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Thermal-Mechanical Modelling around the Cavities of Underground Coal Gasification

Dongmin Yang[1,*], Vasilis Sarhosis[1,*], Yong Sheng[2,#]

[1] Research Fellow, Institute for Resilient Infrastructure, School of Civil Engineering, University of Leeds, UK, d.yang@leeds.ac.uk, v.sarhosis@leeds.ac.uk
[2] Associate Professor, Institute for Resilient Infrastructure, School of Civil Engineering, University of Leeds, UK, y.sheng@leeds.ac.uk

Abstract

Underground coal gasification (UCG) is an efficient method for the conversion of the deep coal resources into energy. This paper is concerned with a feasibility study of the potential of deeply lying coal seams (> 1200 m) for the application of UCG combined with subsequent storage of CO_2 for a site located in Bulgaria. A thermal-mechanical coupled model was developed using the ABAQUS software package to predict the heat transfer, the stress distributions around the UCG and the consequent surface subsidence. Material properties of rocks and coal were obtained from existing literature and geomechanical tests which were carried out on samples derived from the demonstration site in Bulgaria. Three days of gasification has been simulated by assigning a moving heat flux on a cell of 2 m × 2 m × 2 m at a velocity of 2 m/day. Results of temperature and stress distribution showed that the developed numerical model was able to simulate the heat propagation and the stress distribution around cavities under a thermal-mechanical coupled loading during the UCG process. Also, the surface subsidence was found to be 0.08 mm after three days of gasification for the case studied. It is anticipated that the results of this paper can be used for the prediction and optimization of the UCG process in deep coal seams.

Keywords: *Underground coal gasification, thermal-mechanical modelling, finite element method, surface subsidence*.

[#]**Corresponding Author:** Dr. Yong Sheng

1.0 Introduction

Underground coal gasification (UCG) is a process in which coal is converted into product gas without mining by artificially enhancing gas permeability in a section of a coal seam, igniting the coal, partially combusting and gasifying coal by means of injected oxidants, and producing the product gas for cleanup and processing for a variety of end uses. During UCG process, the volume of the cavity increases progressively with coal consumption and thermo-mechanical spalling, if any, from the roof. As the cavity shape is irregular in three dimensions, the flow pattern inside the UCG cavity is highly non-linear.[1] The complexity increases further due to several other processes occurring simultaneously, such as heat transfer by convection and radiation, spalling, water intrusions from surrounding aquifers, several chemical reactions and other geologic aspects.[2] UCG research and industrial scale operations are gathering pace in recent years, with Australia, China, Canada, USA leading the development and several UK sites in preparation for UCG tests.[3] Since UCG process takes place underground it is difficult to use instruments to monitor the entire coal reaction conditions and its effect on the seam and strata. Post-burn drillings into the UCG chambers can provide useful information on operating features such as highest rock temperature and coal reaction temperature.[4, 5] In addition, a number of laboratory tests have been performed in the past to investigate this process.[6, 7] However, experimental tests on UCG are time consuming and expensive. Also, since the

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[*] These two authors contribute equally to this paper.

UCG process involves complex physical and chemical phenomena, such as mass and heat transport, chemical reactions and geo-mechanical behaviour, limited data on cavity growth and the and stress distribution around cavities have been obtained from those tests due to the difficulty of controlling the operating variables. Thus, computational modelling of the UCG process can provide an alternative to achieve a comprehensive and qualitative understanding of such a complex process. Biezen [8] have considered the three dimensional modelling of the UCG process with some simplifications such as the absence of the heat transfer calculation or a constant gasification temperature. Also, Perkins *et al.* [9] developed a one dimensional numerical model to investigate the effects of operating conditions (e.g., temperature, pressure, water influx, gas composition) and coal properties (e.g., thermo-mechanical spalling behaviour, reactivity, composition) on the rate of local cavity growth and the effectiveness of energy utilization. The thermo-mechanical spalling behaviour of coal, the behaviour of the ash and the amount of fixed carbon in coal were found to most affect the cavity growth rate. Yang [10] presented a 3D nonlinear numerical model of UCG with free channel (*i.e.* a channel without solid phases) to study the temperature field, concentration field as well pressure field in the gasification panel. Khadse [11] also developed a model for UCG in which a coupled UCG channel was viewed as similar to a packed bed where coal particles are filled in the reactor and go through the processes of oxidation and gasification. Seifi *et al.* [12] carried a 3D simulation of UCG process to investigate the cavity shapes, temperature variation, product gas composition and flow rates with the consideration of heat and mass transport phenomena in conjunction with chemical reactions. However, the above thermal-mechanical models are focused on the mechanism of UCG cavity growth at small geometric scale without considering any detailed geologic information, faults reaction and surface subsidence.

This study aims at evaluation of the potential of deeply lying coal seams for the development of UCG combined with subsequent storage of CO_2 in the affected areas by utilizing the same borehole infrastructure. The development of a thermal-mechanical coupled model to analyze the heat transfer and stress distribution around the UCG cavities is presented in this paper. During gasification process, the temperature in the reactor can be up to 1200°C. [13] Also, the strength and deformation characteristics of coal and rocks under high temperature are different from those at ambient temperature. Therefore, a coupled thermal-mechanical model is essential for the corresponding analysis of UCG, such as roof deformation and ground subsidence. The computational software ABAQUS [14] is used in which a coupled temperature-displacement procedure is adopted to simultaneously solve the stress/displacement and temperature fields. The heat transfer equations are integrated using a backward-difference scheme, and the coupled system is solved using Newton-Raphson approximation method (ABAQUS, 2010). Cavity shapes and temperature profile in the coal seam during gasification are investigated by assuming the coal consumption at a specific temperature. This paper consists of four sections. The first section describes the geological structure of a Bulgarian coal deposit. The next section provides a description and modelling of the heat propagation and stress distribution around UCG cavities. The third section presents the results of the analysis and discussions. Finally, conclusions and recommendations for future works are presented.

2.0 Geological structure of the Bulgarian site

The geological structure and location of coal seams are essential for the UCG simulation study that aims to analyze the strata deformation under overburden mechanical loading and gasification heating effect. The Bulgarian site is situated is in a geologically complex area with various geological layers, numerous normal faults and few reverse faults. The available coal seams at this area have been estimated to be 36 million tones approximately. Fig. 1 shows the geological West-East cross section of the Bulgarian site. These geological layers have different properties. The geological cross sectional area A, shown with a blue square box in Fig. 1 was selected for the study, because: a) It includes all of the lithologic ages of the site area; b) there is a presence of a fault which dipping angle is 89°; and c) there are different layers of coal seams. A cross section of the study area, 'Section-A', is presented in Fig. 2. In this study, only one coal seam has been adopted for the thermal-mechanical modelling of gasification process. The coal seam is located at about 1,750m below ground. It is approximately 10m thick and 1,000m long. The ignition has been assumed to take place at a distance of 300m from the left hand side of the section. After ignition the gasification point has been assumed to move towards left boundary at a speed of two meters per day for a period of three days. Also, the thickness of the 3D model has been set to be 400m to avoid any significant boundary effects.

