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THE NUMERICAL SIMULATION OF A SUDDEN INFLOW OF METHANE INTO THE END SEGMENT OF A LONGWALL WITH Y-TYPE VENTILATION SYSTEM**SYMULACJA NUMERYCZNA NAGLEGO DOPŁYWU METANU DO KOŃCOWEGO ODCINKA ŚCIANY WYDOBYWCZEJ PRZEWIETRZANEJ W SYSTEMIE NA Y**

Present paper is an analysis of the propagation of methane in the end segment of a longwall ventilated by means of the Y-type ventilation system. The propagation in question occurs as a result of sudden inflows of methane from the adjacent goaf. Relevant simulations for multiple variants were carried out using the Finite Volume Method. As part of the process of verifying the adopted numerical methods, the simulation of the stationary propagation of methane under conditions corresponding to in-situ measurements, and in relation to the end segment of the CW-4 longwall in the „Budryk” colliery, was carried out. The dimensions adopted were consistent with the data obtained in the course of in-situ measurements. The model encompassed eight sections of a powered roof support, a segment of a temporary support, and a fragment of the CW-4 heading. The distributions of velocity for the SST $k-\omega$ and SAS turbulence models were compared with the data from the in-situ measurements. The highest compatibility with the results of the flow velocity measurements was demonstrated in the case of the SAS model. The verified models were subsequently used in the process of simulating the results of sudden, local methane inflows from the goaf adjacent to the temporary support, as well as from underneath the shield of the fifth section. The simulation results were presented as a sequence of methane concentration distributions, on selected internal surfaces of the computational domain.

Keywords: methane hazard, longwall, Scale Adaptive Simulation

Rozpatrywano zagadnienie propagacji metanu w końcowym odcinku ściany przewietrzanej w systemie na Y wywołanej przez nagłe dopływy od strony zrobów. Przeprowadzono wielowariantowe symulacje wykorzystując metodę objętości skończonej. W ramach weryfikacji użytych metod numerycznych przeprowadzono symulację stacjonarnego rozprzysku metanu dla warunków odpowiadających pomiarom *in-situ*, w odniesieniu do końcowego odcinka ściany CW-4 z KWK Budryk. Przyjęto wymiary zgodne z danymi z pomiarów *in-situ*. Model składał się ośmiu sekcji obudowy zmechanizowanej, odcinka w obudowie doraźnej, oraz fragmentu chodnika CW-4. Porównano rozkłady prędkości dla modeli turbulencji $k-\omega$ SST i SAS z danymi z pomiarów „in-situ”. Najlepszą zgodność z wynikami pomiarów prędkości przepływu otrzymano dla modelu SAS. Zweryfikowane modele użyto do symulacji skutków nagłych

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dopływów metanu od strony zrobów obudowy doraźnej i spod osłony odzawałowej piątej sekcji. Wyniki symulacji przedstawiono w postaci sekwencji rozkładów stężeń metanu na wybranych przekrojach obszaru obliczeniowego.

Słowa kluczowe: zagrożenie metanowe, ściana wydobywcza, symulacja z adaptacją skali

1. Introduction

Inflows of methane from goaf are among the ways in which the methane hazard is manifesting (Dziurzyński, 2012; Szlązak, 2012; Skotniczny, 2013). In particular, the problem is connected with sudden outflows of methane. Data concerning such events is scarce, and adequate counter-measures difficult to establish. However, the phenomenon in question can be successfully analyzed by means of computer simulations. The present article discusses cases involving sudden inflows of methane from goaf adjacent to the end segment of a longwall ventilated using the Y-type ventilation system.

Prior to conducting a computer simulation, a researcher has to verify the adopted methods. To this end, data obtained during in-situ measurements, concerning the stationary conditions of methane release, was used. After generating a model consistent with the data from the measurements, two sources of a sudden inflow were analyzed: goaf next to the temporary support of a longwall and the area underneath the shield of the fifth section, counting from the longwall outlet (see Fig. 1). The computations were performed for various turbulence models so that the obtained descriptions could be compared with each other.

At the beginning, the flow of air through the intersection of the longwall and the heading was estimated. Due to the complex structure of the numerical model (which contained a lot of elements influencing the image of the flow), the authors decided to perform the initial computations upon simplified models. As the computations progressed, new elements were gradually introduced into the numerical models. Those elements were supposed to reflect, in the most accurate manner possible, the conditions of the real intersection.

The initial computations were carried out for the simplest model of flow. The operating pressure was given, which corresponded to the conditions in the mine. For the non-stationary gas migration, it was necessary to take into consideration the equations of the transportation of components. This was completed in several stages. After convergence was obtained, a model of the transportation of a gas mixture was introduced. The initial given composition of the mixture corresponded to dry air, without methane. Subsequently, the composition was enriched with steam in such a proportion that the resulting humidity was ca. 90 percent. Thus, humid air free from methane was obtained. After that, some additional computations were carried out, which resulted in generating the initial state.

2. The simulation of the stationary propagation of methane under conditions corresponding to in-situ measurements

Based on the documentation and data obtained in the course of measurements performed in the CW-4 longwall of the „Budryk” colliery, a series of multiple variation simulations was carried out. The result was the creation of the final model of the end segment of the longwall and tailgate, whose geometry is presented in Figure 1. In the Y type ventilation system tailgate has

