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ORIGINAL RESEARCH ARTICLE

Utilization of converter gases through energy chemical accumulation

V.S Korolev, M.Y Shevyakov, S.N Petin, A.V Burmakina, I.I Feoktistov

Department of Innovative Tecnologies for High-Tech Industries, National Reserch University "Moscow Power Engineering Institute", Moscow, 111250, Russia

***Corresponding author:** Feoktistov Ilya Igorevich, FeoktistovII@mpei.ru

ABSTRACT

This study presents an exergy analysis of options for efficient converter gases in steel production. The analysis concluded that the most preferable option involves regenerative fuel utilization of converter gas through an energy chemical accumulation process. A geometric model of the energy chemical accumulation reactor was developed and investigated using ANSYS Fluent. The study determined reactor dimensions that ensure an equilibrium syngas composition. Furthermore, it established the correspondence between the energy chemical accumulation reactor's geometric parameters and the dimensions of the inclined gas duct in the converter gas cooling boiler.

Keywords: converter gas; natural gas; metallurgical industry; exergy analysis; carbon dioxide conversion; energy chemical accumulation; reactor; metallic dust carryover; numerical simulation

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1. Introduction

The use of secondary energy resources (SER) is a significant source of fuel savings in industry. One such resource in the ferrous metallurgy industry is gases from steelmaking converters, which are currently used inefficiently due to the following reasons: 1) the variability of the yield and composition of converter gases; 2) the high temperature and dustiness of converter exhaust gases; 3) the cost of purchased energy resources, particularly natural gas, is lower than the cost of converter gas disposal.

Existing domestic schemes for the utilization of converter gases for the production of electricity (based on converter gas cooler steam - CGCS) face problems with unstable and low steam pressure (2.2-2.7 MPa instead of 4.0 MPa) [1], which causes a decrease in the efficiency of electricity production.

A promising approach to converter gas utilization is the use of thermochemical recovery (TCR) [2], where converter gas energy is used for natural gas conversion processes, thereby increasing the enthalpy of natural gas for electrical energy production. Replacing natural gas with syngas saves 18-22% of fossil fuel while maintaining the same electricity output, allowing the company to meet its own needs and generate additional revenue from the sale of surplus energy.

A special case of the TCR process is energy-chemical accumulation (ECA). The term "energy-chemical accumulation" was introduced and used in a number of studies conducted at the Department of High-Temperature Energy Technology at the National Research University "MPEI" under the supervision of Professor A.D. Klyuchnikov. Since the 1980s, numerous works have been written on this topic, most of which are covered in [3]. The ECA process is carried out by directly feeding natural gas into the converter gas stream.

In [4] three main areas of use of ECA products of converter gases are identified:

- use as a secondary fuel [5-7, 8] for generating electricity and steam, heating metal for rolling, etc.;
- reduction processes in a blast furnace [3], reduction of iron ore pellets in a shaft reactor [9];
- hydrogen production [10-12].

The papers [13, 14] focus on the application of ECA in direct reduction iron smelting. The study [15] compares the reducing and fuel properties of natural gas processing products used in reducing iron smelting with carbon and coal. In addition, the authors of the present study developed and investigated (both theoretically and experimentally) the ECA process for producing high-temperature combustion products of natural gas. Furthermore, there are promising methods for using converter gases for the production of synthetic liquid fuels, which are described in the following sources [16, 17]. The above-mentioned sources emphasize the significant potential inherent in the ECA process; however, its practical feasibility becomes apparent only when compared with the common methods of utilizing converter gases.

The paper presents a comparative analysis of the following converter gas utilization options: 1) cooling of converter gas in a converter gas generator with combustion on a candle (a method in use in the Russian Federation) [1]; 2) cooling of converter gas in a converter gas generator with compression and collection in a gas holder [18]; 3) cooling and afterburning of converter gas in a waste heat boiler (maximum production of superheated steam) [18]; 4) regenerative fuel utilization of converter gas based on energy-chemical accumulation (ECA) - a process of physicochemical interaction of high-temperature waste gases with natural gas with the aim of converting them into a fuel gas for a wide range of applications, with heat consumption of the process due to the heat of the waste gases.

If the effectiveness of the proposed converter gas utilization method based on ECA is proven, the primary research object will be the ECA reactor. The problem is that, to date, there are no design recommendations for this reactor that would fully account for the aforementioned characteristics of converter gas.

The papers [10, 19] present schematic solutions for the production of energy resources based on the ECA of converter gas from steelmaking. The papers [20, 21] consider numerical models of the ECA process without taking into account the presence of carryover—fine particles—in the converter gas.

In this paper, a model of an ECA reactor is proposed that takes this presence into account. There are software packages that are potentially suitable for modeling conversion processes, in particular processes with the presence of solid particles in the gas. Some of them allow for studies using LSTM models and transformers for accurate forecasting of time series data. For example, work [22], which discusses the use of LSTM for forecasting the concentrations of pollutants, including gases, taking into account seasonal and short-term changes. This study proposes using the ANSYS software package Fluent, since the use of this package resulted in high convergence compared to other calculation programs under the same boundary conditions for ECA reactor prototypes without taking into account solid particles in the gas [20, 21].

2. Methodology

2.1. Analysis of converter gas utilization efficiency

an exergy analysis is proposed. Exergy analysis of thermal systems is a type of energy analysis that allows for calculating the efficiency of the solution under consideration.

