

CFD SIMULATION OF TEMPERATURE VARIATION IN CARBONIFEROUS ROCK STRATA DURING UCG

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Abstract

The numerical simulation was based on the computational fluid dynamics formalism in order to identify the change of temperature in rock strata during underground coal gasification (UCG). The calculations simulated the coal gasification process using oxygen and water vapour as a gasification agent in 120 hours. Based on the selected software (Ansys-Fluent) a model of underground coal gasification (UCG) process was developed. The flow of the gasification agent, the description of the turbulence model, the heat-exchange model and the method of simulation of chemical reactions of gasification are presented herein.

Keywords

underground coal gasification, computational fluid dynamics, modelling

1. INTRODUCTION

Fuel acquisition, mainly underground fuels, has undeniably contributed to the development of civilisation in the modern world. Fossil fuels are currently the main source of energy, which were originally used as thermal energy, generally as a raw material for the generation of electricity. However, in the case of the exhaustion of natural resources of raw materials and the need to use zero-emission technology for their processing this has resulted in the most economically developed countries of the world being forced to search for new methods of energy production. This issue is very clearly seen in the countries of the European Union, and hence also in Poland. In addition, the situation is complicated by the prospect of future restrictions regarding the supply of crude oil and natural gas, which threatens the stability and energy security for many countries of the world (Białecka 2008; Borowiecki eds. et al. 2008).

In the case of a country that has huge amounts of deposits of hard or lignite coal, the development of clean coal technologies is invaluable. Poland is undoubtedly in the ranks of these states, as a country whose economy depends on energy manufactured from coal combustion. The forward-looking method, which opposes the mentioned threats, is the underground coal gasification process (Białecka 2008). According to the results of the model and experimental research (Białecka 2008; Kozaczka 1994; Stańczyk et al. 2012; Tomeczek 1991), the *in situ* coal gasification method could be an innovative method of chemical mining of out-of-

balance coal deposits, unavailable within the usage of conventional extractive techniques.

The coal gasification process in *in-situ* conditions, poses a potential threat to the original state of the rock strata. The georeactor formed underground, in a coal seam, affects layers of rocks in the vicinity. One of the mechanisms of this interaction is the natural flow of heat from the gasification area (gasification channel) to the rock strata. The study of georeactor-rock strata interaction is important for the determination of the potential impact of gasification technologies by specifying the dynamism of changes of physical and mechanical properties of rocks constructing a rock mass. Such research can be carried out using computer simulation methods. The advantages of software for computational fluid dynamics (CFD) is the possibility of modelling the phenomena related to fluid flow (combustion, turbulence, multiphase flows, chemical reactions, heat conduction, radiation, etc.) (ANSYS... 2009).

2. CHARACTERISTICS OF THE UNDERGROUND COAL GASIFICATION PROCESS

Under the conditions of the underground coal gasification process (UCG), along the gasification channel, three zones of gasification reaction were developed, namely (Białecka 2008):

- oxidation zone
- reduction zone
- pyrolysis zone

The oxidation zone is determined by a number of exothermic chemical reactions between components of a gasification agent and a coal mass, accompanied by an energy effect in the form of heat. The products arising from the oxidation reactions constitute substrates of secondary reactions in the reduction zone. However, the pyrolysis zone includes thermal processes, as a result of which gas and fluid products are produced at the expense of heat collected from a stream of the flowing syngas (Białecka 2008; Borowiecki eds. et al. 2008; Kozaczka 1994; Tomczek 1991).

The UCG process is determined thanks to a chemical interaction between the gasification agent (oxygen, a mixture of oxygen and water vapour, air or air enriched with oxygen) and coal, which accompanies large amounts of heat emitted to the rock strata. In the work of Białecka (2008), based on the results of experimental research on the gasification process with the participation of oxygen, the possibility of temperature along the gasification channel of 2270 K and higher, for a distance of 2–3 meters of its length were shown. Thus, high temperature disrupts the initial balance in the vicinity of the rock mass. The result of heat transfer into the rock strata is the change of the physical-chemical properties of rocks strata, which may result in their destruction. This creates a potential threat to mine crews and reduces the efficiency of the process.

3. MODEL OF COAL GASIFICATION PROCESS BASED ON THE APPLICATION OF CFD

The main assumption was to base the simulation on the reactive flow of fluid. Gas moving through the fire channel simulates the physical-chemical phenomena related to the transportation of mass and energy as well as the occurrence of chemical reactions. The description of chemical reactions is a kinetic description. In the framework of the prepared model, the interaction of gas from the gasification channel with the vicinity layer of the Carboniferous rocks has been taken into account. This description is related to the transportation of heat energy. The coal layers as well as the geological layers in the vicinity of a georeactor are treated as a homogeneous body. Due to the complexity of equations and the complexity of numerical methods used for solving them, it was decided to use the non-commercial CFD code.

3.1. Georeactor geometry

Studies on the underground gasification technology were shown that a useful form of syngas can be obtained even from coal with a thickness of at least 1 meter. Carrying out the gasification process at these types of coal seams enables eliminating the arising mining difficulties (Białecka 2008).

For the purpose of implementing a simulation of the underground coal gasification process, a georeactor model was developed and located in the coal seam of the thickness of 1 metre, the width of 2 metres and the length of 5 metres. The coal seam is available for the gasification process thanks to a gasification channel in the form of a cylinder with a diameter of 0.18 metres and a length of 5 metres, located in the symmetry plane of the georeactor. The gasification channel ensures the supply of the gasification mixture to the reaction area of the georeactor and ensures the reception of syngas. The effects of the adopted considerations led to the develop-

ment of 5 geometrical models of the georeactor which were shown in Figure 1.

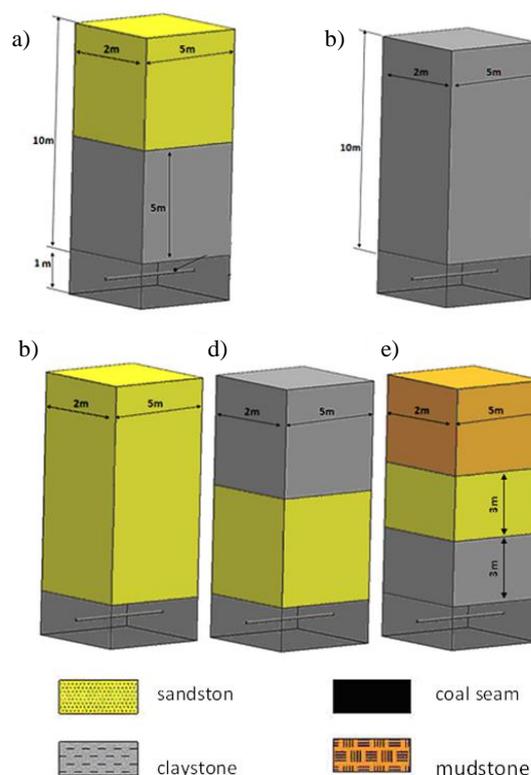


Fig. 1. The geometric model of the georeactor developed for the simulation of the UCG process

The geometry used in the calculations is based on the following information (Fig. 3):

- solid model of the coal layer – $1 \times 2 \times 5$ m
- solid model of the gasification channel – $\varnothing 0.18 \times 5$ m
- solid model of claystone, mudstone and sandstone layer.