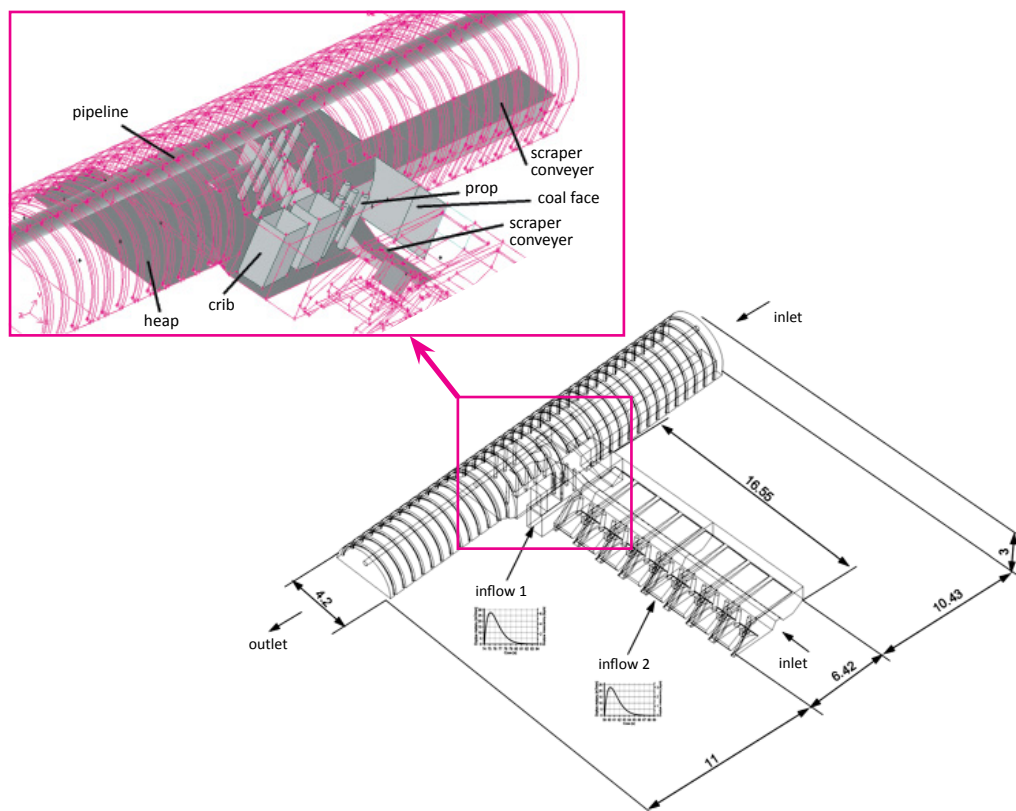


Fig. 1. The intersection of the CW-4 longwalls – a model

two sections: one along unmined coal and the other along goaf, starting at intersection with the longwall outlet. The part adjacent to coal seam provides additional fresh air to dilute methane exhausted from the longwall.

The adopted dimensions corresponded to the data from in-situ measurements. The model encompassed eight sections of a powered roof support, a 2.15 m long segment of a temporary support, and a fragment of the CW-4 heading. The description of the heading took into account the 10.43 m long segment next to the unexploited seam, the intersection 6.42 m long with the longwall, and the 9.97 m long segment adjacent to goaf.

In the segment through which the fresh air was supplied, the height of the heading was 3 m, and its width – 4.2 m. In the heading, a scraper conveyor was placed. The area of the cross-section of the heading was 11 m². It was assumed that 582 m³ of methane-free air was supplied through the heading per one minute, which gives us the mean velocity of 0.98 m/s. The flow rate corresponded to the results of velocity traversing in the heading. The velocity distributions and turbulence parameters at the inlet of the modeled heading were calculated by means of generating a developed flow profile, which was done with the computations performed on the auxiliary model. At the intersection, there is a transfer station and the propulsion of a longwall conveyor – both being major obstacles to the flow. Additionally, the presence of props was taken into account. In the intersection area, the

floor of the heading rises progressively, creating a heap. Its height decreases from 3 to 2 meters. The cross-section of the further part of the heading, in the considered model, is smaller ($6,53 \text{ m}^2$).

The height of the longwall was 1.55 m, and the area of its cross section was 7.5 m^2 . The total length of the eight sections was 14.4 m, and the whole analyzed longwall segment was 16.55 m long. In the sections adjacent to the inlet and outlet powered roof support is not used. Instead a temporary support is made of wood and steel beams supported by props. The position of the props was adjusted so that it corresponded to the information provided by notes and photographs. The arches of tailgate adjacent to goaf are supported by cribs evenly spaced at the goaf border. The space between the cribs was described as a permeable porous partition.

A three-dimensional model of the intersection was meshed by means of an unstructured tetrahedral grid, which was subsequently converted to a polyhedral grid. The initial flow calculations, performed for the segment comprising eight sections of the support, made it possible to generate the boundary conditions at the model inlet. As a result, the calculated and the measured velocity distribution proved to be highly consistent.

As the velocity distribution was given, it was possible to calculate the volumetric flow rate of the air flowing through the longwall. The obtained value was 792 m^3 per minute, which gives us the mean velocity of 1.62 m/s. Particularly high compatibility of the calculated and measured velocities concerned the SAS model.

For the sake of numerical simulations, during the initial calculations, the classic $k-\varepsilon$ model was used. In the final calculations, the $k-\omega$ SST (Ansys, 2013) turbulence models, as well as a scale-adaptive method (SAS – Menter, 2012) were adopted. The SAS model involves a hybrid approach, which provides exact and simplified descriptions suited to the scale of given phenomena. If a grid is thick enough, the model allows quite accurate simulations of vortex structures (which are responsible for the phenomenon of the turbulent diffusion) and can be used in modeling flows characterized by strong reverse pressure gradients and separation of the boundary layer.

The measured field of methane concentrations was diversified only to a minor extent, and thus it was difficult to observe any regularities in its distribution. Therefore, a homogenous mean concentration of 0.38% was given at the inlet. The field of methane concentrations starts to demonstrate signs of diversification in the spot where the stream of the ventilating air and the stream flowing out of the longwall are combined. At the intersection and at the further segment of the CW-4 heading, there runs a stream of mixed air and methane, which is a case of a jet in a crossflow (Galeazzo, 2013), initially containing just air.

For the final intersection model, a non-stationary description was adopted, which – for each of the considered turbulence models – required generating the initial state by means of performing unsteady flow calculations lasting several flow passage times, in the segment considered. The flow occurs alongside two routes – from the longwall inlet and from the heading inlet. For the first route, along the segment in the longwall, the velocity inside the stream was ca. 3 m/s. Further, in the CW-4 heading, along goaf, the velocity values would sometimes reach 6 m/s. The total flow time is ca. 9 seconds. The flow along the other of the two routes, i.e. from the inlet of the longwall, was 25 seconds, and the velocity of the ventilating air current was 0.6 m/s. However, this low-speed segment was characterized by the absence of methane, which is why the first estimation was taken into account. As a result, the initial stationary propagation was calculated for the duration of at least eight flow times passage (more than two for each estimation). The initial states were characterized by velocity zones and methane concentration fields that were changeable in time, but different for each particular description. The nature of this changeability could be compared to quasi-periodical or chaotic oscillations typical of the turbulent flow.