Exergy, like energy, is a thermodynamic potential. However, energy is associated with a fundamental property of matter, while exergy characterizes the maximum useful work a system can perform when it reaches equilibrium with its environment. The environment is defined as a system whose parameters are constant and independent of the system under consideration.

Energy analysis, based on the first law of thermodynamics, considers only changes in the total energy of a system. Exergy analysis, based on the second law of thermodynamics (the increase in entropy in irreversible processes), considers the loss of useful work associated with the irreversibility of processes.

The first widely known works on the implementation of exergy analysis were carried out by various authors, including J. Shargut and Z. Ranta, whose works and methods are mentioned in the source [23].

These methods were used and developed by V.M. Brodyansky [24, 25]. This method was successfully used in various works, in particular, in the analysis of the thermodynamic efficiency of using expander-generator units [26].

The following initial data are used for the calculation of converter gas [27]: CO_2 = 23.52%; CO = 57.35%; H_2 = 0.29%; O_2 = 4.22%; N_2 = 14.62%;

- heat of converter gas combustion: 7280.42 kJ/m^3;

- characteristics of natural gas composition – CH_4 = 100%.

The calculation of exergy efficiency is carried out using the formula:

$$\eta_e=\frac{\sum E_{out}}{\sum E_{in}}=\frac{E_{out}^{water}+E_{out}^{sg}}{E_{in}^{water}+E_{in}^{cg}+E_e+E_{in}^{ng}+E_{comp}}, \tag{1}$$

where $\sum E_{\mathrm{in}}$ and $\sum E_{\mathrm{out}}$ are the resulting exergy flow at the input and output of the plant, respectively, in MW; E_{in}^{water} and E_{out}^{water} — exergy water flows at the inlet and outlet of the waste heat boiler, E_{in}^{cg} — exergy flow of converter gases at the input, E_{in}^{ng} — exergy flow of natural gas at the inlet, E_{out}^{sg} — exergy flow of syngas at the outlet of the waste heat boiler, these flows can be found using formula (2); E_e — the exergy flow of electrical energy for which expression (3) is valid; E_{comp} — exergy during gas compression.

$$E_{flow}=G_{flow}\cdot[(h_{flow}-h_0)-T_0\cdot(s_{flow}-s_0)], \tag{2}$$

where G_{flow} is the volumetric flow rate of the fuel, kg/s; h_{flow} is the enthalpy of the flow at given parameters, kJ/kg; s_{flow} is the entropy of the flow at given parameters, kJ/(kg·K); h_0 is the enthalpy of the flow at ambient parameters, kJ/kg; s_0 is the entropy of the flow at ambient parameters, kJ/(kg·K); T_0 is the ambient temperature, K.

$$E_e=N_e, \tag{3}$$

where N_e is the amount of electricity for the studied period of time, kJ/h or MW.

2.2. Development of design features of ECA reactor

This paper proposes an ECA reactor design similar to a gravity-driven pneumatic classifier for bulk materials. Among several pneumatic classifier options, the multi-row design is the most suitable, as it is compact, its design allows for high flow turbulence, and achieves a high degree of particle separation. This is due to the presence of transfer shelves. Centrifugal vortices are formed above and below these shelves, promoting stratification and dispersion of the material and increasing the residence time of the particles in the apparatus [28].

The next step is to construct a 3D model of the reactor. This requires determining the required reactor dimensions. Table 1 summarizes the data for calculating the ECA reactor dimensions.

Table 1. Initial data for calculating the overall characteristics of the ECA reactor

Parameter	Numerical meaning
Volumetric flow rate of converter gas, m^3/s	190
Reaction time to equilibrium composition, s	0.5
Average diameter of fly ash, m	0.0015
Density of fly ash, kg/m^3	5200
Gas density inside the reactor, kg/m^3	0.2

When compiling the initial data, the following boundary conditions were adopted: based on numerical calculations using the method [28], a slight change in the density of the gas mixture was detected during the reaction; therefore, the gas density inside the reactor was assumed to be constant. The reaction time to the equilibrium composition was obtained using the same method, and the average diameter of the entrained particles was adopted based on [7, 29].

The speed inside the reactor is calculated using the formula for pneumatic classifiers with transfer elements [30]:

$$w=\sqrt{\frac{g\cdot\left(\rho_p-\rho_g\right)\cdot x_{50}}{2.175\cdot e^{-0.164\cdot\mu}}}, \tag{4}$$

where g is the acceleration due to gravity, m/s^2; ρ_p is the particle density, kg/m^3; ρ_g is the gas density, kg/m^3; x_{50} is the fraction size that corresponds to the equal distribution of the material into large and small products, µm; μ is the flow concentration of the material at the top of the reactor, kg/m^3.

The velocity was calculated for x_{50}=1.5 mm, which corresponds to the average diameter of the entrained particles. As the fraction size decreases, the gas velocity decreases, so for better separation of large entrained particles, it is more advantageous to reduce the velocity. For this reason, and to reduce the reactor's dimensions, a gas velocity of 8 m/s was adopted.

The cross-sectional area of the flow inside the reactor is calculated using the formula:

$$S=\frac{Q_g}{w}, \tag{5}$$

where Q_g is the volumetric gas flow rate, equal to the converter gas flow rate.

The cross-sectional area was 24 m^2. It can be conveniently divided into four sections with dimensions: width – 3 m, length – 2 m. The reactor height is calculated using the formula:

$$h=w\cdot\tau\cdot 1.3, \tag{6}$$

where τ is the reaction time to equilibrium composition; 1.3 is a 30% margin to account for mixing of the reactants inside the ECA reactor. The resulting height was 5.2 m.