3.2. Simulation grid

Figure 2 shows the results of the numerical grid. It was decided to generate unstructured grids in the form of tetrahedron in a pyramid shape with the base of a triangle, namely:

- an unstructured grid of a solid model of the georeactor heat system (system I – Fig. 2a) consisting of gasification channel formed by 11,761 nodal points combined with 54,352 simple elements, forming a geometric image of the area occupied by the fluid (volume of 0.0603 [m³]), coal layer formed by 43,230 nodal points combined with 237,821 simple elements, forming a geometric image of the area occupied by the coal mass (volume of 24.87 [m³]), the sandstone layer formed from 2,635 nodal points, combined with 12,872 simple elements, a geometric image of the area occupied by the matrix of rock (volume of 125 [m³]), claystone layer formed by 2,661 nodal points combined with 12,979 simple elements, a geometric image of the area occupied by the matrix of rock (volume of 125 [m³]);
- unstructured grid of a solid model of georeactor heat system (system II – Fig. 2b) consisting of a gasification channel formed by 11,761 nodal points combined with 54,352 simple elements, forming a geometric image of

the area occupied by the fluid (volume of 0.0603 [m³]), coal layer formed by 43,230 nodal points combined with 237,821 simple elements, forming a geometric image of the area occupied by coal mass (volume of 24.87 [m³]), claystone layer formed by 1,887 nodal points combined with 9,010 simple elements, a geometric image of the area occupied by the matrix of rock (volume of 125 [m³]);

- unstructured grid of a solid model of the georeactor heat system (system III – Fig. 2c) consisting of a gasification channel formed by 11,761 nodal points combined with 54,352 simple elements, forming a geometric image of the area occupied by the fluid (volume of 0.0603 [m³]), coal layer formed by 43,230 nodal points combined with 237,821 simple elements, forming a geometric image of the area occupied by coal mass (volume of 24.87 [m³]), sandstone layer formed from 1,887 nodal points, combined with 9,010 simple elements, a geometric image of the area occupied by the matrix of rock (volume of 250 [m³]);
- unstructured grid of a solid model of georeactor heat system (system IV – Fig. 2d) consisting of a gasification channel formed by 11,761 nodal points combined with 54,352 simple elements, forming a geometric image of the area occupied by the fluid (volume of 0.0603 [m³]), coal layer formed by 43,230 nodal points combined with 237,821 simple elements, forming a geometric image of

the area occupied by coal mass (volume of 24.87 [m³]), claystone layer formed by 2,635 nodal points combined with 12,872 simple elements, forming a geometric image of the area occupied by the matrix of rock (volume of 0.125 [m³]), sandstone layer formed from 2,661 nodal points, combined with 12,979 simple elements, a geometric image of the area occupied by the matrix of rock (volume of 125 [m³]);

- unstructured grids of a solid model of the georeactor heat system (system V – Fig. 2e) consisting of gasification channel formed by 11,761 nodal points combined with 54,352 simple elements 11,761, forming a geometric image of the area occupied by the fluid (volume of 0.0603 [m³]), coal layer formed by 43,230 nodal points combined with 237,821 simple elements, forming a geometric image of the area occupied by coal mass (volume of 24.87 [m³]), claystone layer formed by 2,228 nodal points combined with 10,778 simple elements, forming a geometric image of the area occupied by the matrix of rock (volume of 75 [m³]), sandstone layer formed from 2,221 nodal points, combined with 10,775 simple elements, forming a geometric image of the area occupied by the matrix of rock (volume of 75 [m³]), mudstone layer formed from 410 nodal points, combined with 1,187 simple elements, a geometric image of the area occupied by the matrix of rock (volume of 100 [m³]);

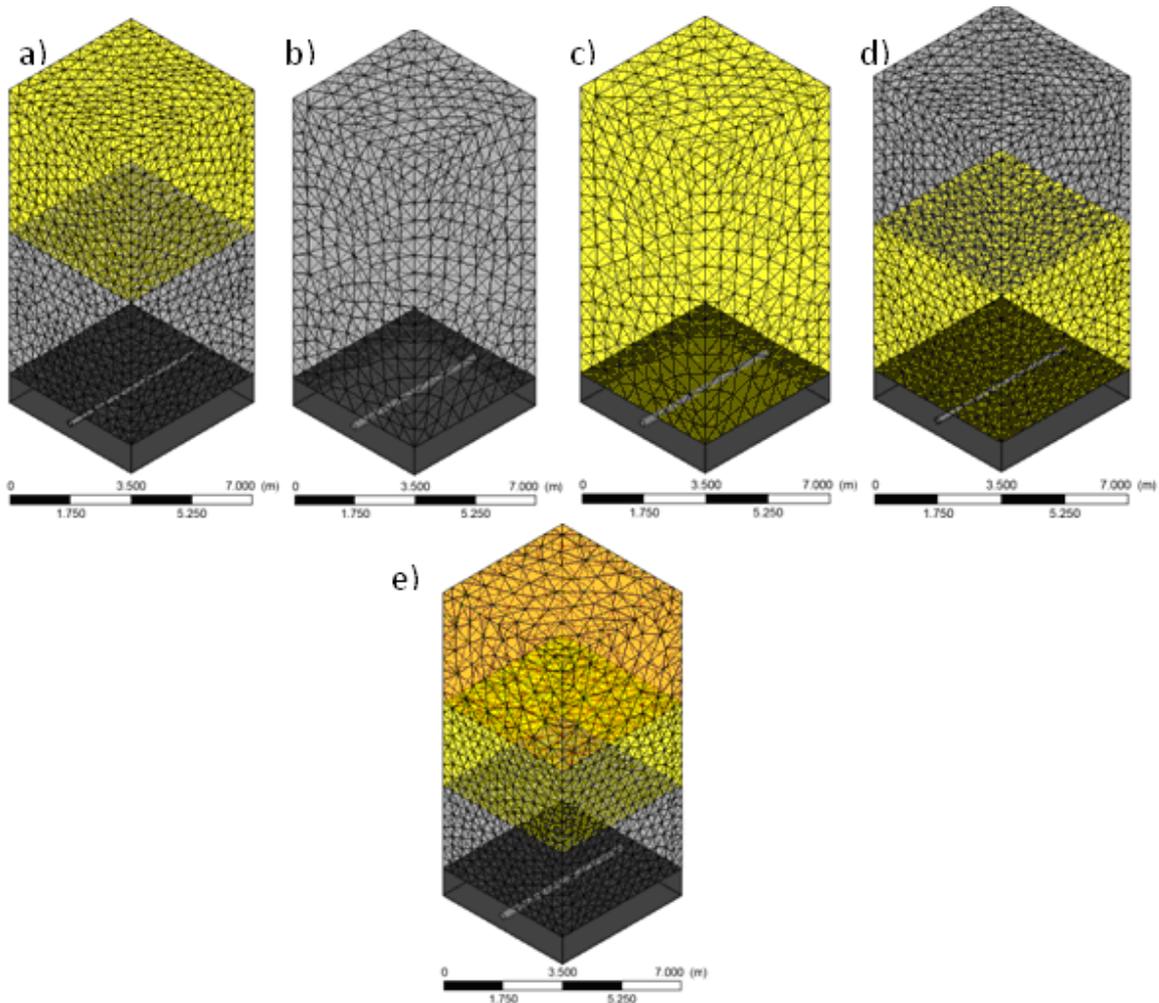


Fig. 2. Simulation grid: a – system I, b – system II, c – system III, d – system IV, e – system V, f – system VI