2.1. Comparing the velocity and concentration distributions for the considered turbulence models, using data obtained during in-situ measurements

In order to verify the model of the longwall segment, the results of the in-situ measurements, carried out at the CW-4 longwall of the „Budryk” colliery, were used. The measurements made it possible to determine the boundary conditions for the simulations, in particular – the flow rates in the CW-4 heading and the velocity field in the longwall. The latter was determined by means of the multi-point system for methane velocity and concentration measurement developed at the Strata Mechanics Research Institute (Dziurzyński et al., 2012). The system encompasses methane-anemometric sensors that register (pointwise) the flow velocity and methane concentration. The sensors are hanged on a truss spragged across the cross-section (Fig. 2). So far, the system has been used to perform simultaneous multi-point measurements in cross-cuts of galleries. Here, it has been used for the first time to perform measurements in a cross-cut of a longwall. The measuring spot was at the fourth section, counting from the longwall outlet. The adopted arrangement made it possible to conduct the measurements in one point behind the hydraulic supports, in a passage used by humans and in one measurement line, above the scraper conveyor (Fig. 3). In this longwall the roof support sections were not equipped with a movable lid – a segment of the roof at the unmined body of coal was not propped by anything. The roof could collapse which would destroy measuring probes. Pieces of coal separating from the coal face are another threat. Thus, the sensors had to be placed at a safe distance from those surfaces.



Fig. 2. The discussed section with visible sensors of the multi-point system for methane velocity and concentration measurements

The obtained velocity field and concentration field were subsequently compared with the simulation results. First, the geometry of the area was developed. Then, the results were compared for two turbulence models: the $k-\omega$ SST and SAS models.

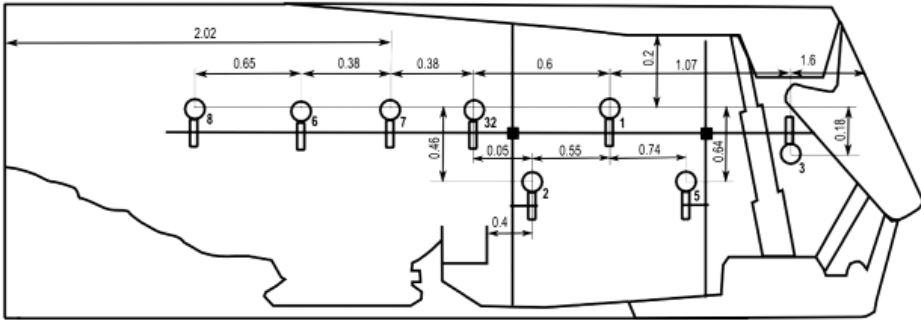


Fig. 3. The arrangement of methane-anemometers in the longwall cut (dimensions given in meters)

The results were presented in the form of a table (Table 1, Table 2).

The SAS model ensures a higher compatibility with the results of the flow rate measurements. The biggest registered difference in readings between an anemometer and the calculation results concerns anemometer no. 32, placed above the cable channel. The difference is 0.52 m/s. In the case of the $k-\omega$ SST turbulence model, the biggest registered difference is much higher: it is 1 m/s, and it concerns anemometer no. 5

TABLE 1

Comparing the readings of the anemometric sensors with the values calculated using the $k-\omega$ SST turbulence model

Sensor no.	Measured values, flow rate [m/s]	Calculated values, flow rate [m/s]	Difference
1	1,71	1,01	-0,70
2	2,49	3,06	0,57
3	0,55	0,61	0,06
5	1,51	0,51	-1,00
6	2,70	2,89	0,19
7	2,59	2,85	0,26
8	2,94	3,06	0,12
32	1,88	2,53	0,6

TABLE 2

Comparing the readings of the anemometric sensors with the values calculated using the SAS turbulence model

Sensor no.	Measured values, flow rate [m/s]	Calculated values, flow rate [m/s]	Difference
1	1,71	1,30	-0,41
2	2,49	2,91	0,42
3	0,55	0,65	0,11
5	1,51	1,03	-0,48
6	2,70	2,79	0,09
7	2,59	2,81	0,22
8	2,94	2,93	-0,01
32	1,88	2,40	0,52

2.2. A sudden inflow of methane from goaf adjacent to the temporary support

It was assumed that goaf gases, whose concentration was 8.27%, flowed along a rectangular 1.6 m² surface from the point where the longwall goaf bordered the temporary roof support. In accordance with the information found in relevant sources (McPherson, 1995), it was assumed that the variability course of the inflow stream was that of strongly suppressed oscillations (Fig. 4). At the maximum flow, the mean velocity at the goaf borderline would reach the value of ca. 0.3 m/s. In the first variation, a 6 second period and amplitude 27 m³/min were considered. The impulse would occur when a stationary inflow of methane of the concentration of 0.38%, corresponding to the real conditions, took place. The inflow would start at the inlet of the longwall.

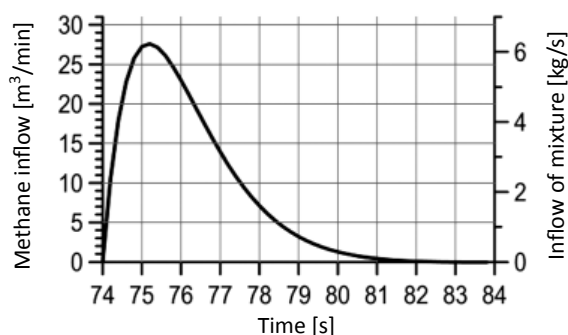


Fig. 4. A sudden inflow of methane from the goaf bordering the temporary roof support

Before the transient states were computed, initial calculations concerning the steady state for the maximum inflow value had been carried out. In this way, a potential range of the stream of the inflowing gases was estimated, and the sensitivity of the solution to the inflow intensity was checked.