The reaction time $\tau$to the equilibrium composition in seconds is determined from the formula:

$$\frac{1}{C_{CH_4}}=k\tau+\frac{1}{C_{0\ CH_4}}, \tag{7}$$

The next step is modeling the ECA reactor. This is a multi-step process and includes the following steps:

1) development of a three-dimensional model of the reactor;
2) modeling the dynamics of entrained particles in an ECA reactor without taking into account chemical reactions;

3) calculation of the completeness of the chemical reaction in a simplified formulation without taking into account metal carryover;

4) Combined modeling of an ECA reactor taking into account the dynamics of fly ash and chemical reactions.

The first step can be implemented in various third-party CAD programs. Steps 2-4 are performed in the ANSYS software package Fluent.

3. Results and Discussion

3.1. Results of the analysis of the efficiency of converter gases use

Table 2 presents the data reduced to 1 ton of converter steel for conducting an exergy analysis of the input and output exergy flows of various options.

The parameters of the steam output streams in options 1 and 3 are: steam pressure 4 MPa, saturated steam temperature 249 °C (option 1), superheated steam - 450 °C (option 3).

The volumetric composition of the syngas obtained in option 4: CO_2 = 6.89%, H_2O = 2.73%, CH_4 = 0.038%, CO = 59.33%, H_2 = 21.19%, N_2 = 9.82% [31].

Table 3 presents the results of the exergy analysis. Figure 1 clearly shows the resulting exergy flows [32].

Table 2. Initial data for exergy analysis

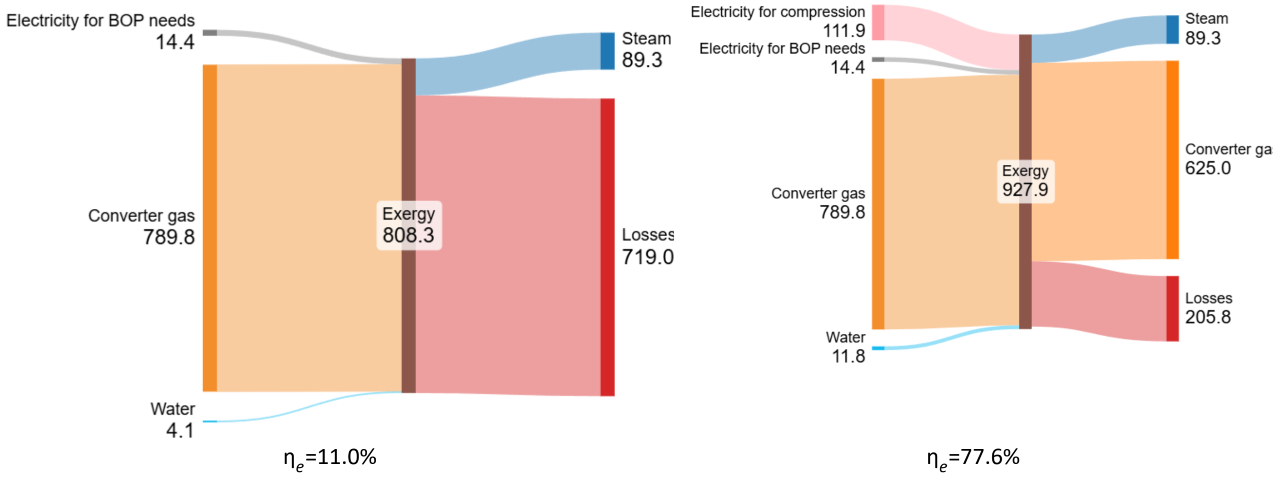
Parameter	**Way disposal converter gas**			
	1	**2**	**3**	**4**
Input streams				
Specific volume of converter gas, m^3/t of steel	87			
Electricity consumption for own needs kW·h/t of steel	4	4	10	6
Electricity consumption for additional compression kW·h/t of steel	-	31	-	46
Specific volume of water, t/t of steel	87.1	87.1	254 .4	20.7
Specific volume of natural gas, m^3/t of steel	-	-	-	15.41
Output streams				
Steam consumption, tons/ton of steel	78.4	78.4	229	18.6
Output of cooled gas/combustible gas, m^3/t of steel	–	87	–	129.5

Table 3. Exergy analysis for various converter gas utilization schemes

Name flow	**The considered variant of the method for utilization of converter gases**			
	1	**2**	**3**	**4**
	Exergy streams on input:			
Exergy of the boiler at the inlet, MJ/t of steel	789.8	789.8	789.8	789.8
Exergy of electrical energy for own needs, MJ/t of steel	14.4	14.4	35.5	19.7
Exergy of electrical energy for compression, MJ/t of steel	-	111.9	-	166.4
Exergy of water at the boiler inlet, MJ/t of steel	4.1	4.1	11.8	1.0
Exergy of natural gas at the boiler inlet, MJ/t of steel	-	-	-	610.2