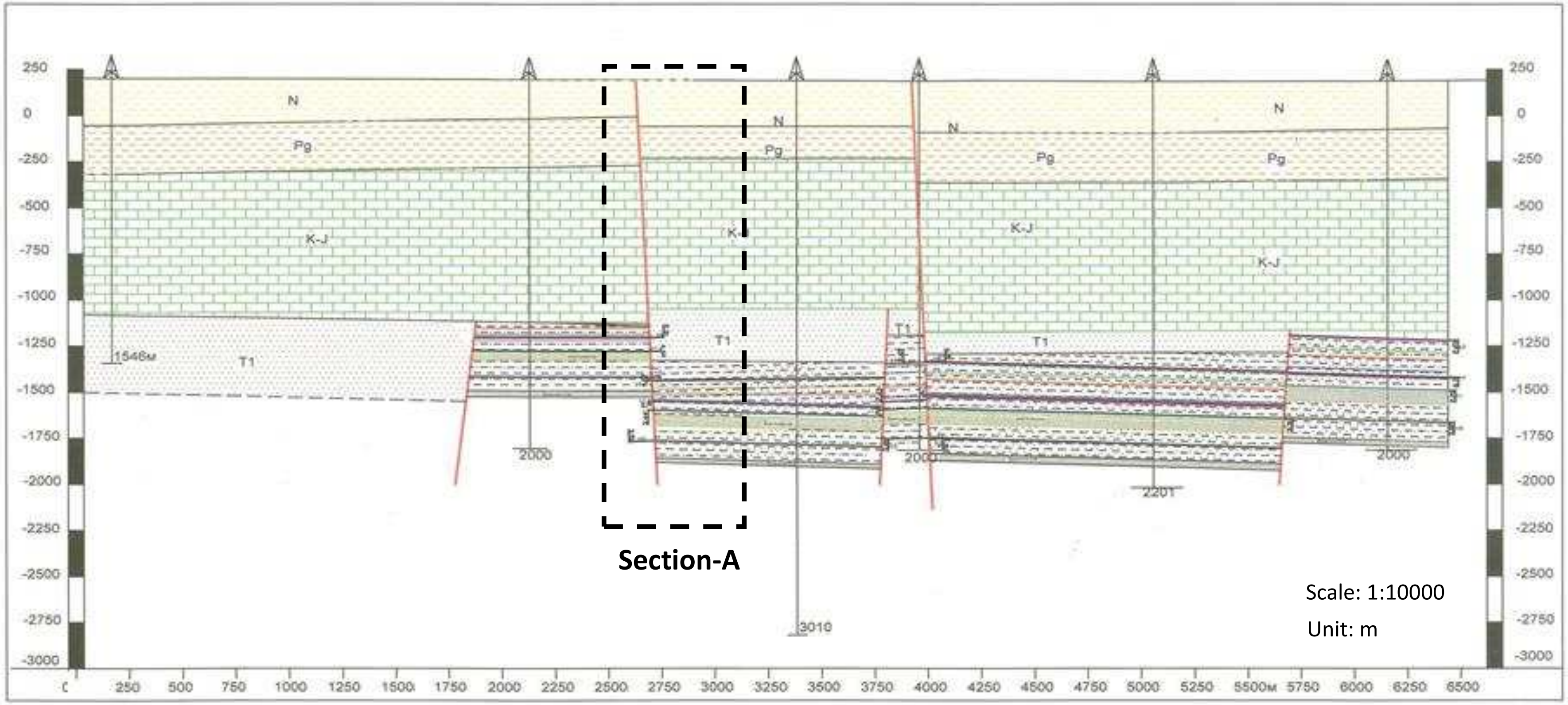

Fig. 1 Geological west-east cross section of the Bulgarian site

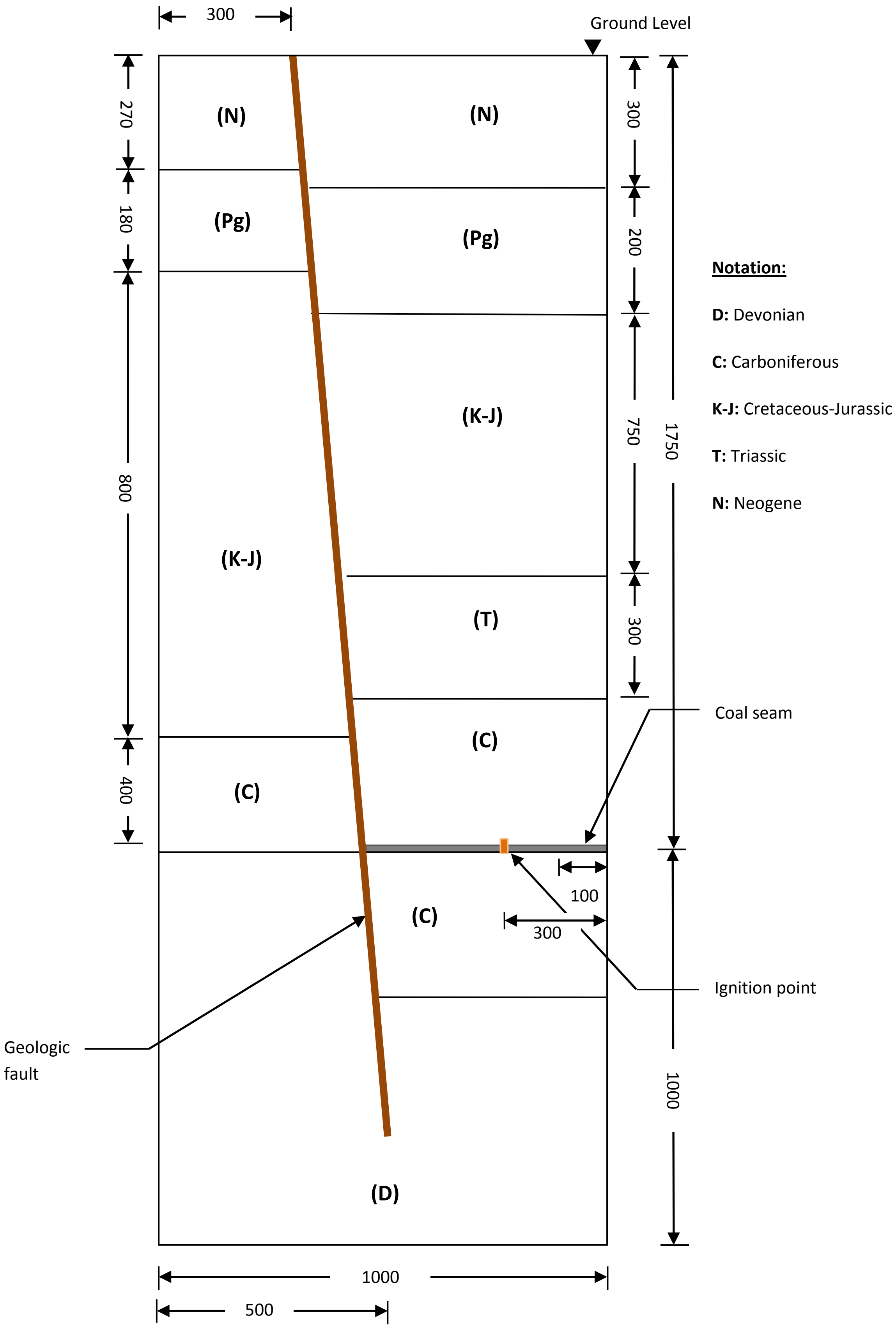

Fig. 2 Geometric coordinates of Section A. (All dimensions are in meters. Not to scale)

3.0 UCG modelling

3.1 Model geometry

A geometric three dimensional model representing the geologic cross section A of the Bulgarian site was created in ABAQUS. Finite element mesh has been generated in the model. Mesh generation plays an important role for accuracy results and economy of computational time. Since very high temperature and stress gradients will occur near the gasification point at the coal seam, a fine mesh has been assigned for the coal layer and a course mesh for the surrounding area. After a series of trail tests, a fine mesh with a size of $2m \times 2m \times 2m$ was chosen for the coal seam. Model using meshes smaller than this size would encounter a severe distortion under the gravitational force of overburden rock with a height of 1750m. Each finite difference element was assumed to behave in a linear elastic manner. The ignition point is positioned 2m above the bed of the coal seam and at a distance of 300m from the left hand side of the model.

3.2 Boundary conditions

The bottom edges of the geological section were fixed in the vertical and horizontal direction while the vertical edges were treated as roller support so that the model is allowed to move only in the vertical direction. The fact that the vertical edges of the model were allowed to move in the vertical direction was to simulate the possible displacement as a result of the faults. Also, the underground temperature has been assumed constant and equal to 10 °C and the temperature at the top surface of the model was assumed to be constant and equal to 20 °C. During UCG process, machinery and pipe networks would be located on top of the site. However, owing to the large depth at which the UCG process is taking place, the effect of surface load has been ignored. Self weight effects of the rocks were assigned as gravitational force according to their densities as listed in Table 1.

3.3 Fault simulation

In ABAQUS model, the fault has been represented as a contact of two surfaces. The normal behaviour of the contact has been simulated using the "hard contact" approach in ABAQUS to restrict the penetration between the two surfaces. [14] Conversely, the tangential behaviour of the fault contact has been simulated using the "frictional" approach, to allow sliding as a result of the self-weight of the rocks. The coefficient of friction assumed to be constant along the length of the fault and equal to 0.2. [15] Also, thermal conductivity was allowed between the two surfaces on each side of the fault to account for the temperature distribution.

3.4 Heat flux at the ignition point

The gasification process has been assumed to last for three days. Experimental combustion testing of coal samples obtained from the coal seam has been carried out at the laboratory of the Centre for Research and Technology Hellas (CERTH). From the experimental testing, the lower heating value (LHV) of the coal was measured to be 25MJ/kg. Also, the energy intake (E) for the coal of volume (V) with a density of (ρ) can be calculated as:

$$E = V \times \rho \times LHV \qquad \text{eq. 1}$$