2.2.1. Calculating the steady state for the maximum stream of goaf gases

Prior to calculating the transient states induced by a sudden inflow of methane, an initial estimation of the inflow impact zone had been performed. This was done by calculating a particular case of the steady flow. The starting point was to provide a solution for the non-stationary flow with a constant inflow of methane. In the simulation software, the numerical model was replaced with the stationary one. The maximum inflow value (i.e. the local inflow – 27 m³/min 8,27% CH₄), from a chosen surface (where the goaf bordered the temporary roof support), was given. Then, the new state of equilibrium was calculated. Such calculations were performed for both the k - ϵ model and the k - ω SST model. It was impossible to perform such an estimation for the SAS model, as this model, by definition, describes processes that are changeable in time. Concentration fields of methane, for the steady maximum inflow, are shown in Fig. 5 (the k - ϵ model) and Fig. 6 (the k - ω SST model). It was decided that the concentration distributions of methane (volume shares expressed as %), for selected internal surfaces, would be depicted against the outline of the computational area. Horizontal sectional views of both the longwall and the tailgate were selected, as well as the following vertical sectional views: the one of the longwall, of the intersection inlet, and the heading next to the goaf.

The inflow of methane resulted in the change in pressure distributions. In the area of the inflow, overpressure could be observed. The stream that carried gases from goaf narrowed down the main flow in the longwall, in a fashion typical of a jet in a crossflow.

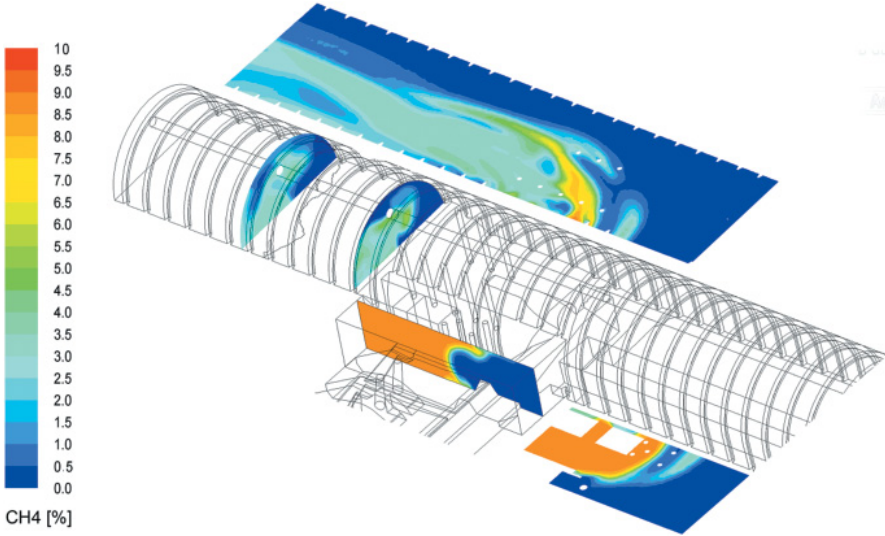


Fig. 5. The stationary field of methane concentrations for the steady maximum inflow of 27 m³/min – the $k-\epsilon$ model

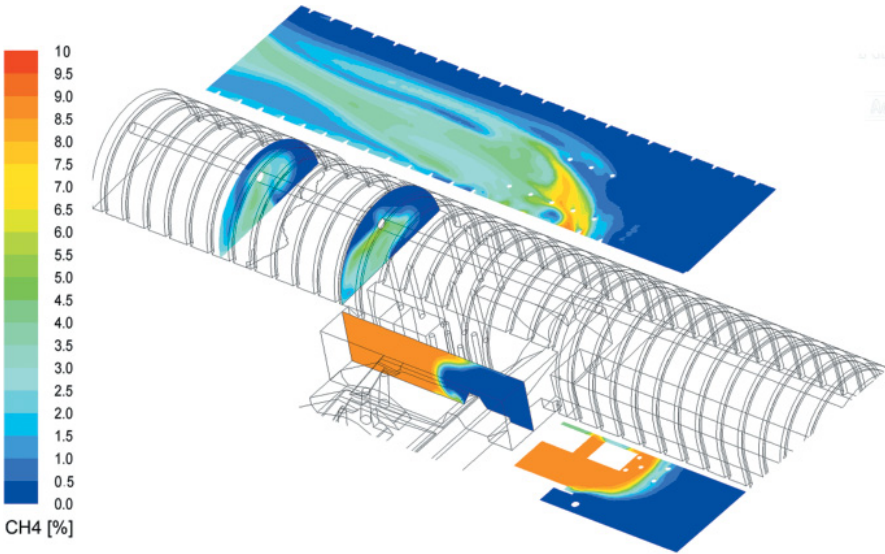


Fig. 6. The stationary field of methane concentrations for the steady maximum inflow of 27 m³/min – the $k-\omega$ SST model

2.2.2. Calculating the impact of a sudden methane inflow for the $k-\omega$ SST turbulence model

The inflow resulted in a change in the distribution of pressures in the model, just like in the stationary case. In the area of the inflow, overpressure was observed. As the intensity of the inflow increased, a stream would form in the cavity, and it started to change the initial state of the flow. The stream that carried the goaf gases narrowed down the main flow in the longwall. It can be seen in the graphic representations of the distributions of methane concentrations – for the initial state and for the consecutive flow stages.

In the cavity, next to the cribs, a cloud of methane appeared, expanding from the goaf towards the passage used by humans. The structure of the cloud was diluted by the system of vortices within the cavity. Due to the forces of buoyancy, the concentration values increased together with the altitude. This tendency was coupled with the impact of the vortices, which caused the gas to mix with air. A small amount of gas leaked through the seal between the cribs. After some time, the zone of the increased methane concentration reached the stream flowing in the longwall from the passage used by humans to the longwall outlet, left of the conveyor. As a result, the stream would start to carry away methane. The process of methane propagation is shown in the figures below (Figs 7-11).

At the longwall outlet, the stream that flows through the passage used by humans enters the current of the ventilation air supplied the CW-4 heading. Thus, it is yet another issue of a jet in a crossflow. The current of fresh air gets accelerated locally in the intersection area – this is due to the constraints that narrow down the cross-section: the conveyors, motor, transfer station, and floor elevation (uplift).