3.3. Modelling of the fluid flow

Basic equations describe the behaviour of the fluid flowing along the gasification channel were presented by the following equations (ANSYS... 2009):

- equation of conservation of mass:

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \bar{u}) = S_p \quad (1)$$

where:

- t – time [s]
- ρ – fluid density [$\text{kg}\cdot\text{m}^{-3}$]
- \bar{u} – vector of fluid element speed [$\text{m}\cdot\text{s}^{-1}$]
- S_p – source element related to the exchange of mass [$\text{kg}\cdot\text{m}^{-3}\cdot\text{s}^{-1}$]

- equation for the conservation of momentum:

$$\frac{\partial}{\partial t}(\rho \bar{u}) + \nabla(\rho \bar{u} \bar{u}) = -\nabla p + \nabla(\mu \nabla \bar{u}) + S_u \quad (2)$$

where:

- t – time [s]
- \bar{u} – vector of fluid element speed [$\text{m}\cdot\text{s}^{-1}$]
- p – fluid pressure [Pa]
- μ – dynamic viscosity of fluid [$\text{Pa}\cdot\text{s}$]
- S_u – source element related to change in the fluid momentum [$\text{kg}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$]

- equation of the conservation of energy:

$$\frac{\partial}{\partial t}(\rho h) + \nabla(\rho \bar{u} h) = \nabla(k \nabla T) + S_h \quad (3)$$

where:

- t – time [s]
- \bar{u} – vector of fluid element speed [$\text{m}\cdot\text{s}^{-1}$]
- h – enthalpy [$\text{J}\cdot\text{kg}^{-1}$]
- T – fluid temperature gradient [K]
- S_h – source element related to the exchange of energy [$\text{J}\cdot\text{m}^{-3}$]
- λ – coefficient of thermal conductivity [$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$]

- equation of the conservation of the chemical reaction:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla(\rho \bar{u} Y_i) = \nabla(D \nabla Y_i) + S_Y + R_f \quad (4)$$

where:

- t – time [s]
- \bar{u} – vector of fluid element speed [$\text{m}\cdot\text{s}^{-1}$]
- Y_i – mass share of the fluid i -component [-]
- S_Y – source element related to the formation of volatile compounds [$\text{kg}\cdot\text{m}^{-3}\cdot\text{s}^{-1}$]
- R_f – speed of chemical reactions [$\text{kg}\cdot\text{m}^{-3}\cdot\text{s}^{-1}$]
- D – diffusion coefficient [$\text{m}^2\cdot\text{s}^{-1}$].

In addition, the description of the gas flow in the reaction area, which is composed of the gasification channel of the given geometry and changes in the fluid properties resulting from the turbulent nature of the flowing gas were taken into account. Thus, the most widely used CFD turbulence model k - ϵ was included in the calculations. The phenomenon related to the exchange of heat between the flowing fluid (syngas) and the rock strata, is solved on the basis of the following expressions (9) (ANSYS... 2009):

$$\frac{\partial}{\partial t}(\rho h) = \nabla(k \nabla T) \quad (5)$$

where:

- ρ – fluid density [$\text{kg}\cdot\text{m}^{-3}$]
- k – coefficient of thermal conductivity of the rock layer [$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$]
- T – temperature gradient [K]
- h – enthalpy of fluid

The left side of the equation (5) interprets the phenomena related to the convective heat transport in the syngas flow, while the right side of the equation describes the transport of heat energy.

The amount of heat conducted to the rock mass determines the thermal conductivity coefficient λ . The value of this parameter for the ground of the Upper Silesian Coal Basin was examined (Pawiński, Roszkowski, Strzemiński 1995), and the results are presented in table 1.

Table 1. Thermal conductivity coefficient of rocks (Pawiński, Roszkowski, Strzemiński 1995)

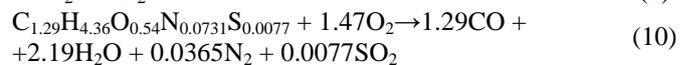
Rock types	Value of the λ parameter [$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$]
Conglomerates	3.4
Coarse-grained sandstones	3.5
Close-grained sandstones	3.1
Sandy stone	2.2
Clay stone	2.1
Coal seam	0.60

Basic gasification process reactions are expressed in the form of three equations of primary reactions between coal and the gasification agent, as well as three equations of secondary reactions between products of primary reactions. Gasification reactions do not occur individually and their effect, expressed by a specific volume of product gas components, involves the resultant change to the course in terms of preferences for certain chemical reactions and the creation of specific chemical compounds, the decisive role of such parameters as temperature, pressure or mass fraction of gasification agent compounds. The chemical composition of coal is listed in table 2.

Table 2. Ultimate/proximate analysis of coal (Stańczyk et al. 2012)

Technical analysis	coal	63.83%
	volatiles	32.41%
	ash	2.21%
	moisture	1.55%
Elementary analysis	C	83.84%
	H	4.94%
	O	9.79%
	N	1.15%
	S	0.28%
heat of combustion		$3.34 \cdot 10^7 \text{ J}\cdot\text{kg}^{-1}$

The following chemical reactions of the gasification process were adopted for the calculations:



The following parameters of the kinetic model, expressed in the form of the dependence (12), were adopted (ANSYS... 2009):

$$k = AT^\beta e^{-E/RT} \quad (12)$$

- reaction No. (6) (Vikram 2012):
 - activation energy – $E = 6.1e^{+07}$ [J·mol⁻¹]
 - power factor of temperature – $\beta = 0$
 - exponential coefficient – $A = 0.052$ [s⁻¹]
- reaction No. (7) (Vikram 2012):
 - activation energy – $E = 1.15e^{+08}$ [J·mol⁻¹]
 - power factor of temperature – $\beta = 0$
 - exponential coefficient – $A = 0.0782$ [s⁻¹]
- reaction No. (8) (Vikram 2012):
 - activation energy – $E = 7.53e^{+07}$ [J·mol⁻¹]
 - power factor of temperature – $\beta = 0$
 - exponential coefficient – $A = 6e^{-07}$ [s⁻¹]
- reaction No. (9) (Askarova et al. 2009):
 - activation energy – $E = 3800$ [J·mol⁻¹]
 - power factor of temperature – $\beta = 0$
 - exponential coefficient – $A = 0.9740509$ [s⁻¹]
- reaction No. (10) (ANSYS... 2009):
 - activation energy – $E = 2.027e^{08}$ [J·mol⁻¹]
 - power factor of temperature – $\beta = 0$
 - exponential coefficient – $A = 2.119e^{+11}$ [s⁻¹]
- reaction No. (11) (ANSYS... 2009):
 - activation energy – $E = 1.7e^{08}$ [J·mol⁻¹]
 - power factor of temperature – $\beta = 0$
 - exponential coefficient – $A = 2.239e^{11}$ [s⁻¹]