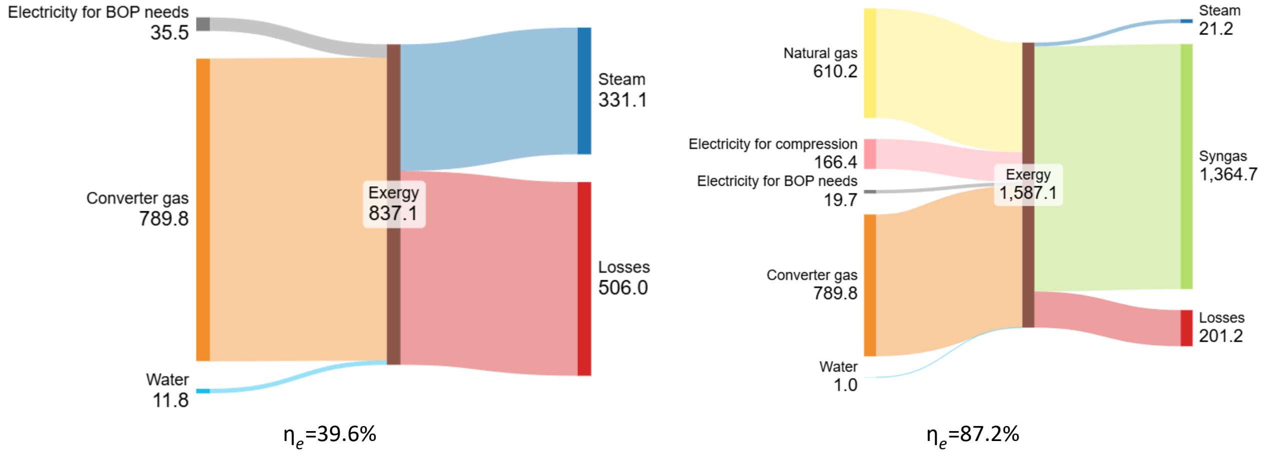
Name flow	The considered variant of the method for utilization of converter gases			
	1	2	3	4
TOTAL on input:	808.3	920.1	837.1	1587.1
	Exergy streams on output:			
Exergy of steam at the boiler outlet, MJ/t of steel	89.3	89.3	331.1	21.2
Exergy (kg/sg) at the boiler outlet, MJ/t of steel	0	625.0	0	1364.7
TOTAL on output:	89.3	714.3	331.1	1385.9
Exergy losses:				
kJ/t steel	719	205.8	506.0	201.2
%	89	22.4	60.4	12 8
Exergy efficiency, %	11.0	77.6	39.6	87.2

Table 3. (*Continued*)



1) Cooling in CGC with flaring

2) Cooling in CGC with compression and storage in a gas holder



3) Cooling and complete post-combustion in CGC

4) Regenerative fuel utilization

Figure 1. Results of exergy analysis (MJ/ton steel)

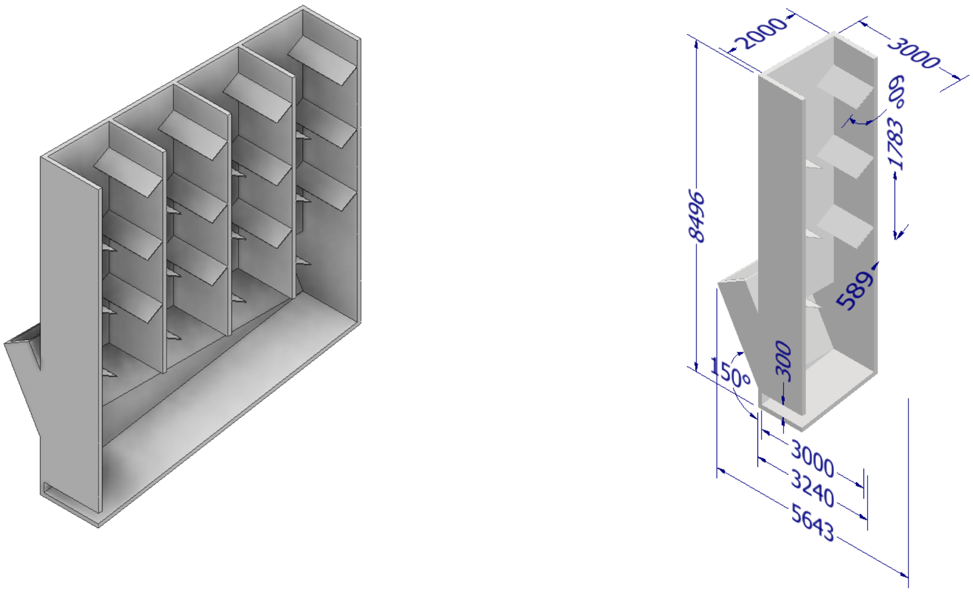
Using exergy analysis, it was found that the most efficient converter gas utilization scheme is one with regenerative fuel use of converter gas based on energy-chemical accumulation (ECA), which has an exergy efficiency of 87.2%. The current Russian scheme, which cools converter gas in a converter gas generator with combustion on a candle, has an exergy efficiency of 11%.

3.2. Results of ECA reactor modeling in ANSYS Fluent

3.2.1. Development of a three-dimensional model of the reactor

Figure 2(a) shows a cross-section of the ECA reactor model. Converter gas is supplied from both sides at an angle of 60° to the horizon, as this will create the initial separation of large entrained particles, and gas supply from both sides improves mass transfer, as it corresponds to the heat engineering principle of "counter-flows" proposed in the theory of intensive energy conservation [33].