The current deflects the stream that carries methane in the direction of the sidewall next to the goaf. The presence of the system of vortices, generated by the constraints enhances the process of mixing the stream. Due to the diversion of the methane stream, the fields of increased

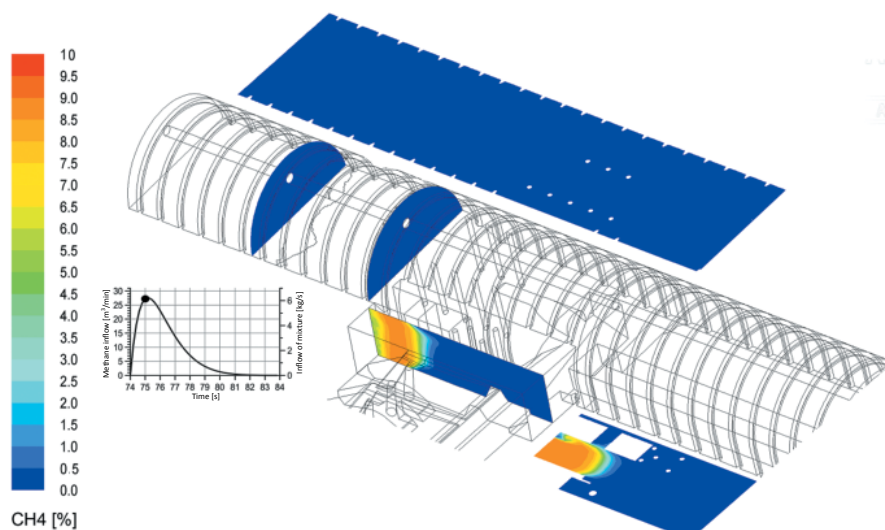


Fig. 7. The field of methane concentrations in the first second of the outflow, the $k-\omega$ SST model

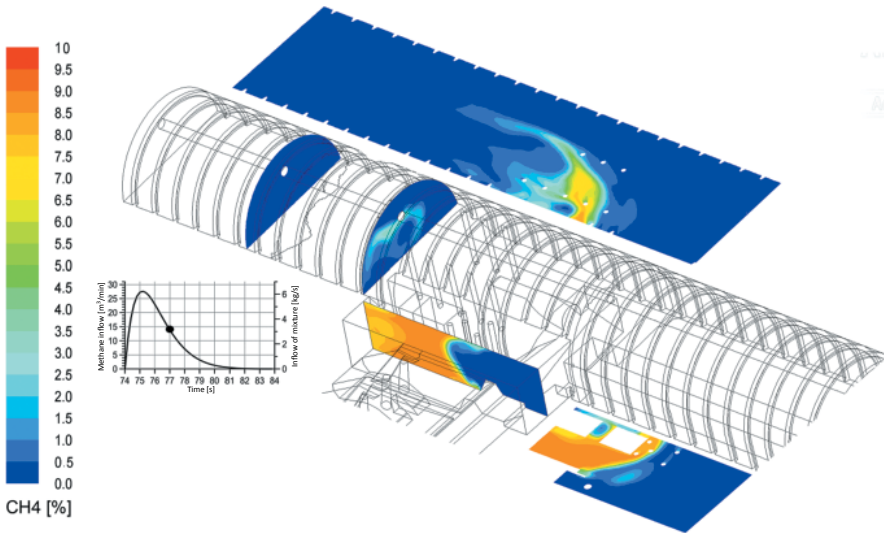


Fig. 8. The field of methane concentrations in the third second of the outflow, the $k-\omega$ SST model

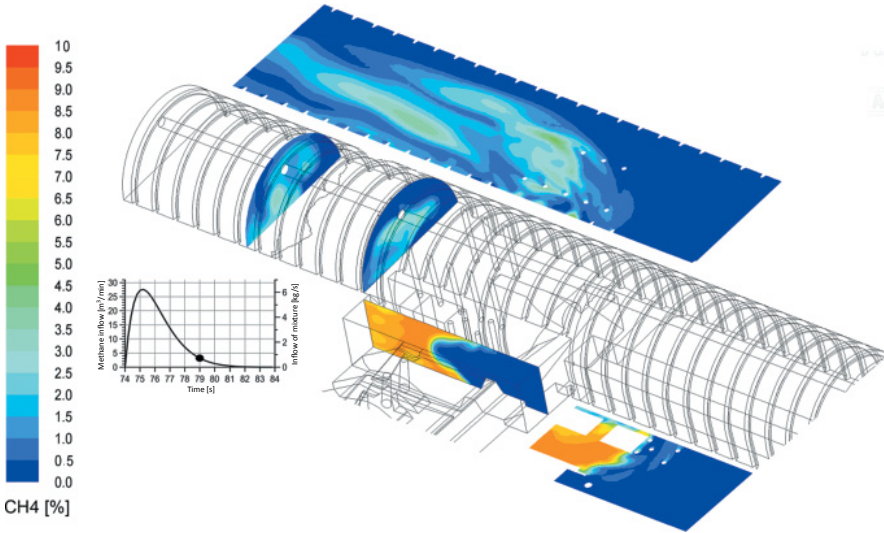


Fig. 9. The field of methane concentrations in the fifth second of the outflow, the $k-\omega$ SST model

methane concentrations – in the segment of the CW-4 heading that is adjacent to the goaf – are moved to the left (looking in the direction of the air current).

The distributions of methane concentrations bear out the validity of the common practice of placing methane sensors at the possibly highest altitude on the left sidewall. The current of fresh air protects the instruments in the initial segment of the intersection and next to the

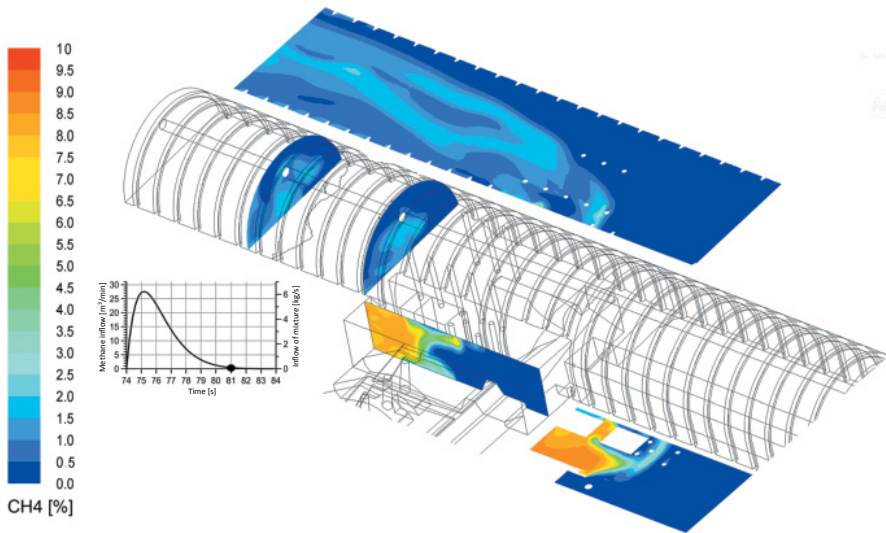


Fig. 10. The field of methane concentrations in the seventh second of the outflow, the $k-\omega$ SST model