According to Couch (2009), the gasification progress is between 1m/day to 10m/day, depending on the coal seam thickness. Assuming a reasonable gasification progress to be 2m/day and the total volume gasified per day to be 8m^3, the gasification of this coal will theoretically result in energy of,

$$E = 8\mathrm{m}^3 \times 1500\mathrm{kg/m}^3 \times 25 \times 10^6 \mathrm{J/kg} \\ = 3 \times 10^{11} J \qquad \text{eq. 2}$$

Therefore, the body heat flux (Q) can be calculated as:

$$Q = \frac{E}{T} = \frac{3 \times 10^{11} J}{24 \times 60 \times 60 s} = 3{,}472{,}000 W \qquad \text{eq. 3}$$

It was assumed that when the ignition point starts to move from the first ignition point to the second one, the heat flux of the first ignition point is gradually decreased to half. This is to represent the moving behaviour of the gasification chamber.

Time integration of transient thermal transfer is done using the backward Euler method in the coupled displacement-temperature elements in ABAQUS. Time increment is manually controlled with an initial value of 3,600 seconds (or 1 hour), so as to get the modelling results at every hour during the gasification process. Four numerical steps were used. The first step dealt with the equilibrium of the system due to gravitational forces. The other three steps dealt with the three ignitions.

3.5 Material properties

Different geological ages have different geological layers with different mechanical properties and thermal characteristics. In ABAQUS model, assigning material properties for each geological layer is computationally expensive. So, material properties for each geological age have been taken as the average of the properties of each geologic layer contained according to their thickness. A detailed library of mechanical and thermal properties of the different geological ages is presented at Table 1. Such values obtained from the experimental testing of rock samples taken from the Bulgarian site. Experimental testing has been carried out according to the ASTM Designation D 3148-72 [16] to determine the strength and elastic properties of the rock materials. Also, temperature dependant mechanical properties of rocks and coal have been obtained from the published literature. [17-21] These properties have later been implemented in a tabular format in the numerical model developed with ABAQUS. From the material properties at Table 1, both elastic modulus and strength of the rocks decreases with increase of the temperature.

Table 1 Material properties used for the development of the UCG thermal-mechanical model

Geological age	**Temperature (^{o}C)**	**Density ρ (Kg/m^3)**	**Elastic Modulus E (GPa)**	**Poisson's ratio v**	**Specific heat c (J/(Kg^{o}C)**	**Thermal Conductivity k (W/m ^{o}C)**	**Thermal expansion α (/^{o}C)**
Neogene (N)	0	2440	55.28	0.27	1152	1.84	8.4 x 10^{-6}
	600	2404	14.27	0.27	1664	0.37	1.15 x 10^{-6}
Paleogene (Pg)	0	2471	40.1	0.26	1007	1.96	9.18 x 10^{-6}
	600	2467	10.2	0.26	1343	0.42	0.87 x 10^{-6}
Lower Cretaceous-upper Jurassic (K-J)	0	2350	80.0	0.31	1530	1.60	6.00 x 10^{-6}
	600	2256	35.2	0.31	2540	0.32	2.28 x 10^{-6}
Triassic (T)	0	2350	80.0	0.31	1530	1.6	6.00 x 10^{-6}
	600	2256	24.0	0.31	2540	0.32	2.28 x 10^{-6}
Carboniferous (C)	0	2465	29.9	0.22	1070	2.00	8.40 x 10^{-6}
	600	2465	10.9	0.22	1532	0.50	1.49 x 10^{-6}
Devonian (D)	0	2350	80.0	0.31	1530	1.60	6.00 x 10^{-6}
	600	2256	24.0	0.31	2540	0.32	2.28 x 10^{-6}
Coal	0	1500	4.0	0.3	800	0.27	5 x 10^{-6}
	400	1500	0.12	0.3	1120	0.81	1.5 x 10^{-6}
	1000	750	0.000012	0.3	960	0.025	1.5 x 10^{-6}