4. NUMERICAL SOLUTIONS OF THE UCG PROCESS

The following local conditions of the numerical solution, separately for each of the discretization areas, were included, namely:

- a) for the gasification channel (fluid element):
 - temperature and value of the flow of mass O₂ – 25 [°C] and 5.4 [kg·s⁻¹]
 - specific heat of oxygen O₂ c_{pO_2} based on the relation (ANSYS... 2009) – $c_{pO_2} = 876.317 + 0.122828T - 0.000558304T^2 - 1.20247e^{-06}T^3 - 1.14741e^{-09}T^4 - 5.12377e^{-13}T^5 + 8.56597e^{-17}T^6$ [J·kg⁻¹·K⁻¹]
 - temperature and value of the flow of mass H₂O – 100 [°C] and 5.4 [kg·s⁻¹]
 - specific heat of water vapour H₂O c_{pH_2O} based on the relation (ANSYS... 2009) – $cp_{H_2O} = 1937.8 - 1.18077T + 0.00364357T^2 - 2.86327e^{-06}T^3 + 7.59578e^{-10}T^4$ [J·kg⁻¹·K⁻¹]
 - the coefficient of heat conduction (ANSYS... 2009) – 0.0454 [W·m⁻¹·K⁻¹]
 - mass fraction of oxygen and water vapour – O₂ – 0.4, H₂O – 0.6;
- b) for the georeactor model (coal seam):
 - density – 1450 [kg·m⁻³] (Chmura 1968)
 - porosity – 5% (Białecka 2008)

- permeability $\beta - 1e^{-15}$ [m²] (Białecka 2008)
- specific heat of coal mass c_{pC} based on the relation (Johnson 1979; Shirazi 2012):

$$c_{pC} = \begin{cases} 0.1116 - 0.001417T & T < 598 \text{ [K]} \\ 2.14618 - 0.0006483T & T \geq 598 \text{ [K]} \end{cases}$$

- temperature $T - 298.15$ [K]
- thermal conductivity – (Chmura 1968; Shirazi 2012):

$$\lambda_c = \begin{cases} 0.535 \text{ [W·m}^{-1}\text{·K}^{-1}] & T < 673 \text{ [K]} \\ 0.11 - 0.0002 \text{ [W·m}^{-1}\text{·K}^{-1}] & T \geq 673 \text{ [K]} \end{cases}$$

- c) for the sandstone layer (porous medium):
 - density – 2690 [kg·m⁻³] (Chmura 1968)
 - porosity – 0.6 [%] (Chmura 1968)
 - permeability in the plane (X, Y, Z) $\beta - 1e^{-14}$ [m²]
 - specific heat $c_p - 1120$ [J·kg⁻¹·K⁻¹] (Chmura 1968)
 - initial temperature $T - 298.15$ [K]
 - thermal conductivity – 3.5 [W·m⁻¹·K⁻¹] (Pawiński, Roszkowski, Strzemiński 1995);
- d) for the claystone layer (porous medium):
 - density – 2710 [kg·m⁻³] (Chmura 1968)
 - porosity – 2.4 [%] (Chmura 1968)
 - permeability in the plane (X, Y, Z) $\beta - 1e^{-15}$ [m²]
 - specific heat $c_p - 800$ [J·kg⁻¹·K⁻¹] (Chmura 1968)
 - initial temperature $T - 298.15$ [K]
 - thermal conductivity – 2.1 [W·m⁻¹·K⁻¹] (Pawiński, Roszkowski, Strzemiński 1995);
- e) for the mudstone layer (porous medium):
 - density – 2600 [kg·m⁻³] (Chmura 1968)
 - porosity – 5 [%] (Chmura 1968)
 - permeability in the plane (X, Y, Z) $\beta - 2e^{-15}$ [m²]
 - specific heat $c_p - 1000$ [J·kg⁻¹·K⁻¹] (Chmura 1968)
 - initial temperature $T - 298.15$ [K]
 - thermal conductivity – 2.88 [W·m⁻¹·K⁻¹] (Chmura 1968).

The following global settings in the CFD program were adopted, namely:

- transient state
- gasification pressure – 101325 [Pa]
- gravity acceleration – 9.81 [m·s⁻²]
- gasification agent is a mixture of oxygen and water vapour
- time – 120 hours
- roughness of the gasification channel – 0.1 [m]
- convergence of calculations – $1 \cdot 10^{-4}$

5. STUDY OF MODEL TEST RESULTS

Below, the temperature field change results were presented, which is the solution of the numerical model of the UCG process.

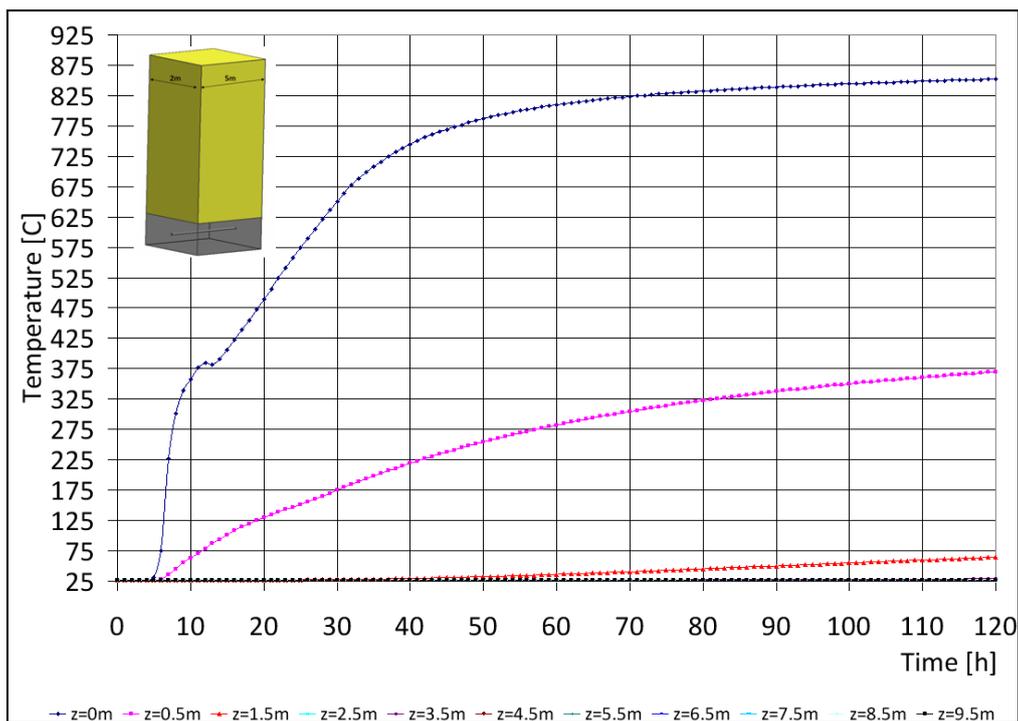


Fig. 3. Change of average temperature in the sandstone layer under the conditions of the UCG process in time interval of 120 hours