Since the reactor is evenly divided into four sections, it was decided to calculate one section at a time to speed up the calculations (Fig. 2(b)). In this case, the converter gas flow rate must be reduced by a factor of four.



a) Model of a four-section reactor

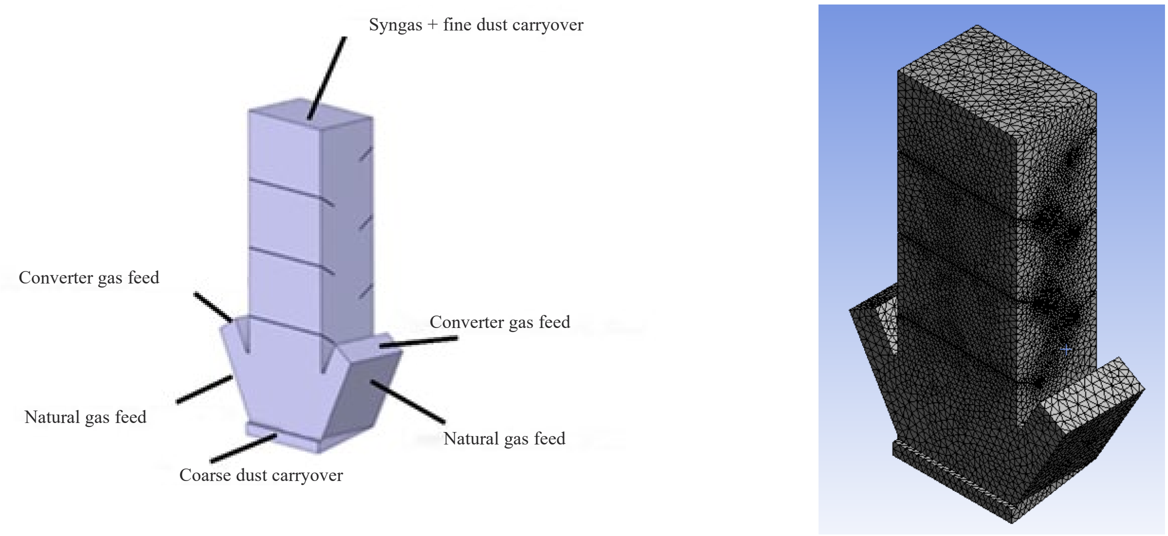
b) One reactor section

Figure 2. Three-dimensional model of the ECA reactor

3.2.2. Modeling the dynamics of entrained particles in an ECA reactor without taking into account chemical reactions

After constructing the 3D model, the reactor's internal volume is created and then the mesh is generated. The ANSYS software package was used to create the internal volume SpaceClaim. Figure 3(a) shows the resulting internal volume of one section of the ECA reactor.

Next, a tetrahedral mesh was constructed to allow for the ECA process simulation. As mentioned earlier, the simulation is divided into several additional steps. The first step is to "purge" the reactor to identify simulation errors and determine whether mesh refinement is necessary. Standard was used for this purpose. The k - ε turbulence model was used, with velocities of 15 m/s at both reactor inlets and pressures of 0 at the lower and upper outlets. Figure 3(b) shows the computational grid for the internal volume of the ECA reactor.



a) Internal volume of one reactor section

b) Calculation grid

Figure 3. Internal volume with a computational grid for one section of the ECA reactor

Figure 4 shows the current lines in the ECA reactor.

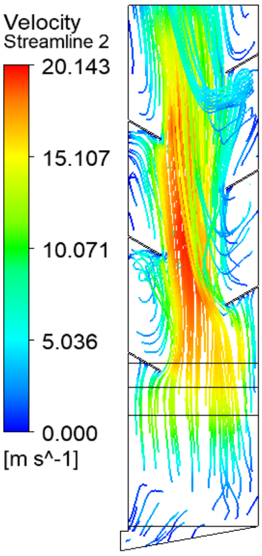


Figure 4. Distribution of current lines in the ECA reactor

Modeling of the entrained particle dynamics is based on the methodology [34, 35]. As a turbulence model, based on [34, 35], k - ε was chosen RNG. This turbulence model was obtained using a static method called renormalization group theory. It is similar in form to the Standard k-ε - turbulence model, but has the following improvements [36]:

- the RNG model contains an additional term in its equation that significantly improves the accuracy for flows with fast stresses;

- the RNG model includes the effect of vortex on turbulence, which improves accuracy for swirling flows;

- the RNG theory provides an analytical formula for turbulent Prandtl numbers, while the Standard k-ε model uses user-specified constant values;

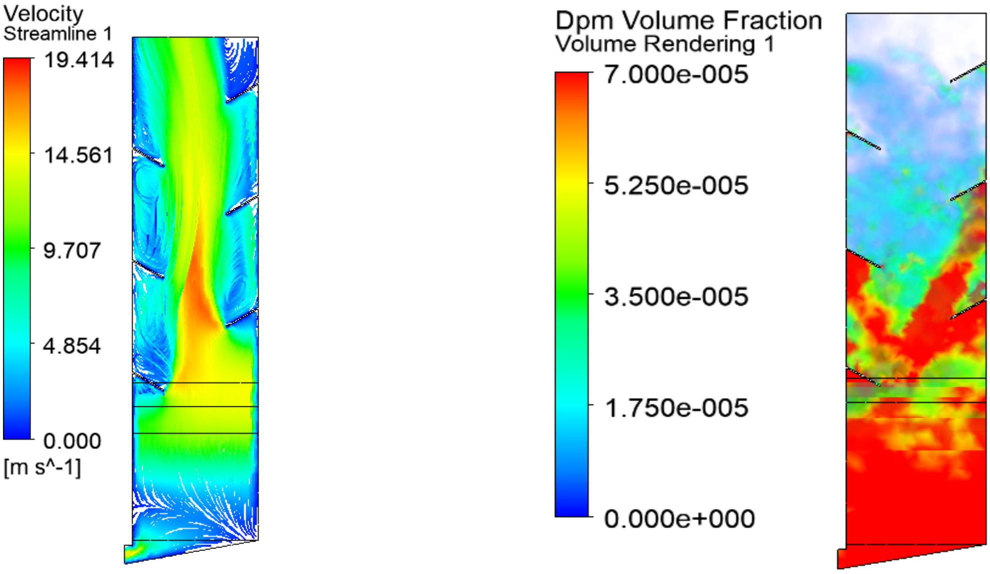
- where as the Standard *k*-ε model is a high-Reynolds-number model, and RNG theory provides an analytically derived differential formula for the effective viscosity that accounts for low-Reynolds-number effects. However, effective use of this function depends on proper treatment of the near-wall region.