4.0 Results and discussion

4.1 Temperature distribution

Figures 4, 5 and 6 respectively show the temperature distributions around the gasification point after every 24 hours during the first three days of the UCG process. From the results analysis, it was found that high temperatures are concentrated at the area surrounding the ignition point owing to the constant heat flux applied at this location. As the ignition point is changing position, the area with high temperature changes accordingly. Also, the thermal affected area increases as the gasification process is taking place. According to Couch [13], coal is gasified at a temperature of approximately 400 ^{0}C or even above, however, to maintain the heat transfer and model integrity, elements with a temperature higher than 400 ^{0}C were allowed to be active. This was implemented to allow the heat to be transferred between finite elements. Also, in order to realistically represent the mechanical failure of coal after gasification, the elastic modulus of coal was assumed to linearly decrease with temperature. The area with gray colour at Figures 3, 4 and 5 represents the estimated evolution of the cavity shape. In order to give a 3D view, X-Y and Y-Z cutting planes were used. In each case the injection point has been located on the intersection of the two cutting planes, and two cutting planes move together with the injection point for each day to produce a symmetric view. From the results analysis, it was found that the shape of the cavity is gradually growing as the injection point is moving place. It is worth mentioning that thickness of the coal gasified for all three days was found to be constant and equal to 6 m. It is anticipated that if a higher value of heat flux is applied at the ignition point, then the thickness of the coal gasified will increase.

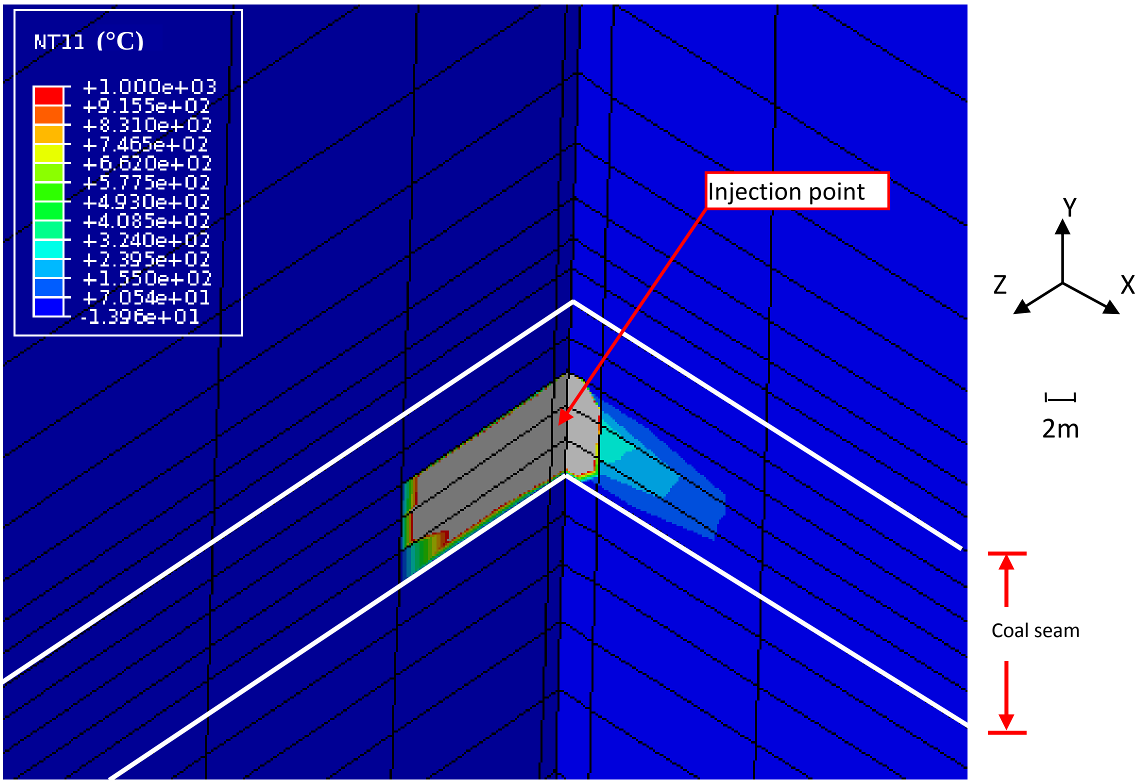

Fig. 3 Temperature distributions obtained from ABAQUS (one day after ignition)