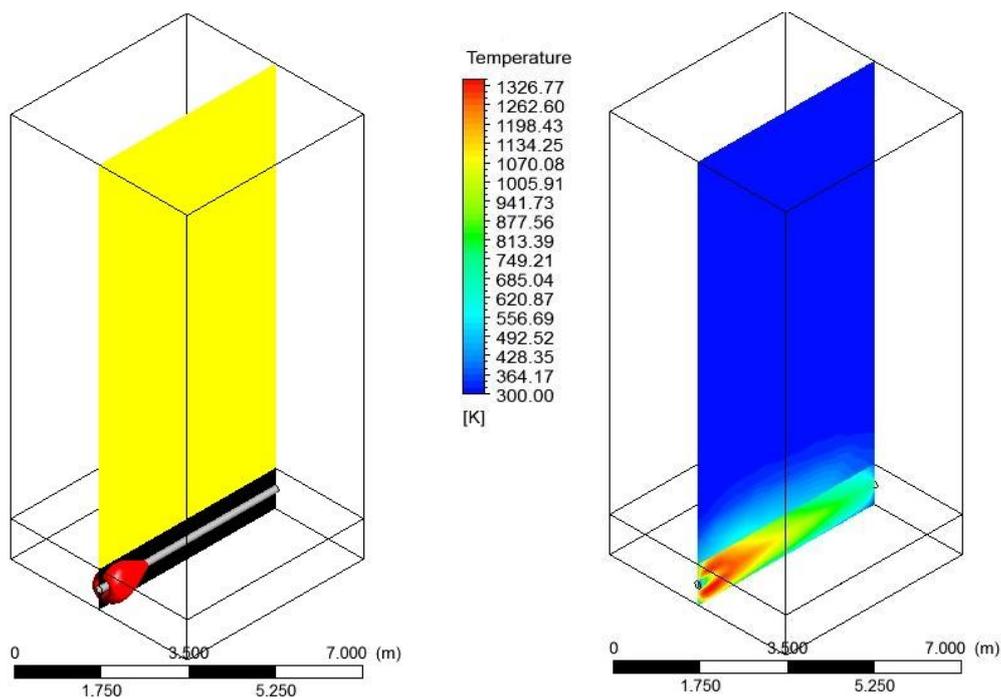


Fig. 4. The shape of the cavity (red area) and the changes of temperature in a layer of sandstone during UCG after 120 hours

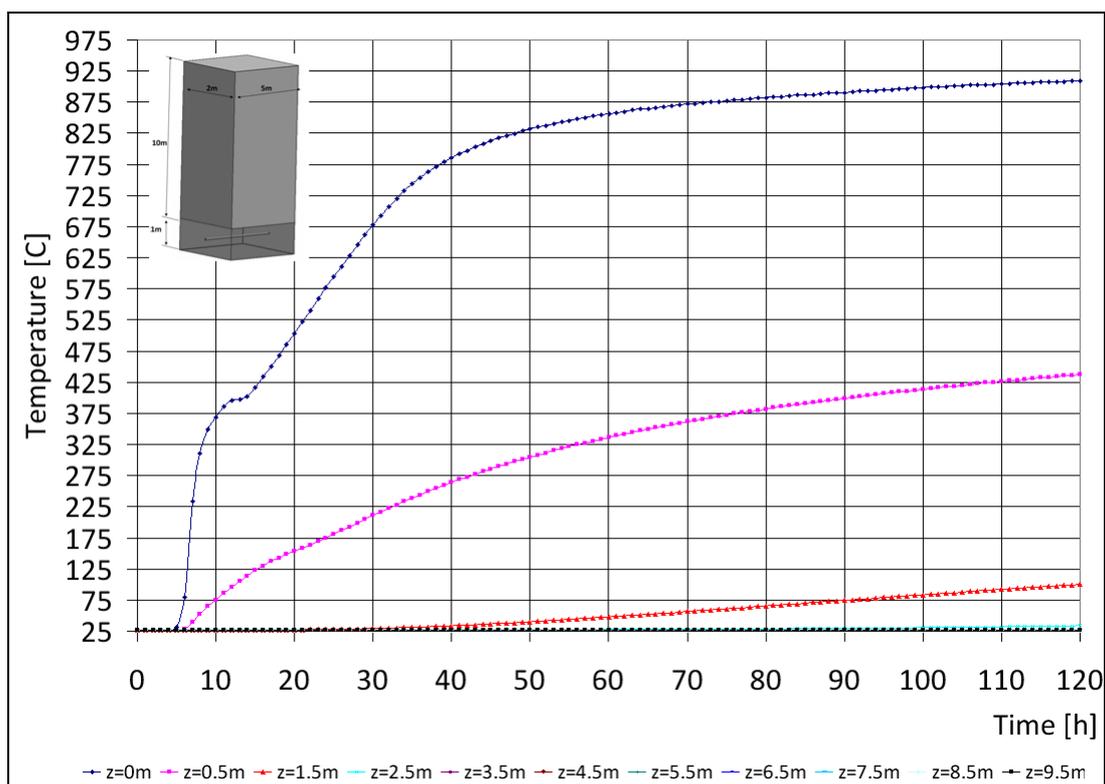


Fig. 5. Change of average temperature in the claystone layer under the conditions of the UCG process in time interval of 120 hours

