 - kmol of CO_{4} .

The connection between the i and jindices for $(M_{r}^{*})_{l}$ in the (6) formula is shown in Table 3.

The main ratios in the developed mathematical model are regular differential equations that reflect the energy conservation law for one-dimensional stationary flow in an annular channel of the gasifier and the mass conservation law for the components, participating in chemical reactions (Table 1).

In a vertical one-dimensional flow, an infinitely small element with the length of dz is distinguished (Fig. 1).

The notation on Fig. 1 is as follows:

 d_{o} , d_{i} – outer and inner diameter of the annular channel, m;

 q_{i} , q_{i} – density of the heat flow on the outer and inner cylindrical surface of the annular channel, $kJ/(m^2 \cdot s);$

 q_r – density of the resulting radiant heat flow on the cross-section of the annular channel (directed along the z axis), $kJ/(m^2 \cdot s)$;

 h_{mix} - specific enthalpy of the multicomponent, flow kJ/kg;

 G_i – mass flow rate of the *j*-th component, kg/s;

 Q_{i}^{V} – volumetric heat generation as a result of the *i*-th chemical reaction (5), $kJ/(m^3s)$.

The energy balance for the one-dimensional stationary flow between the z and z + dz sections (Fig. 1) can be written as:

$$dQ_{\Sigma} = G_{\min} dh_{\min} dQ_{\Sigma} = G_{\min} dh_{\min}$$
 ...(6)

where dQ_{s} - the total amount of heat, put into the multicomponent flow in a unit of time, kJ/ s; G_{mix} – mass flow rate of the mixture, kg/s.

Note that the (6) dependence is written down without taking into account the change in kinetic and potential energy of the flow that was specified in the assumptions [12].

$$dQ_{\Sigma} = \left(F\sum_{i=0}^{i_{\max}} Q_i^{v} - q_o \Pi_o - q_i \Pi_i\right) dz - Fq_{r}, \quad \dots (7)$$

$$G_{\min} = \sum_{j=0}^{j=j_{\max}} G_j = (\rho w)_{\min} \cdot F$$
, ...(8)

$$dh_{\rm mix} = c_{\rm mix} dT, \qquad \dots (9)$$

where F- cross-section of the annular channel, m ²;

 Π_o , Π_i , – outer and inner perimeters of the channel respectively, m;

 $(\rho w)_{mix}$ - mass rate of the mixture, kg/(m²·s);

 c_{mix} – specific isobaric heat capacity of the mixture of gaseous and solid components, kJ/kgK;

 \dot{O} – absolute temperature, K.

By inserting the (7) - (9) dependence in the (6) formula, we obtain the following energy equation for the one-dimensional stationary flow of a multicomponent mixture:

$$\left(\rho_{W}\right)_{mix}c_{mix}\frac{dT}{dz} = \sum_{s=0}^{t_{mix}} \mathcal{Q}_{s}^{r} - q_{s}\frac{\Pi_{s}}{F} - q_{s}\frac{\Pi_{s}}{F} - \frac{dq_{r}}{dz} \dots (10)$$

The mass rate of the mixture in the (10)

i				Compor	ent and it	s number <i>j</i>			
	C 0	$\begin{array}{c} \mathbf{O}_2 \\ 1 \end{array}$	H ₂ O 2	CO ₂ 3	$\begin{array}{c} \mathrm{H_2} \\ \mathrm{4} \end{array}$	CO 5	CH_4 6	N ₂ 7	Ash 8
0	-1	-1	0	1	0	0	0	0	0
1	-2	-1	0	0	0	2	0	0	0
2	-1	0	-1	0	1	1	0	0	0
3	-0.5	0	-1	0.5	1	0	0	0	0
4	-1	0	0	-1	0	2	0	0	0
5	-0.5	0	0	0	-1	0	0.5	0	0
6	0	0	-1	1	1	- 1	0	0	0
7	0	-0.5	0	1	0	- 1	0	0	0
8	0	-0.5	1	0	-1	0	0	0	0
9	0	-2	2	1	0	0	-1	0	0

Table 1. Matrix of moles N_{ii}

Table 2. Connection	between <i>i</i> and	<i>i</i> in formula 1
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Table 3. The connection between the *i* and *j* indices for $(M_v^{km})_{ii}$ in the (6) formula.

											· v	′1J	(<i>'</i>			
i	0	1	2	3	4	5	i	0	1	2	3	4	5	6	7	8	9
					3												

Table 4. Connection between air excess and relative consumption of steam

a	0.25	0.2	0.3	0.35	0.4
d _n	0.02265	0.01812	0.02718	0.03171	0.03624

Table 5. Volume fractions of generator gas components, % (with the excess air coefficient α =0.2).