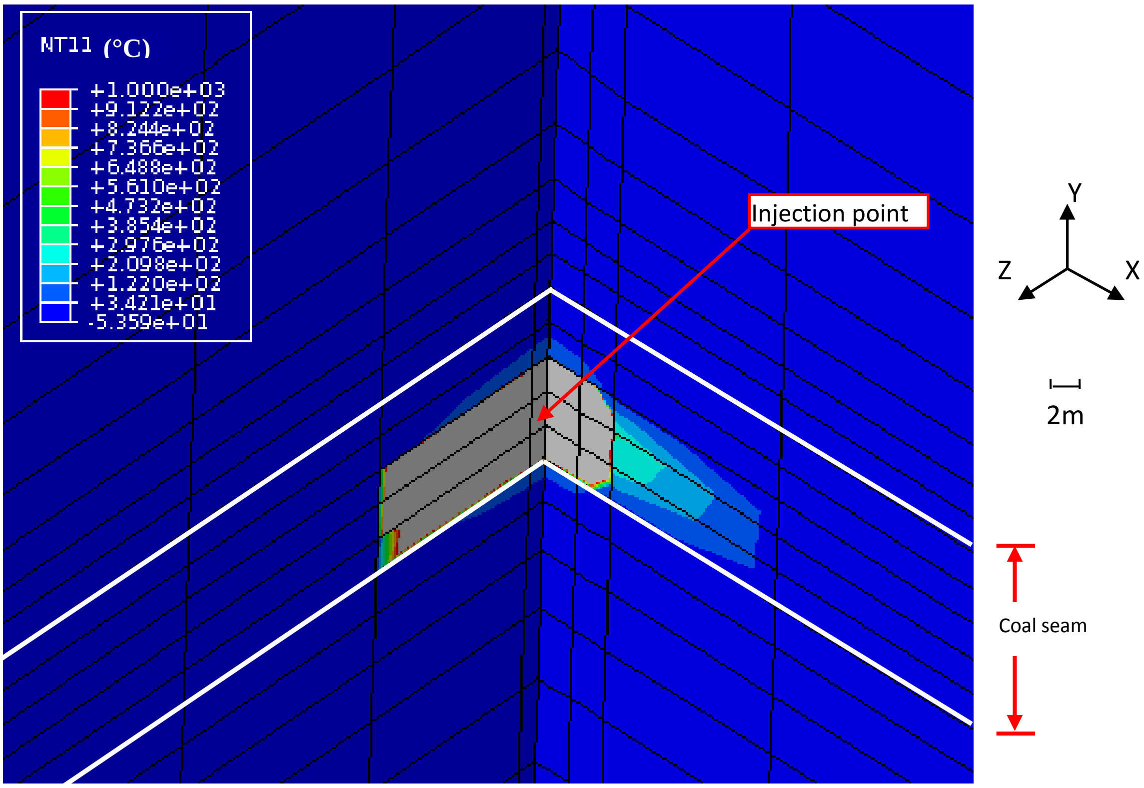

Fig. 4 Temperature distributions obtained from ABAQUS (two days after ignition)

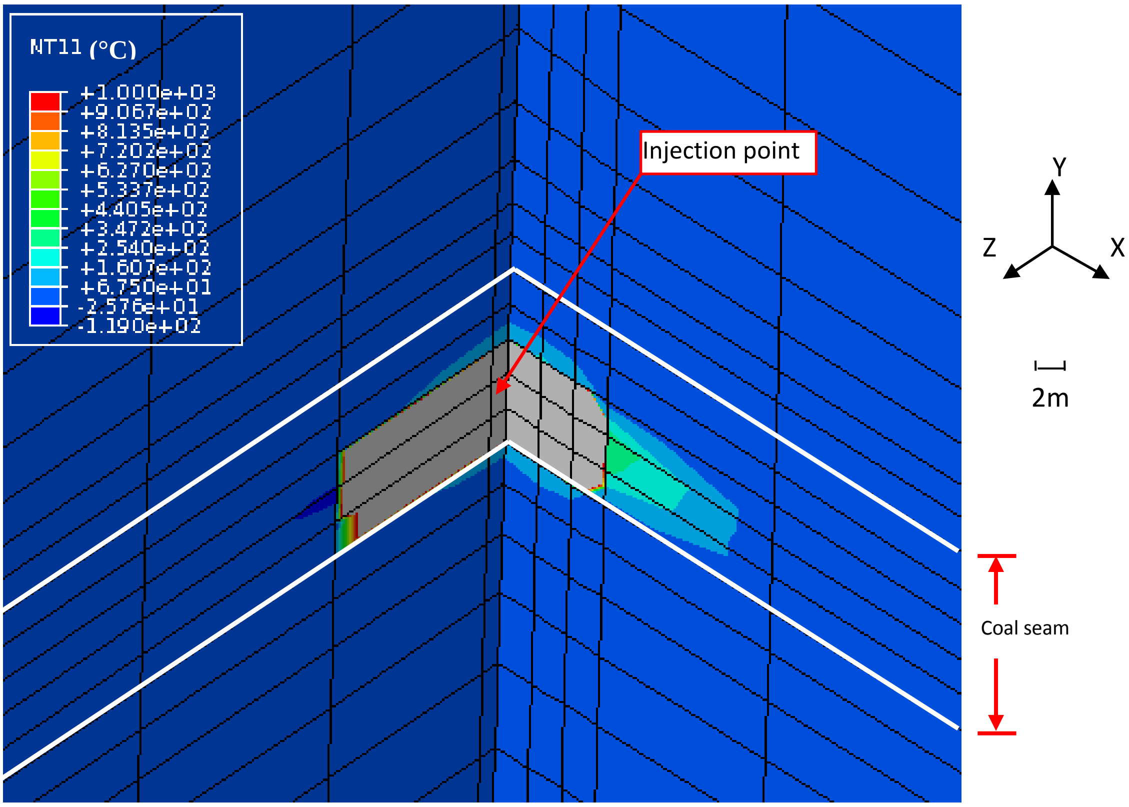

Fig. 5 Temperature distributions obtained from ABAQUS (three days after ignition)

4.2 Vertical displacement distributions

Figures 6, 7 and 8 show the vertical displacement distributions during the three days of gasification. When the first ignition started, the stiffness of the coal and surrounding rock decreased according to the temperature-dependant properties. Under the gravity of the overburden rocks, larger deformation took place in the area surrounding the gasification cavity, particularly above the injection point. The maximum vertical displacement after the first day of gasification has been found to be in the order of 23 mm just above the injection point (Fig. 6). As the UCG process proceeds, displacement increases up to 49mm at the second day (Fig. 7) and 73mm at the end of the third day of the gasification (Fig. 8).