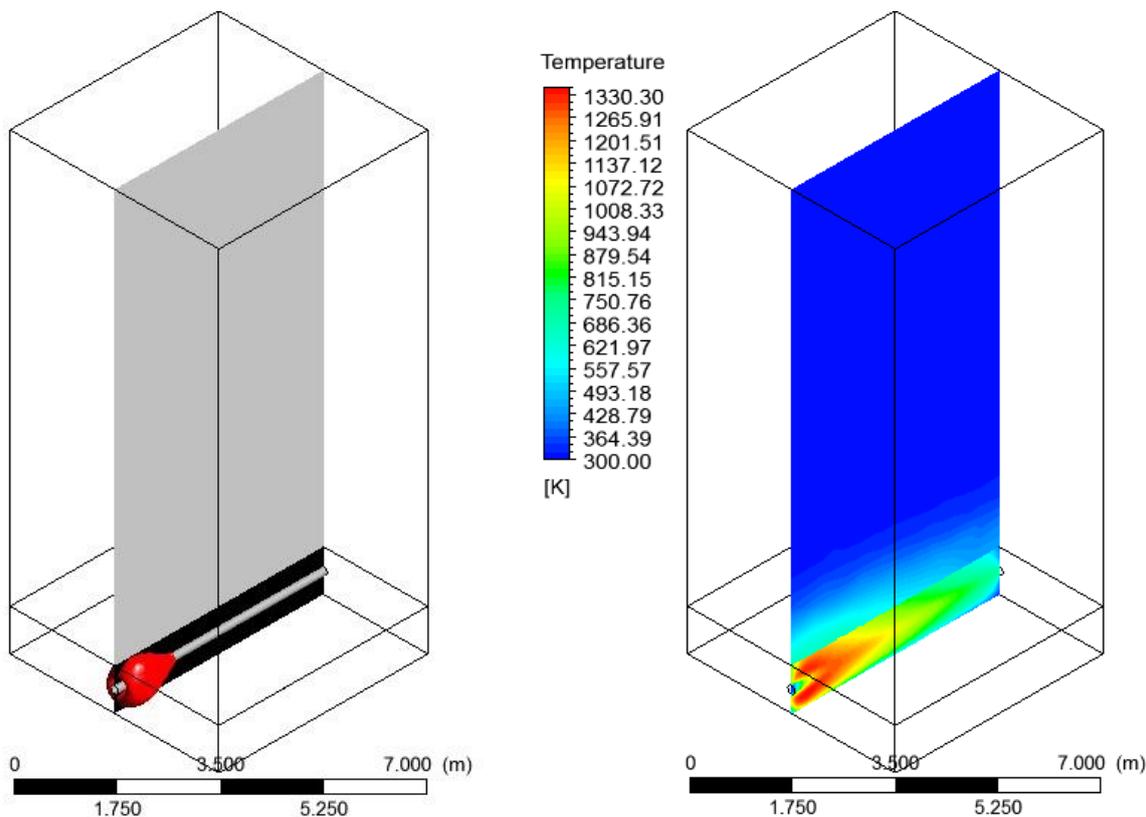


Fig. 6. The shape of the cavity (red area) and the changes of temperature in a layer of claystone during UCG after 120 hours

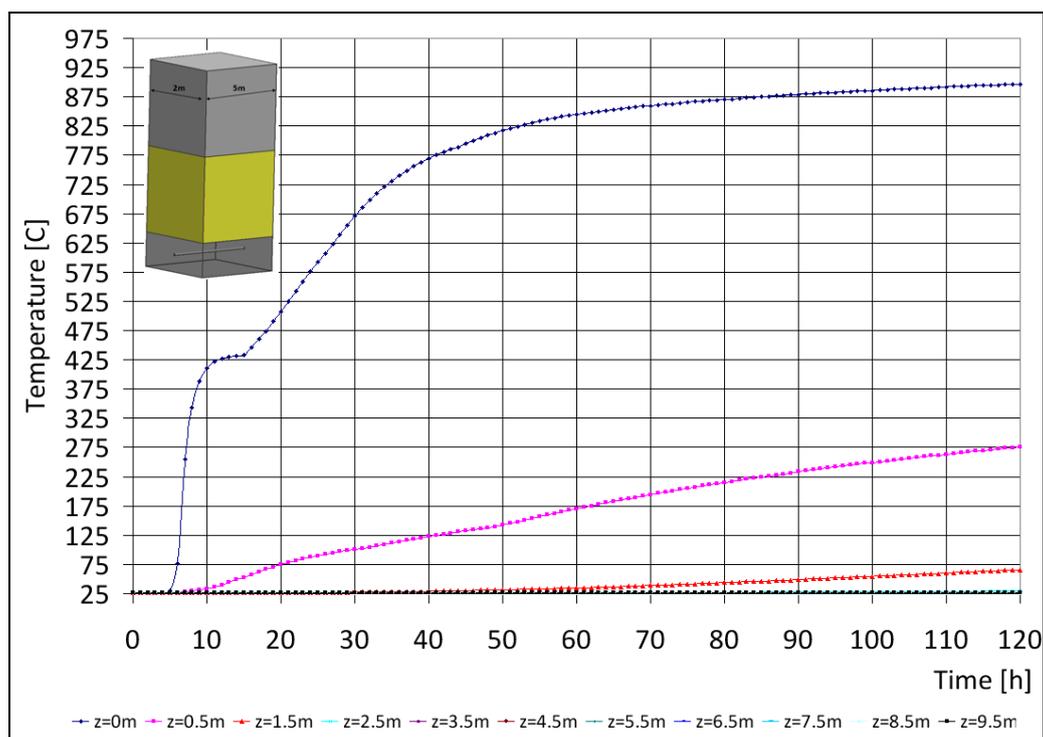


Fig. 7. Change of average temperature in the sandstone and claystone layer under the conditions of the UCG process in time interval of 120 hours

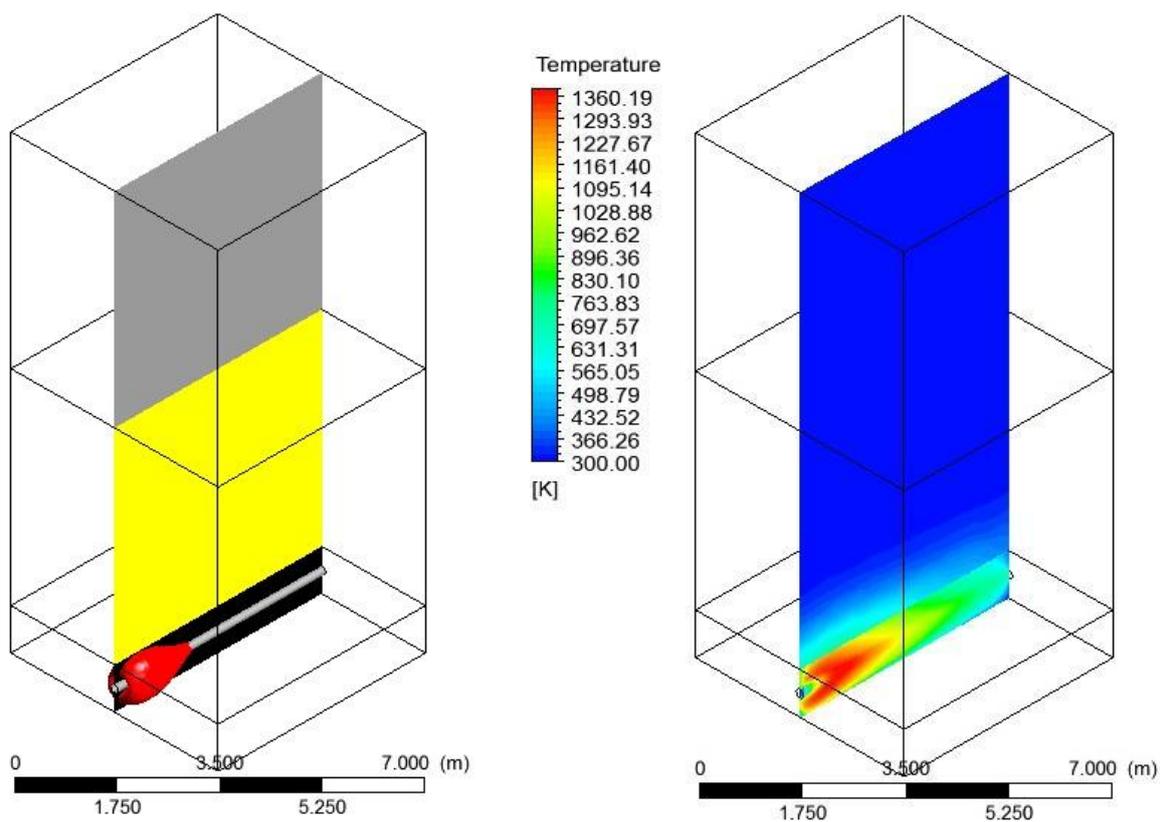


Fig. 8. The shape of the cavity (red area) and the changes of temperature in a layer of sandstone and claystone during UCG after 120 hours