Table 4 shows the parameters for modeling the dynamics of entrained particles.

Table 4. Parameters for modeling the dynamics of entrained particles

Parameter	Established meaning
Model turbulence	k-ε RNG Swirl Dominated Flow
Inlet gas velocities, m/s	15
Excessive pressure on exits	0
Behavior particles on exit	Escape
Density gas, kg/m^3	0.2
Minimum/Average/ Maximum particle diameter, m	0.00015/0.0015/0.015
Mass flow rate of particles at two inputs, kg/s	4.76
Density of fly ash, kg/m^3	5200

Figure 5 shows: a – flow lines taking into account metal carryover, b – distribution of the volume fraction of carryover particles in the reactor.



a) Distribution of current lines in the ECA reactor

b) Distribution of volume fraction

Figure 5. Internal volume with a computational grid for one section of the ECA reactor

The obtained modeling results indicate that entrainment accumulates in the internal volume. This problem for this type of pneumatic classifier is discussed in [28]. It can be solved by periodic purging during periods of converter gas inactivity; the purge entrainment can be accumulated until the next remelting cycle. The positive aspect of entrainment accumulation in the lower section should also be noted, as it allows for the creation of a catalytic layer for the reaction, which, with further research, could lead to a reduction in the reactor's dimensions.

3.2.3. Calculation of the completeness of the chemical reaction in a simplified formulation without taking into account metal carryover

To calculate the chemistry in the ECA reactor, its geometry must be modified by adding methane feed tubes. There are five tubes per side of the reactor, with an outlet velocity of 35 m/s. Figure 6 shows a section of the reactor with methane feed tubes.

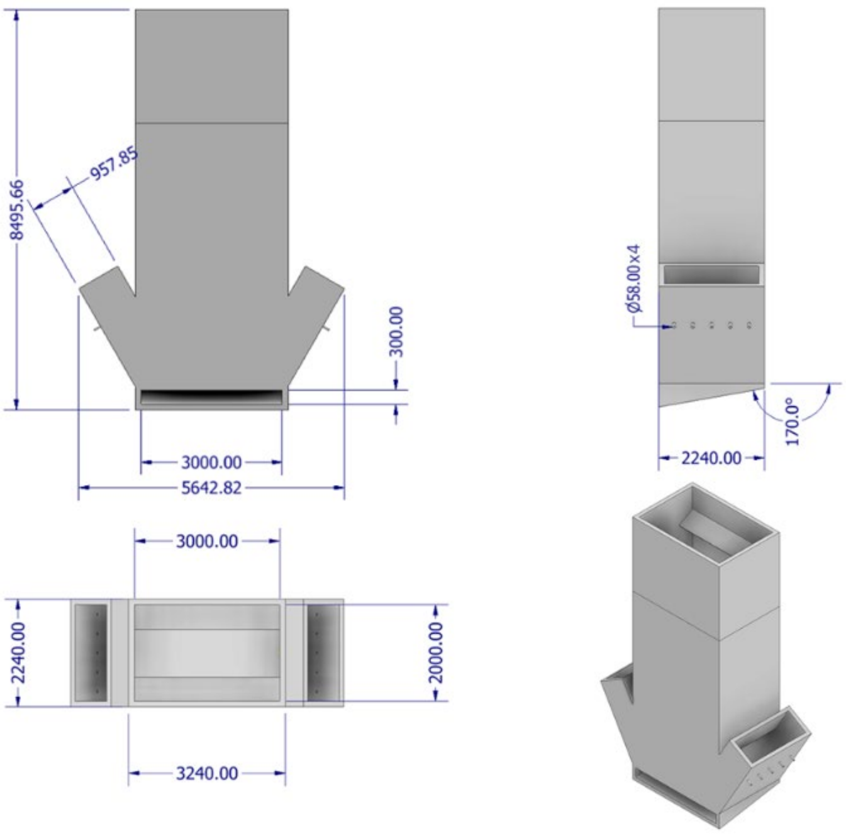


Figure 6. ECA reactor with methane feed tubes

The results are summarized in Table 5. It also reflects the results of calculations in the Mathcad software package [37] using the method described in [38]. A comparison of the parameters obtained as a result of modeling in ANSYS with the results based on the tested method [38] allows us to judge the equilibrium composition of the syngas.

Table 5. Volume fractions at the reactor outlet

Parameter	Methodology [38]	ANSYS Fluent
Temperature syngas , °C	**856**	**839**
	Compound syngas, vol. %:	
CH_4	0.038	0.078
CO_2	6.89	6.15
CO	59.33	59.80
N_2	9.82	9.47
H_2	21.19	22.10
O_2	0	0
H_2O	2.73	2.39

3.2.4. Combined modeling of the ECA reactor

The next step is a combined calculation of the chemical reaction and dispersed entrained particles in the flow, as the calculations for the completeness of the chemical reaction did not take into account the heat introduced by the entrained particles. The same model was used for comparison with previous calculations.