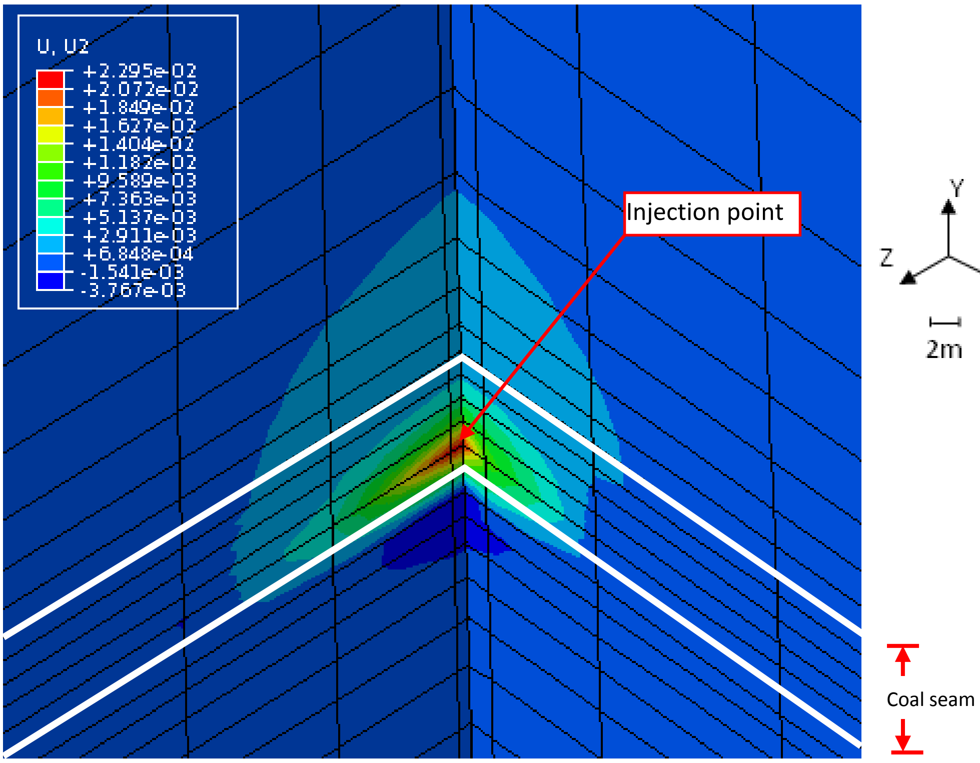

Fig. 6 Vertical displacement U2 (m) after the first day of ignition

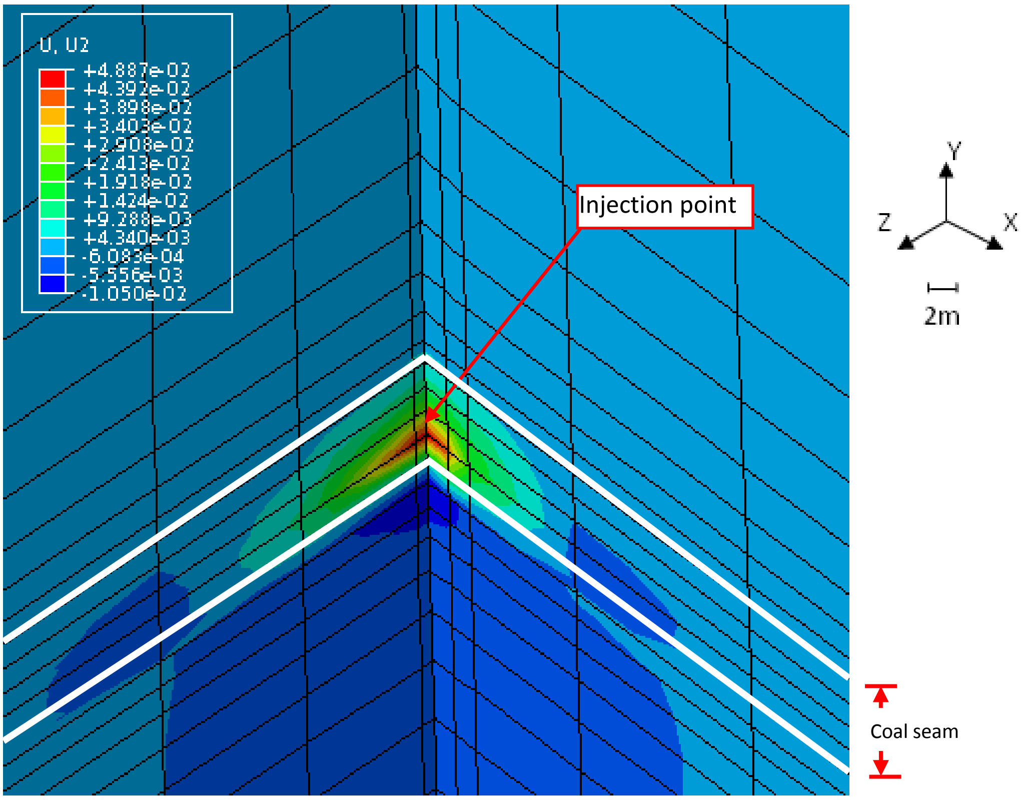

Fig. 7 Vertical displacement U2 (m) after the second day of ignition

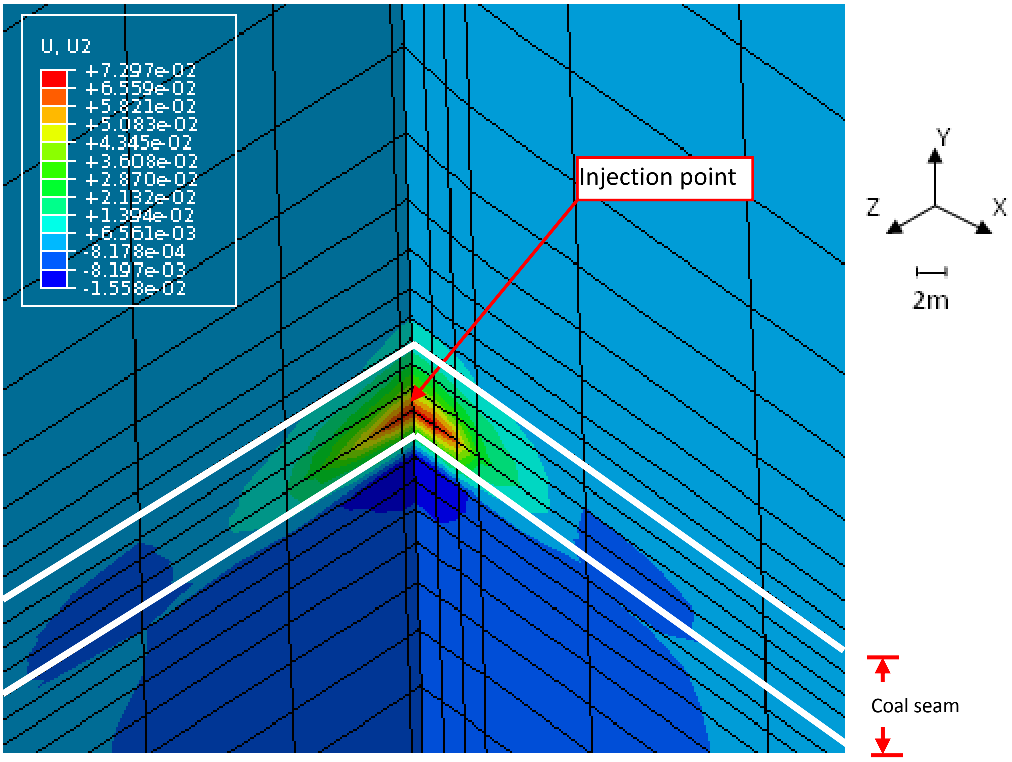

Fig. 8 Vertical displacement U2 (m) after the third day of ignition

4.3 Stress distributions

Figures 9, 10 and 11 show the distribution of stresses under the three ignition points. The nature of the stresses of the overlying from the coal seam formation is very important. The von Mises stress of the overlying from the coal seam is in the order of 20 MPa for the first day of the gasification process (Fig. 9). Also, from the results analysis of the computational model, it was found that as the gasification proceeds there is no significant change of the stresses at the rock layer below the coal seam. The stresses at the layer of rock above the coal seam are in the order of 22 MPa for the second day (Fig. 10) and 24 MPa for the third day (Fig. 11). The dramatic increase of stress in the cap rock is due to the growing cavity below and the heating generated from the coal gasification which makes the rock 'softer' and thus the stress are more concentrated. Also, from the experimental tests on rock samples above the coal seam, it was found that its maximum compressive strength is in the order 40 MPa. The increase in stresses as a result of gasification process indicates that spalling and collapse of the roof strata above the cavity is not likely to be occurring. It is worth noting that fracturing of the formation above an active UCG cavity can: a) provide a passage for gas loss; b) create a connection between the cavity and the overlying aquifers such that water ingress into the cavity increases; and/or create a connection between the cavity and the faults such that synthesis gas can be lost/escape. Also, the type of the rock above the coal seam is very important. For example, some clay rich strata have a self sealing capability, which means fractures will be repaired as the clay naturally swells.