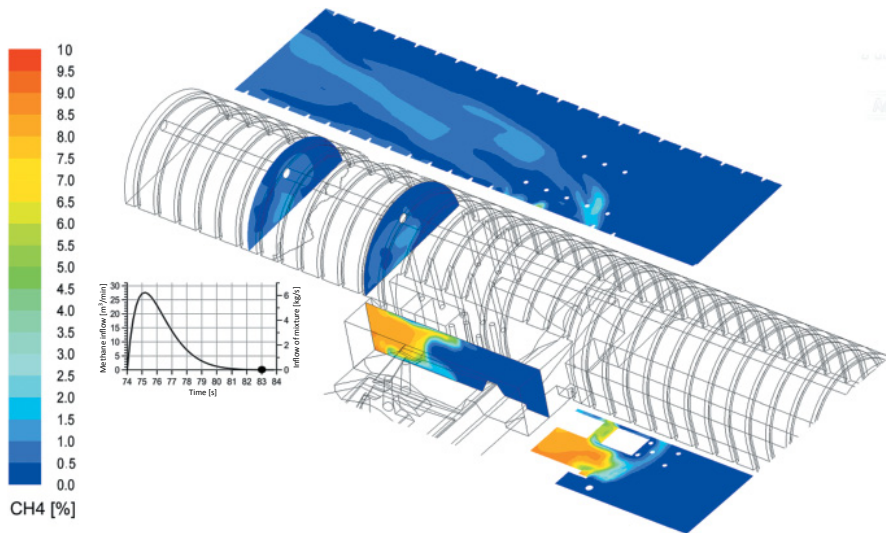


Fig. 11. The field of methane concentrations in the ninth second of the outflow, the $k-\omega$ SST model

right sidewall. However, it can be suspected that, for an outflow from the undisturbed soil, or from underneath the organ of a mining shearer, the stream of methane could reach the right sidewall, too. Thus, placing methane sensors also in this area seems valid. Closer to the outlet, the field of the increased methane concentrations gradually fills in the whole cross-section of the tailgate.

2.3. A sudden inflow of methane from the goaf at the longwall support section

It was assumed that goaf gases of the concentration twice as high as in the case considered in the previous chapter (i.e. 16.53%) flowed the goaf through a rectangular 0.67 m^2 surface from below the shields of the fifth section of the longwall support. In accordance with the information found in relevant sources (McPherson, 1995), it was assumed that the variability course of the inflow stream was that of strongly suppressed oscillations (Fig. 12). The maximum inflow of methane was $23 \text{ m}^3/\text{min}$. The impulse occurred in conditions of stationary inflow of methane of the concentration of 0.38%, calculated in the previous chapter. The mean velocity on the inflow surface would oscillate around the value of ca. 0.7 m/s . Before the transient states were computed, initial calculations concerning the steady state for the maximum inflow value had been carried out. In this way, a potential range of the stream of the inflowing gases was estimated, and the sensitivity of the solution to the inflow intensity was checked.

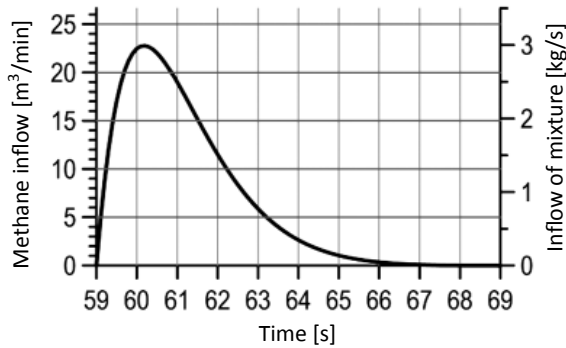


Fig. 12. The course of a sudden inflow of methane

2.3.1. Calculating the steady state for the maximum stream of goaf gases

Just like in the previous case, prior to calculating the transient states induced by a sudden inflow of methane, an initial estimation of the inflow impact zone had been performed. This was done by calculating a particular case of the steady flow. This time, only the $k-\omega$ SST model was considered, as it yields a much more accurate picture of the flow than the $k-\varepsilon$ model. Figure 13 presents the fields of methane concentrations for the state of equilibrium. Again, just like in the previous case, the methane concentration distributions were shown for the horizontal sectional views of both the longwall and the top gate, as well as for the following vertical sectional views: the one of the longwall, the intersection outlet, and the heading next to the goaf. These views were depicted against the outline of the computational area.

In the stationary state, along the segment encompassing the last sections of the powered roof support, the stream fills in the area between the shield and hydraulic supports, and – to a small extent – the passage used by humans. Due to the impact of buoyancy, the stream tends to flow close to the roof. Methane accumulates also in the temporary casing, in an area close

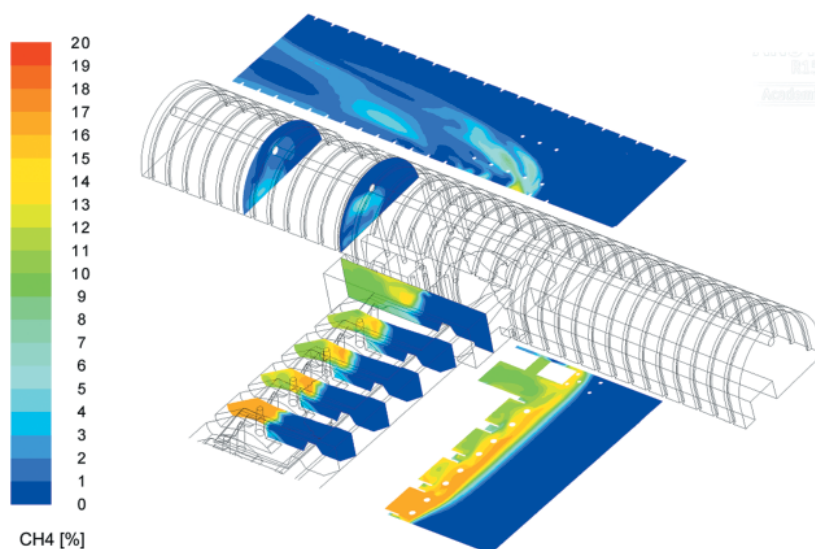


Fig. 13. The stationary field of methane concentrations for the steady maximum inflow of $23 \text{ m}^3/\text{min}$ – the $k-\omega$ SST model

to the longwall goaf – however, the stream does not get any further than to the passage used by humans. At the intersection, as well as in the segment of the CW-4 heading bordering the goaf, the course of the stream is similar to the one calculated for the sake of the previous case.