O ₂ H ₂ O
40 43.52
56 32.92
5920.571879.83
)

794

energy equation for the studies stationary flow does not depend on the z coordinate: $(\rho_W)_{mix} = G_{mix}/F$.

The mass balance of the *j*-th component for the one-dimensional stationary flow between the *z* and z + dz cross sections (Fig. 1) can be written as:

$$dG_{j} = \left(M_{v}^{\Sigma}\right)_{j} F dz \text{ or } \frac{dG_{i}}{dz} = \left(M_{v}^{\Sigma}\right)_{j} F, \qquad \dots (11)$$

where $(M_*^{\Sigma})_j$ – formation rate (plus) and disappearance rate (minus) of the *j*-th component in a volume unit, is determined by the (4) dependence.

$$G_i = \mu_j^p wF \qquad \dots (12)$$

where μ_j^p – expendable concentration of the *j*-th component, kg/m³; w – rate of the flow (gas) in the direction of the z coordinate, m/s.

$$\mu_j^p = \mu_j, \ j \in \{1...,7\} \qquad \dots (13)$$

The equation (13) means that for all the components, except for carbon and ash, the expendable and true concentrations are equal. For carbon and ash it was established that

$$\mu_{j}^{*} = \frac{\rho_{j}\mu_{j}v_{j}}{\rho_{j} + \mu_{j}(v_{j} - 1)} \text{ with } j \in \{0, 8\} \text{ (Table 1)},$$

where ρ_i – density of the coke particle or ash, kg/

$$m^3$$
; V_i – sliding coefficient for solid particles:

$$\nu_j = \frac{w_j}{w},$$

where w_j – rate of solid particles in the direction of the z coordinate, m/s.

The sliding coefficient v_j is connected

with the hovering rate in the following way:

$$v_j = 1 - \frac{w_j^{\text{hov}}}{w}$$
.

The hovering rate $w_j^{hov} = w - w_j$ is calculated for average-sized solid particles.

By inserting the (12) consumption into the (11) material balance equations, we get that

$$\frac{d\left(w\,\mu_{j}^{P}\right)}{dz} = \left(M_{v}^{\Sigma}\right)_{j}, \qquad j=0\dots j_{max}. \dots (14)$$

The system of differential equation (10) and (14) is the basis for the mathematical model of coal gasification in the upward annular flow.

 W_{j}^{hov} Computer programme and computational experiment.

To solve this system, we developed a computer programme in the \tilde{N} # language with 11500 lines. Two characteristic tabs of this programme are shown on Fig. 2 and Fig. 3.

Table 6. Volume fractions of generator gas components,% (with the excess air coefficient α =0.3)

t, °C	Т, К	СО	H_2	CH_4	CO ₂	H ₂ O
700	973	19.47	1.50	0.0252	39.14	39.86
800	1073	38.53	3.23	0.0892	24.94	33.16
900	1173	56.11	6.52	0.3560	12.48	24.57
1000	1273	66.95	10.11	1.0100	5.65	16.26

Table 7. Volume fractions of generator gas components, % (with the excess air coefficient α =0.4)

t, ⁰C	Т, К	СО	H_2	CH_4	CO ₂	H_2O
700	973	8.76	0.724	0.00866	53.97	36.55
800	1073	23.89	1.63	0.02400	41.96	32.45
900	1173	43.14	3.64	0.10300	26.98	26.14
1000	1273	57.59	6.30	0.31800	16.12	19.66

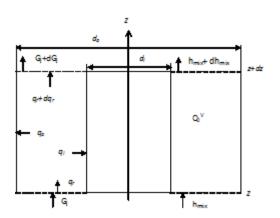


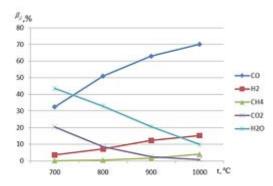
Fig. 1. Computational pattern for making up the energy and material balance

1720		Троверка Перенотры	30001 0	ner qu	a l			
0	45.2	1	00	-		12	0.068	
		-		2250	nr/in/3			
0	-0	1	pet	1115	KT/H/3	de	0.058	
tt:	1.2	1.2	Ožena.	0,21	H'3H'3	L	1,5	м
w	6.8	5	dt	0,01812	sr.kr	ħ	0.0001	
hr.	Z3,5 ;	5	1	1700	w'297			
vo	6.04	n'lir	ve	1				
0	0.2		val	1				
Gyr	0.00027	7 10/10						
TQ.	972	×						