This simulation was performed using the Relax solver. to Chemical Equilibrium. The entrained particles are a mixture of iron oxide Fe_xO_y, each of which has its own heat capacity, melting point, and thermal conductivity. This calculation does not take into account the effects of entrained particle solidification. It was assumed that the particles enter at a temperature of 1650 °C in a solid phase with a density of 5200 kg/m^3 and a heat capacity of 800 J/(kg·K) [39]. Table 6 presents the initial data for the calculation.

Table 6. Initial data for identifying incomplete responses

Name parameter	Parameter characteristic or set value
Model turbulence	k-ε RNG Swirl Dominated Flow
Chemical solver	Relax to chemical equilibrium
Inlet gas velocities, m/s	15
Behavior particles on exit	Escape
Minimum/Average/Maximum particle diameter, m	0.00015/0.0015/0.015
Mass flow rate of particles at two inputs, kg/s	4.76
Temperature converter gas, K	1923
Temperature methane, K	300
Converter gas consumption per input, kg/s	5.425
Methane consumption per side, kg/s	0.48375

The results of the combined modeling of the entrainment dynamics and the kinetics of ECA reactions are presented in Figure 7, and the entrainment distribution is shown in Figure 8.

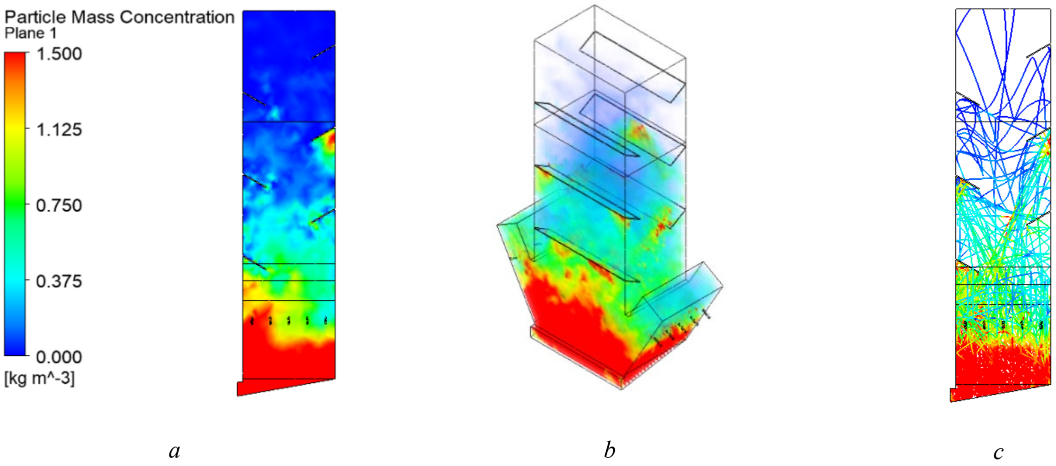


Figure 7. Mass concentration (*a, b*) and particle trajectories (*c*)

The results of the study in the presence and absence of carryover are presented in Table 7. The developed model allows us to estimate how close the chemical composition of the syngas at the outlet of the ECA reactor is to the equilibrium [38]. The final results of the study are presented in Table 8.

Table 7. Mass concentration of fly ash particles at reactor outlets

Parameter	Modeling of gas-dynamic processes without taking into account chemical effects	Modeling of chemical processes taking into account carryover
Upper outlet, kg/m^3	0.00656944	0.00982052
Bottom outlet, kg/m^3	1.3453	1.38859

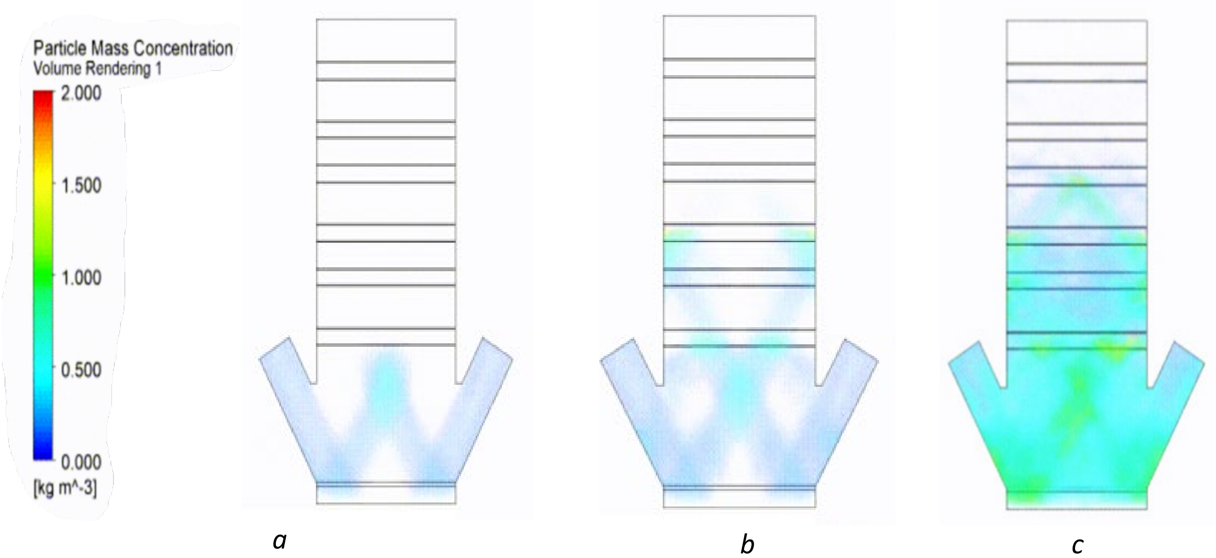


Figure 8. Change in time of the carryover distribution in the frontal axial section of the reactor: *a* – 2 s; *b* – 4 s; *c* – 17 s