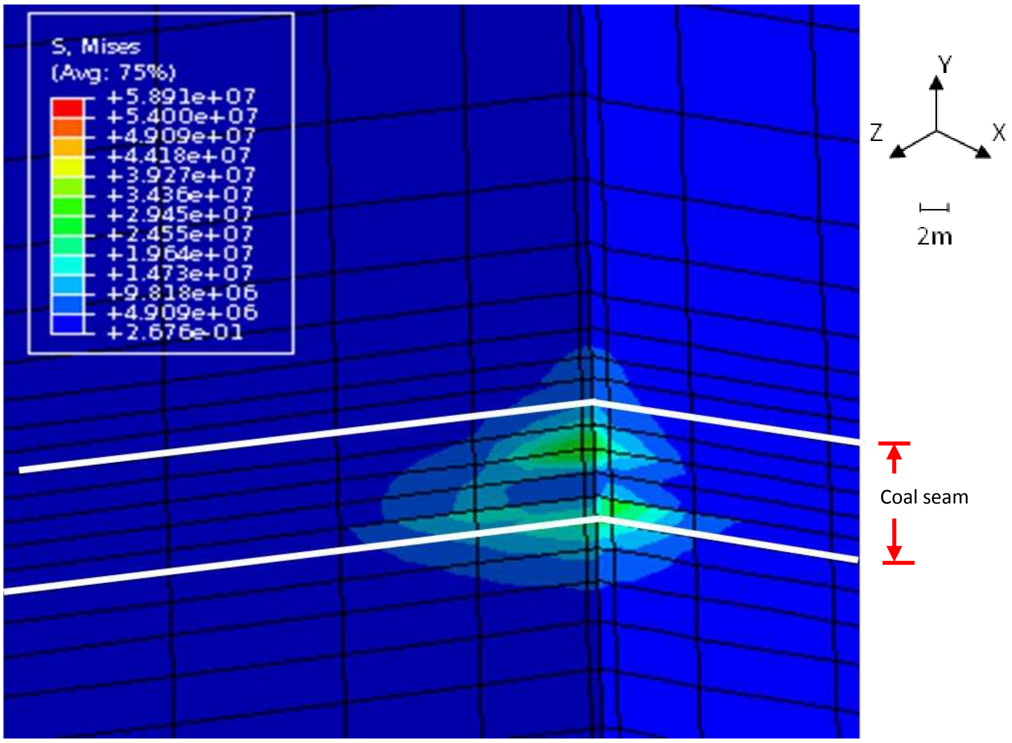

Fig. 9 Stress distributions (Pa) after the third day of ignition

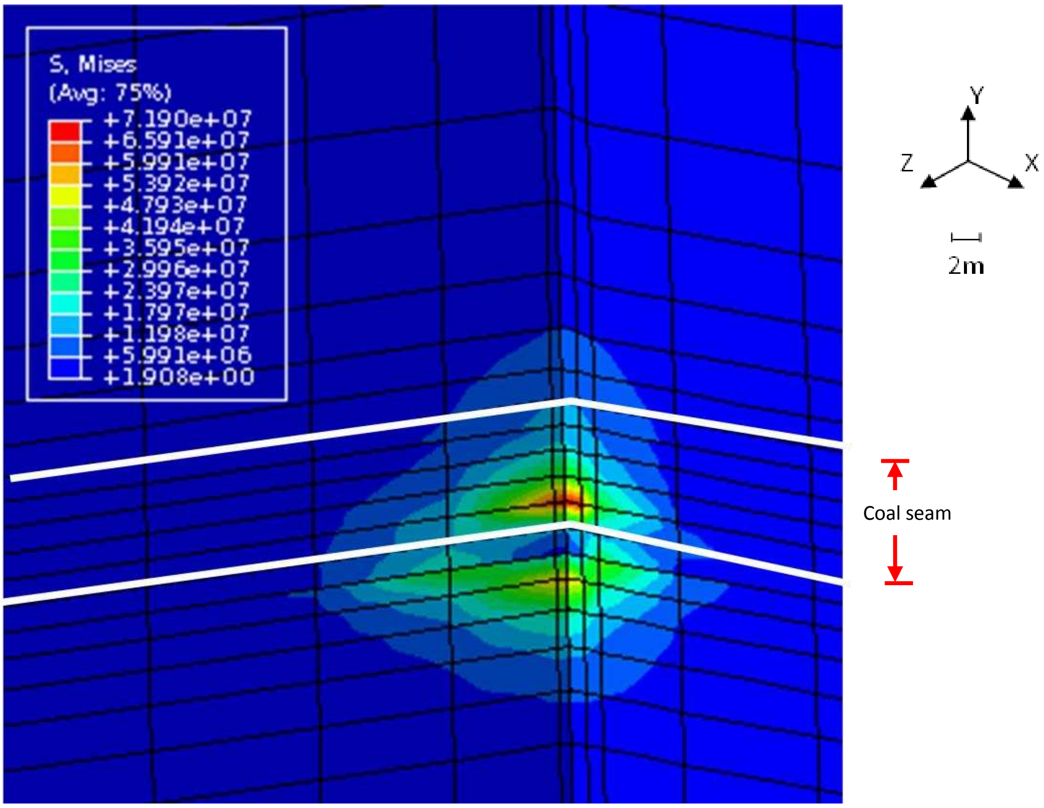

Fig. 10 Stress distributions (Pa) after the third day of ignition

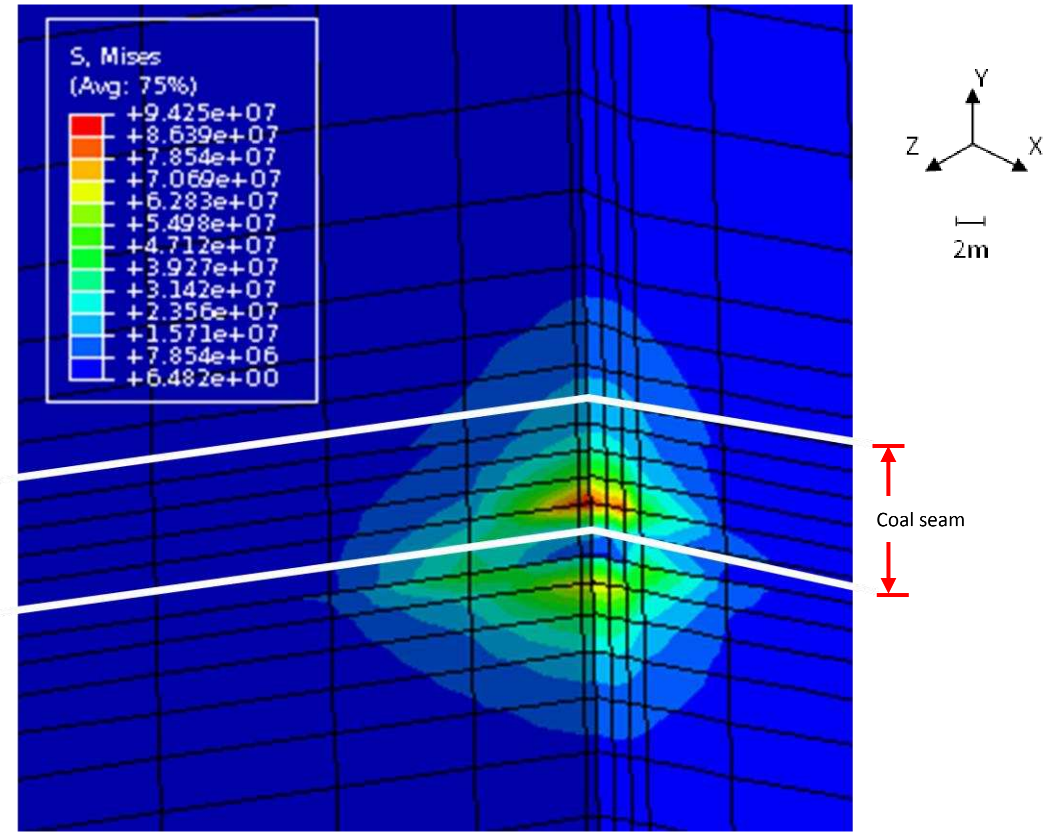

Fig. 11 Stress distributions (Pa) after the third day of ignition

4.4 Surface subsidence

Surface subsidence is a consequence of the cavity growth in the coal seam. During UCG process, a void is created when coal is extracted from the coal seam. This creates stresses and results in a loss of support for the overlying rock formations. Some rock will likely collapse into the void from the roof above the cavity. The factors that influence the stresses developed in the overlying formation, dictating the extent of fracturing and the likelihood of subsidence include: a) the thickness of the coal seam; b) the width, or span of the coal gasified; and c) the depth and strength of the cover (overlying geology). In the ABAQUS model, values of surface subsidence obtained by recording the vertical displacement of the node elements located at the top of the model. The surface subsidence along the Section A after gasification is shown in Fig. 12. Since a geologic fault is included in the model, the subsidence curve is not smooth and there is an obvious jump at the location of the fault. Also, from the results, it was found that as the ignition process is taking place, the surface subsidence is slightly increased. The maximum surface subsidence is approximately 0.025 mm after the first day of the gasification while 0.08 mm after the third day of the gasification.

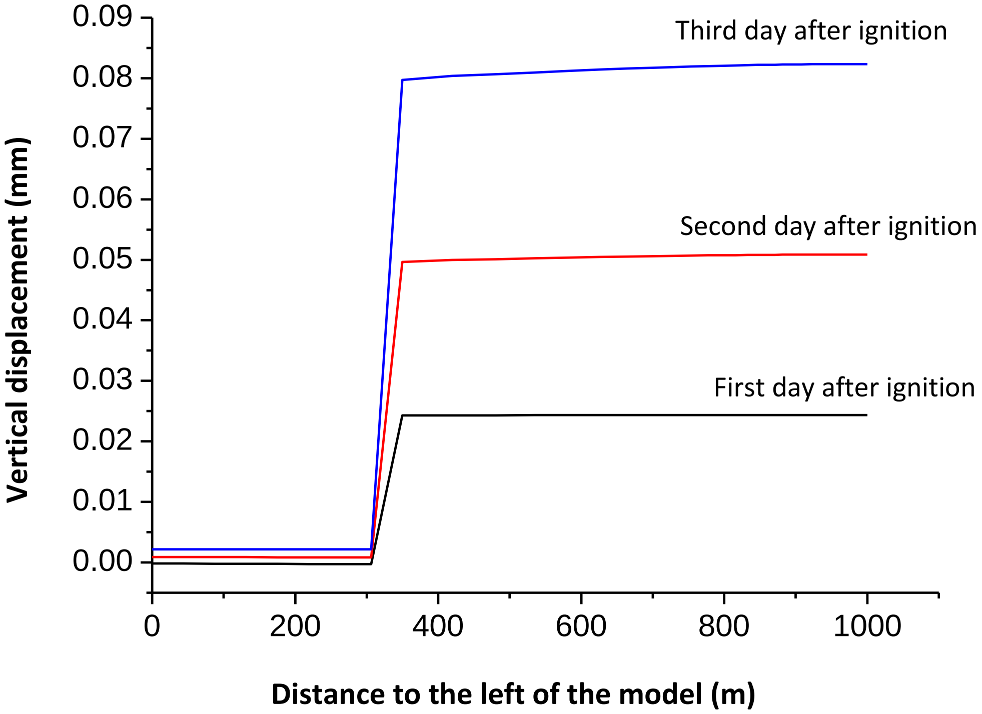

Fig. 12 Surface subsidence across the cross section during UCG for three days

5.0 Conclusions and recommendations