Fig. 2. Data-entry window for entering the initial programme data for gasification in the flow

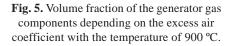
	1040	(Deserve	ichi Tannoe	eacts K										
18	-	T.	W.	ic. RM3	у02. нг/м"Э	µ+00. Kr.M-3	uC02 47.M ² 3	14C	1000 107.0413	4044. 47.5473	µ42, #2,6(3)	anonal ar Ar 'S	unit. Referits	VERONA, Kr.M.'3
	0	973	1,23115653	0.14056411	0.08959587	0.02419668	0	0.00279615	10	0	0.27799604	0.05358292	0.14966411	0.05356292
750	0.075	373	1.44376819	0.11252073	0.0238012	0.03933812	0.03731011	0.00025213	0.00940967	1.1176-05	0.23194146	0.04565221	0.11252073	0.04563221
1500	0.15	573	1.44276522	0.1071652	0.00908544	0.04010995	0.05617437	0.00016853	8.01018172	13725-05	0.23210206	0.04572385	0.1071652	0.04572385
2250	0.225	973	1.44161913	0.10496172	0.00266328	0.04023132	0.0652514	0.00015853	0.00977875	1.617E-05	0.23228722	0.04576000	0.10496172	0.04576033
3000	0.3	970	1.44230342	0.10389326	0.00014685	0.64013311	0.06060306	0.00016656	0.00993557	1,8926-05	0.23217701	0.04573062	0.10389326	0.04573862
3750	0.375	973	1,44008581	0.10281883	0	0.03905007	0.06662076	0.00017874	0.01257448	2.1896-05	0.2312499	0.04555598	0.10281883	0.04555598
4500	0.45	373	1.45410517	0.10176605	0	0.02956511	0.06434843	0.00019054	0.01525081	2.56-05	0.23029247	0.04536737	0.10176605	0.04536737
5250	0.525	373	1.45566139	0.10076386	0	0.03829004	0.06213236	0.00025205	0.01779345	2.8268.05	0.22930144	0.04518789	0.10076306	0.04518789
6000	0.6	973	1.46542706	0.0998085	0	0.03902677	0.06214389	0.00021323	0.0202132	3.165E-05	0.22951339	0.04501689	0.0998085	0.04501689
6750	0.675	975	1.47075738	0.0502966	0	0.03877219	0.05819518	0.00022412	0.02251869	3.518E-05	0.22768521	0.04485374	0.0908966	0.04485374
2500	0.75	973	1.47588533	0.09802511	0	0.03852646	0.09633922	0.00023473	0.02471793	3.8836-05	0.22689412	0.04469789	0.09802511	2,04469729
8250	0.825	973	1.48082281	0.09719129	0	0.038289	0.0545696	0.00024509	0.02681823	4,25E-05	0.22613759	0.04454886	0.09719129	0.04454896
9000	0.9	\$73	1,40558073	0.09639262	0	0.03009828	0.05288056	0.0002582	0.52862617	4.6496-05	0.22541303	0.04440518	0.09639262	0.04443618
\$750	0.975	\$73	1,49010357	0.09562683	0	0,03783682	0.05126662	0.00024567	0.00074778	5.043E-05	0.22471925	0.04426545	0.09962683	0.04425945
10500	1.05	975	1,45455735	0.05485185	0	0.03762118	0.04972359	0.00027473	0.03250853	5,4576.05	0.22405345	0.04413825	0.05429185	0.04413825
11250	1.125	\$72	1.49087397	0.09418576	0	0.03741196	6.04824647	0.00025418	0.03435344	5.8766.05	0.22341418	0.04401235	0.05413576	0.04401225
12000	1.2	\$73	1.50300685	0.01050683	0	0.03720878	0.04683143	0.00029043	1.03604712	6.304E-05	0.22279085	0.04389133	0.00050683	0.04089103
12750	1,275	\$73	1.5070034	0.05295346	¢.	0.03701131	0.04547479	0.0003025	0.00767377	6.742E-05	0.22220899	0.04377493	0.05295346	0.04377483
13500	1.35	\$73	1.51087047	0.09222417	0	0.03681922	0.04417314	0.00031138	0.01923729	7.1886-05	0.22164025	0.04366289	8.09222417	0.04366289
14250	1.425	373	1.51461442	0.09161761	8	0.03663224	8.04292338	E-00032009	8,04074125	7.6436-05	0.22109258	0.04355496	2.09161761	0.04355496
15000	1.5	973	1.5182412	0.09103252	0	0.0364501	0.04172251	0.00032964	0.04218899	8.1068-05	0.22056423	0.04345091	0.09103252	0.04345091

Fig. 3. The results window of the programme for gasification in the flow



P1,% 70 60 50 -00 40 -H2 30 -CH4 -02 20 -H2O 10 0 0,2 0,3 0,4 α

Fig. 4. Volume fractions of the generator gas components depending on the temperature with the excess air coefficient α =0.2



The computational experiment with the mathematical modelling of gasification was carried out with the following initial data.