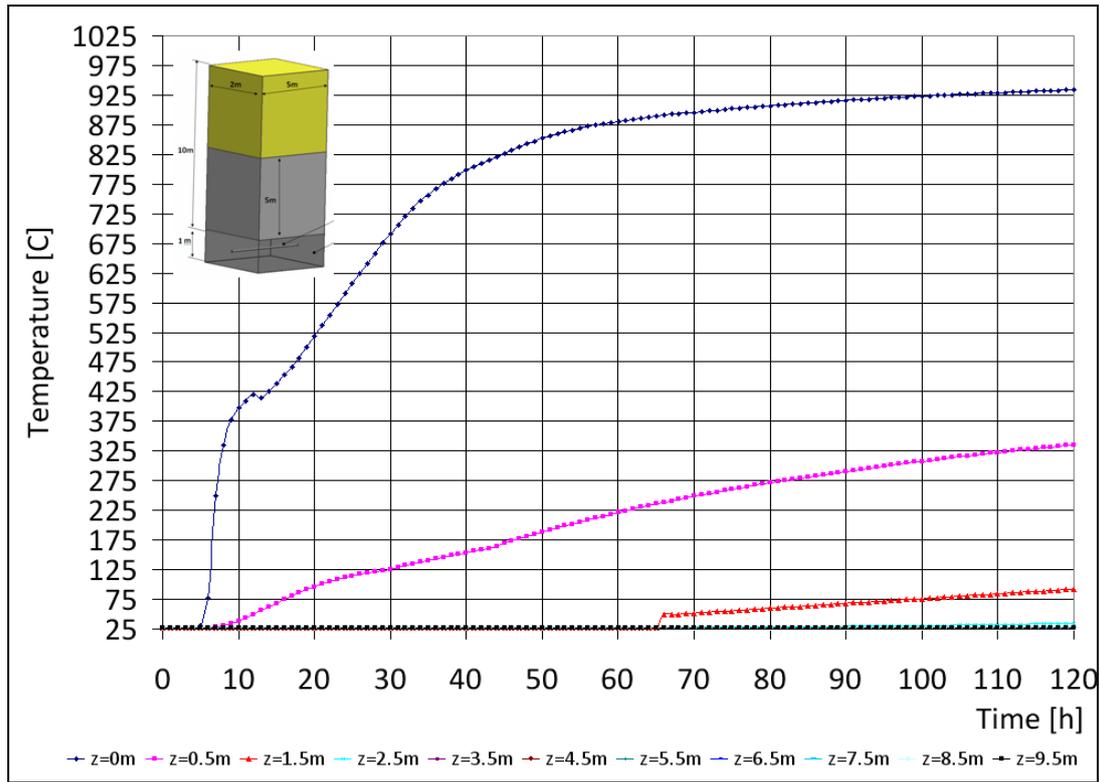


Fig. 9. Change of average temperature in the claystone and sandstone layer under the conditions of the UCG process in time interval of 120 hours

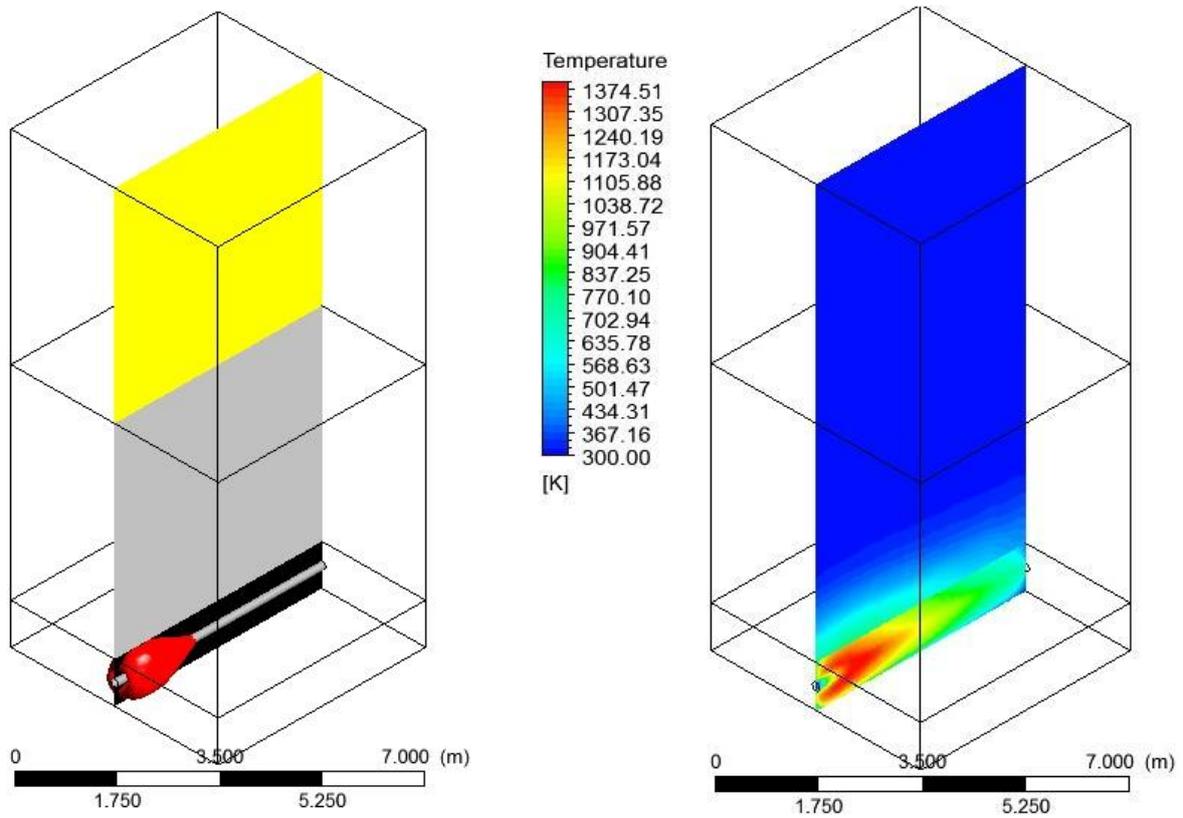


Fig. 10. The shape of the cavity (red area) and changes of temperature in a layer of claystone and sandstone during UCG after 120 hours