2.3.2. Calculations for the SAS turbulence model

The process of methane propagation was depicted in the same way as in previous cases (Figs 14 to 18). In the description of the SAS model, the flow tendencies resemble those calculated for the $k-\omega$ SST model. Still, the increased presence of vortex structures results in the expansion of the area threatened with the impact of methane. In the neighboring sections, however, the process of filling in the area behind the hydraulic supports is delayed.

3. Summary

The authors of the paper carried out a simulation of the effects of a sudden outflow of methane from underneath the shield and from the goaf bordering the temporary roof support, in relation to the final segment of the longwall ventilated by means of the Y-type ventilation system (Dziurzyński et al., 2013), corresponding to the CW-4 longwall in the „Budryk” colliery (Fig. 1). The adopted model recreated, in the most accurate manner possible, not only the geometry of the area, but also the flow phenomenon. This was made possible by in-situ measurements, whose results were used in the study. Consecutively, the description of the investigated segment of the powered support and of the intersection with the top gate were perfected (Table 1 and Table 2). The analysis of the data obtained for two different turbulence models proved that it is the SAS

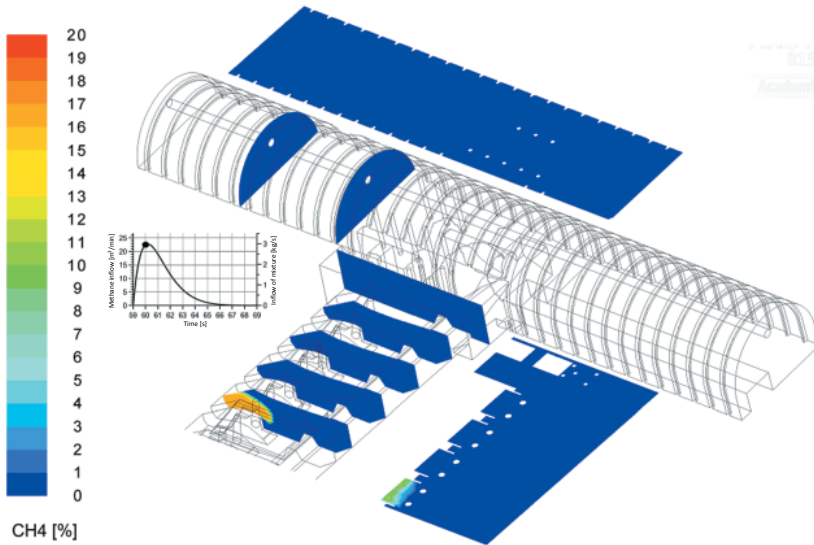


Fig. 14. The field of methane concentrations in the first second of the outflow, the SAS model

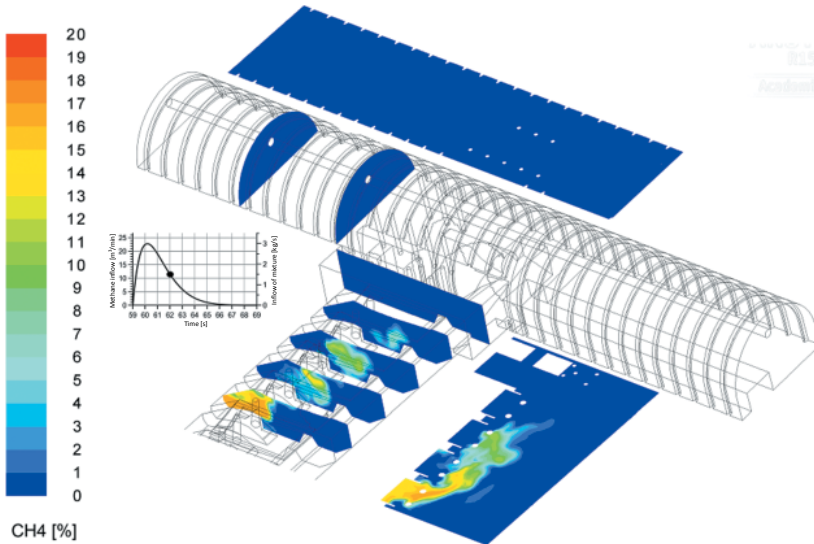


Fig. 15. The field of methane concentrations in the third second of the outflow, the SAS model

model that displays higher compatibility with the results of flow velocity measurements. The verified description was used in the process of performing the simulation of sudden inflows of methane, as well as in the comparative analysis of selected numerical methods. In the initial stages of the computation process, the universal $k-\epsilon$ model was used, thanks to which it was possible to

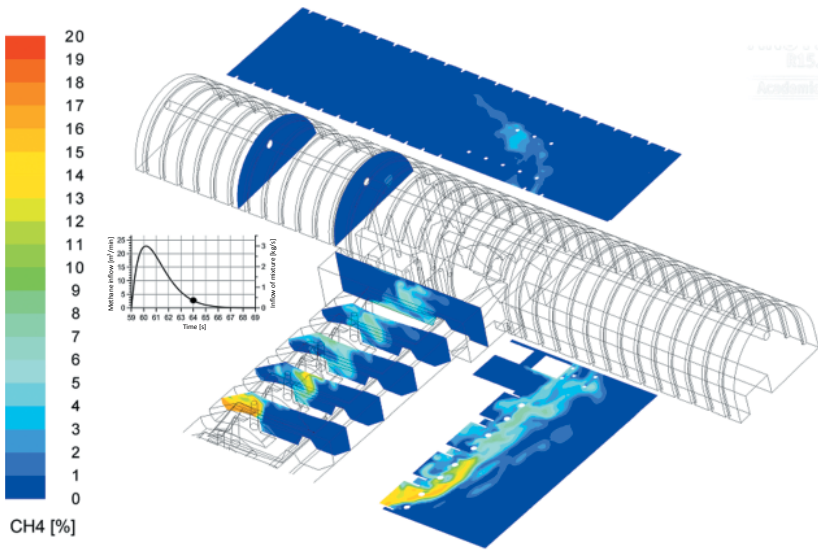


Fig. 16. The field of methane concentrations in the fifth second of the outflow, the SAS model