Fuel: anthracite culm of the Donetsk basin.

Content of the fuel as received (as-received basis ARB) [20]:

 $C^{ARB} = 65.2\% - carbon$,

 $O^{ARB} = 1.3\% - oxygen,$

H^{ARB}=1.2% – hydrogen,

 $W^{ARB} = 8.8\% - water (moisture),$

 $C^{ARB} = 23.5\%$ – ash content.

Theoretical amount of dry air, necessary for total

combustion of fuel:
$$V^0 = 6.04 \frac{m^3}{kg}$$

The α excess air coefficient changes from 0.2 to 0.4.

The relative consumption of water steam, which enters the gasification chamber with air, is determined by the formula:

$$d_{ii} = \frac{G_{ii}}{G_{f}} = \mu_{H2O}^{air} \cdot V^0 \cdot \alpha,$$

where G_{st} , G_{fi}^{-} mass consumption of steam and fuel respectively, kg/s; $\mu_{H20}^{str} = 0.015 \frac{kg}{m^3}$ – absolute air humidity.

The connection between the α air excess and the relative consumption of steam, which enters with this air from the atmospheric d_n , is shown in Table 4.

 $G_{f} = 1 \frac{kg}{hour} = 0.0002778 \frac{kg}{s}$ - consumption of solid fuel;

$$\rho_{e} = 2250 \frac{kg}{m^{3}}$$
 – density of carbon (coke residue);

$$\rho_{axk} = 1115 \frac{kg}{m^3}$$
 – density of ash;

 $O_{2atr} = 0.21 - \text{volume fraction of oxygen in the air;}$

 $f = 1700 \frac{m^2}{kg}$ – specific surface of pulverized coal;

 $d_{o} = 0.068 m$ – outer diameter of the annular channel of the gasification chamber;

 $d_i = 0.058 m$ – inner diameter of the annular

channel of the gasification chamber;

L = 1.5 m – length (height) of the gasification chamber.

The results of the computational experiment are presented in Tables 5-7 and on Fig. 4-10. Presented volume fractions are taken with respect to the volume of the generator gas without nitrogen.

During the analysis of the mathematical modelling results (Tables 5-7, Fig. 4) it was established that the amount of useful components of the generator gas (CO, H₂, CH₄) increases at higher temperatures: volume fractions of CO with 32.4 % at 700 °C to 70.2 % at 1000 °C; fraction of H₂ respectively from 3.5 % to 15.2 %; fraction of CH₄ increased from 0.1 % to 4.0 % (the excess air coefficient α =0.2), which is due an increase in the constants of the chemical reactions rate. Such constants also increase in the combustion (oxidation) reaction of CO, H₂ and CH₄, and , but the rates of these reactions are limited by small oxygen concentration due to small amount of air.

The obtained dependence between the CO, H_2 and CH_4 volume fractions and the excess ar coefficient shows that with the constancy of temperatures the volume fractions of CO, H_2 and CH_4 decrease (Tables 5-7, Fig. 5). It is due to the increasing oxygen concentration and a consequent increasing rate of chemical combustion reaction of these components.

CONCLUSION

We presented a mathematical model of low-reactive coal gasification in the upward annular channel, based on differential equations of the energy and mass conservation for a multicomponent stationary flow. Gasification occurs in an air flow, it is possible to add water steam. The model uses matrixes and vectors to display main characteristic of gasification, which allows modifying it easily by adding new chemical reactions without changing main dependences of the model.

Based on the mathematical model, we developed a C# computer software with the volume of 11500 lines.

A computational experiment aimed at studying the effect of the generator gas in relation to the temperature in the gasifier and the excess air coefficient at the inlet.

The work was financially supported by the Ministry of Education and Science of the Russian Federation within the framework of the Federal Target Program "Research and development in priority directions of the scientifictechnological complex of Russia for 2014-2020" (No. 14.574.21.0018 agreement on "Development of a method of intensifying the gasification process of low-reactive coal in an upward jet-vortex flow of an oxidant", a unique identifier PNI (of the project) RFMEFI57414X0018)

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