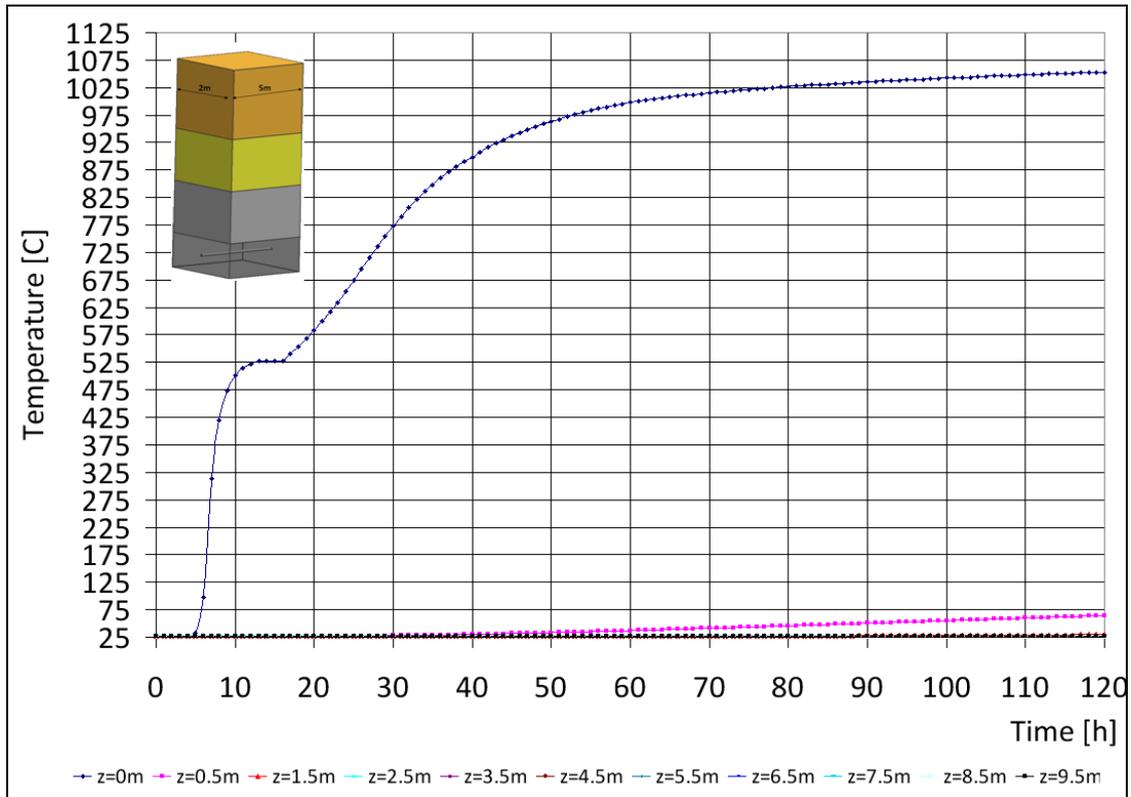


Fig. 11. Change of average temperature in the sandstone, claystone and mudstone layer under the conditions of the UCG process in time interval of 120 hours

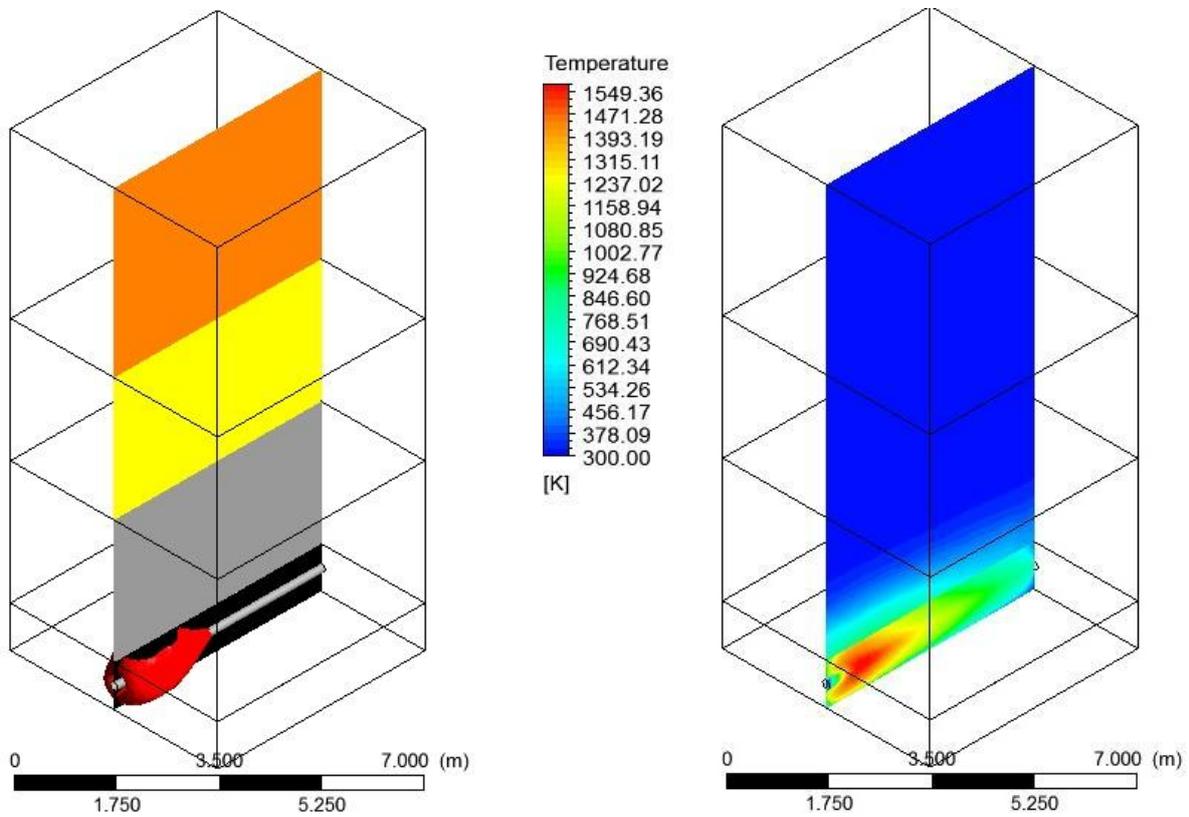


Fig. 12. The shape of the cavity (red area) and change of temperature in a layer of sandstone, claystone and mudstone during UCG after 120 hours

The results of tests showed the possibility to reach the temperature of 1000°C after 120 hours, in a distance of 0.5 metres above the gasification channel. At the height of 1.5 metres the temperature was about 375°C (Fig. 3), for the claystone layer 475°C (Fig. 5), while for the claystone and sandstone layer about 325°C was observed (Fig. 7–9). At the height of 2.5 metres above the gasification channel, in all analysed cases, the same values of temperature of about 75°C were observed. The obtained model results are similar to the results of experimental research presented in work (Stańczyk et al. 2012). According to authors (Stańczyk et al. 2012), in ex-situ conditions of coal gasification processes, with the participation of oxygen and water vapour as the gasification agent, the temperature of about 1200°C at the height of 0.4 metres above the gasification channel was observed, after of 110 hours.

6. SUMMARY AND CONCLUSIONS

The capabilities of Ansys-Design Modeller were used to develop the model of georeactor and rock strata. The next step was to import the geometrical model to the Ansys-Fluent. Based on the geometrical model the discretization area was prepared, which was used to develop a numerical model of UCG.

The research results presented in this work leads to the following conclusions:

1. The applied software turned out to be a tool enabling the creation of models of coal gasification processes occurring in different conditions and, in particular, of the process occurring beneath the ground surface.
2. Due to difficulties arising from the choice of the proper way to implement and carry out coal gasification processes related to the appropriate location in the vicinity of the rock mass, it is justified to predict each time the influence of the adopted solution for the model thermal layout of a georeactor by applying the numerical methods of CFD.

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