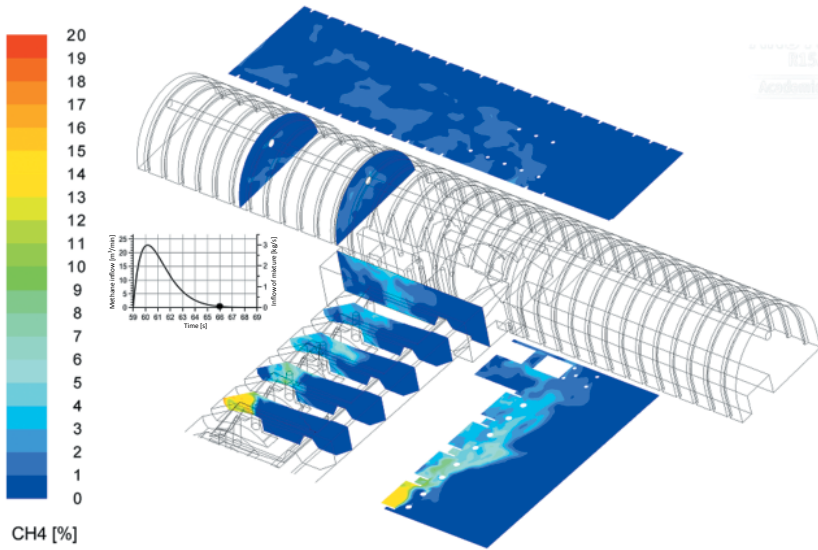


Fig. 17. The field of methane concentrations in the seventh second of the outflow, the SAS model

generate the initial state and create conditions for obtaining convergent and numerically stable solutions with the help of more advanced models.

In these areas of the longwall excavations that are critical from the perspective of safety, the $k-\epsilon$ model does not provide the sufficient accuracy of the description, in particular for the

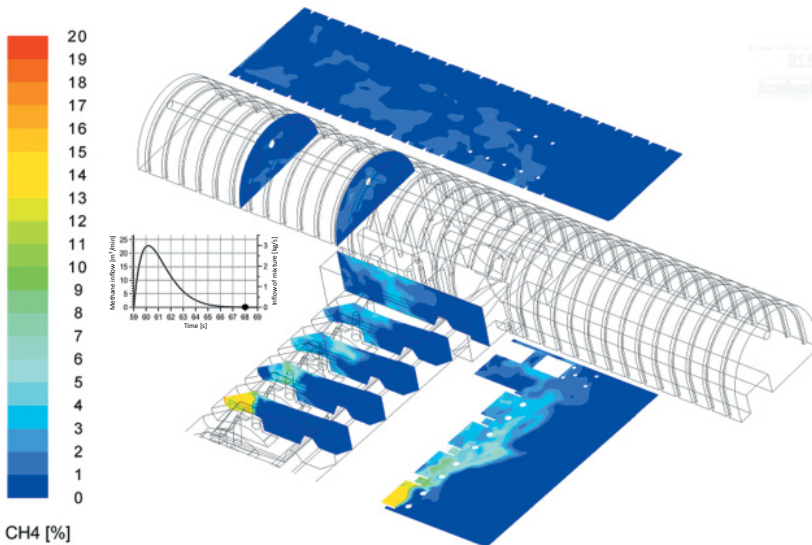


Fig. 18. The field of methane concentrations in the ninth second of the outflow, the SAS model

transient states. This is due to the complicated geometry and the presence of numerous obstacles. Both the scientific sources and the authors' own experiences (some of them were presented in this article) suggest that the $k-\omega$ SST model has an advantage over the $k-\varepsilon$ model. Even better results can be obtained for the two-scale SAS model, which was recently developed with practical applications in mind (i.e., to be used in order to solve flow issues in areas where numerous sources of disturbances can occur, and also in situations where the non-stationary characteristics of the flow have to be represented as accurately as possible).

In the description of the SAS model, the flow tendencies resemble those calculated for the $k-\omega$ SST model. Still, the increased presence of vortex structures results in the expansion of the area threatened with the impact of methane. In the neighbouring sections, however, the process of filling in the area behind the hydraulic supports is delayed.

The 3D description of the neighborhood of the intersection of the longwall and the tailgate, for the Y-type ventilation system, took into account an outflow from the goaf of the temporary casing, or from underneath the shield. In the longwall, higher methane concentrations occur mainly in the area of the passage used by humans (cf. Figs 15-18). Methane accumulates also between the ribs of the support. Additionally, it accumulates closer to the roof, which is the result of the buoyancy impact. The main current ventilating the longwall makes it harder for the zone of increased concentrations to reach the neighborhood of the body of coal. At the intersection with the tailgate, the ventilating air current pushes the methane stream away from the sidewall opposite to the longwall outlet. This phenomenon, to some extent, protects the devices located in this area.

A sudden inflow of methane from goaf can occur in a lot of places. The intensity of the phenomenon can vary, too. Numerous conditions, hard to predict, play a role here (Caliyaza, 1991). Therefore, a lot of various cases should be analyzed. Carrying out a simulation of transient states for each of these cases would be virtually impossible. The authors tested the method of estimating the range of the impact of a given outflow, which involves performing calculations

(with the highest possible accuracy) for the state where no untypical disturbances take place, and then carrying out a multiple variation analysis of stationary solutions, starting with the initial state and changing the location and intensity of the inflow with each succeeding variation. For the cases described in chapters 2.2 and 2.3, the method in questions yielded quite satisfactory results. However, for the most essential and representative cases, it would be advisable to perform calculations for the transient states. At present, a set of analyses of stationary states supplemented with selected transient states simulations seems to be the most appropriate solution.

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