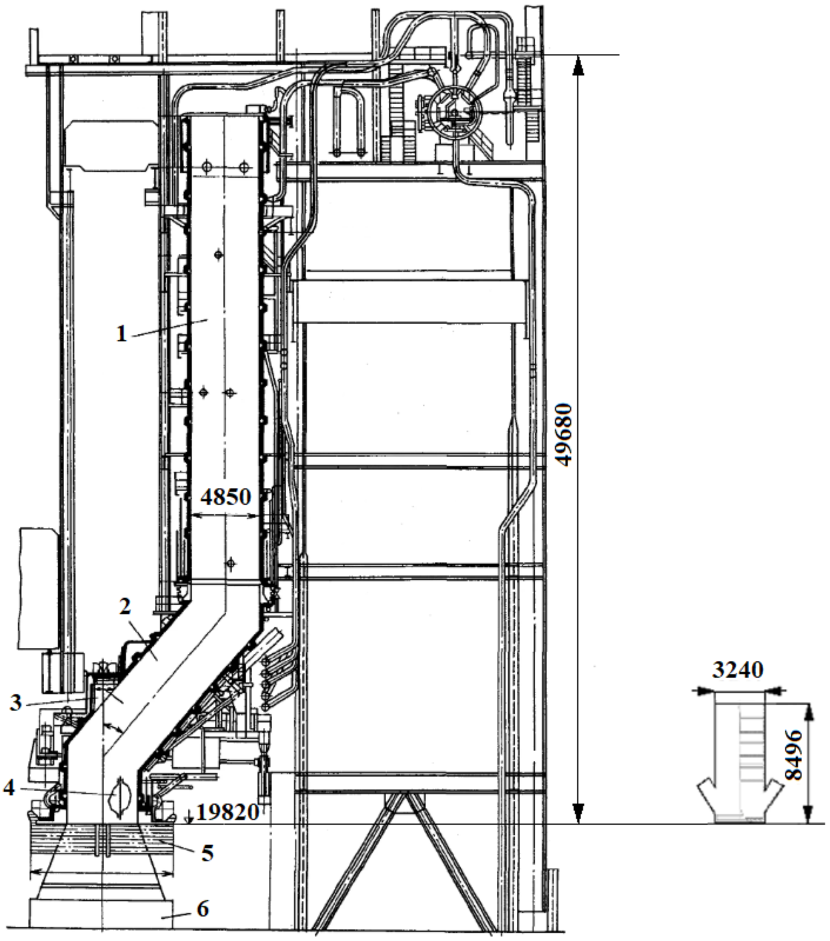
Table 8. Comparison results calculation

Parameter	Numerical modeling in ANSYS Fluent		Calculation of equilibrium state parameters using the method [38]	
	Without accounting metallic dust carryover	Taking into account metallic dust carryover	Without accounting metallic dust carryover	Taking into account metallic dust carryover
Temperature syngas, °C	839	990	856	973
Composition of syngas at the outlet of the ECA reactor, %				
CH_4	0.078	0.0059	0.038	0.003
CO_2	6.15	5.82	6.89	6.251
CO	59.80	60.05	59.327	59.952
N_2	9.47	9.59	9.823	9.816
H_2	22.10	20.83	21.193	20.651
O_2	0	0	0	0
H_2O	2.39	3.21	2.732	3.326

Based on the data presented in Fig. 4 and Table 3, it can be concluded that the composition of the syngas at the reactor outlet is close to equilibrium, while the height of the reactor is 8.5 m.

As can be seen from Fig. 3, the fly ash concentration at the lower section of the reactor is 1389 g/m^3, and at the reactor outlet it is 9.8 g/m^3. This allows us to conclude that the reactor provides effective fly ash separation.

A comparison of the sizes of the ECA and CGCS-400 reactors is shown in Fig. 5, from which it can be seen that the ECA reactor occupies a volume that does not exceed the volume of the inclined flue duct *2*.



a *b*

Figure 9. Comparison of the overall dimensions of CGCS -400 (*a*) and the resulting model of the ECA reactor (*b*):

1 – radiation flue; *2* – inclined flue; *3* – opening for oxygen tuyere; *4* – feed of charge materials; *5* – movable sealing sleeve; *6* – converter

To carry out the ECA process in an inclined shaft of the CGCS, it is necessary to ensure its gas density for the purpose of explosion safety and increasing efficiency [40].

4. Conclusion

1. Using exergy analysis, converter gas utilization options were analyzed. A regenerative fuel system based on the ECA process was proposed as a promising option, characterized by an exergy efficiency of 82.7%. The current converter gas utilization system has an exergy efficiency of 11%.
2. A design for an ECA reactor based on a gravity-driven pneumatic classifier with transfer elements—inclined shelves—was proposed. A mathematical model was developed and implemented in ANSYS. Fluent numerical modeling of fly ash dynamics and the chemical reaction of converter gas with natural gas. The numerical study determined the geometric characteristics of the ECA reactor necessary for achieving complete reagent conversion and effective fly ash removal.

3. The possibility of placing the developed ECA reactor within the volume occupied by the inclined shaft of the converter gas cooler has been established.

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Conflict of interest

The authors declare no conflict of interest

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