A three dimensional thermal-mechanical modelling around UCG cavities using the computational software ABAQUS has been performed. The model was able to simulate the heat propagation, stress distribution and surface subsidence in UCG process. The proposed method has simplified the modelling of the UCG process and thus only studied the thermo-mechanical behaviour. In reality the chemical reactions, heat and mass transfer, pore pressure, moisture content variations, evaporation, reactor void pressure, water influx and development of cracks affect the total behaviour of a system. Inclusion of pore pressure variation with heat and pressure and the interaction of thermo-mechanical model with process chemical model will be very challenging, but will provide more realistic insights of UCG cavity growth than any existing numerical models. Although simplifying some parts of the UCG process may affect the final outcome, the results of this study have shown that the proposed thermal-mechanical model is capable to be used for future preliminary studies which aim to simulate the UCG process at full scale geological formations. The stress concentration above the coal seam has not increased significantly, around 10%, as a result of the cavity generated during the gasification process. The amount of surface subsidence as a result of the cavity generated during UCG process is negligible for the case studied in this paper. In the future work, the 3D ABAQUS model will be further improved by incorporating the faults distribution surrounding the studied coal deposit in Bulgaria so as to assess the risk of synthesis gas leakage though the geological faults. In addition, detailed knowledge of the hydrogeology of the overlying formations is necessary to make an informed decision about the risks of fracturing on aquifers and forming connections to overlying rocks.

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