Simulation of cmouldering combustion in porous media using the finite element system FEFLOW

Michael Plagge
michael.plagge@st.ovgu.de
Hochschule Magdeburg-Stendal (FH) and Otto-von-Guericke-University Magdeburg, Germany
Klaus-Jürgen Kohl
klaus-juergen.kohl@idf.uni-magdeburg.de
Institute of Fire Department Saxony-Anhalt, Germany
Prof. Dr.-Ing. Eckehard Specht
eckehard.specht@ovgu.de
Otto-von-Guericke-University Magdeburg, Germany
Prof. Dr. sc. tech. Hans-Jörg Diersch
h.diersch@wasy.de
DHI-WASY GmbH, Germany

ABSTRACT: The class of porous media may include fills from coal, lignite, wood strands, and granules or waste material. The space between those anisotropic solids is often filled with air. Materials coming into contact with air oxidize. Especially filled porous media are affected by smouldering fires caused by endothermic reaction. Due to the potentially massive environmental and economic impact, scientific approaches to arrive at new solutions for fire fighting and fire prevention were forced in the last few years. Different simulation models are used to understand and model the internal physical and chemical reactions on porous media for various geometries. The finite element system FEFLOW includes several possibilities for modeling flow, mass and heat transport as well as reactive multi species transport. For a two-dimensional approach to simulate a self-heating coal stockpile a known thesis from literature is used as a basis for the implementation in FEFLOW. Equation systems and input data, however, are to be derived and modified. The equation system contains a modified momentum equation, two equations for generation and degradation of coal and ash, two equations for transportation of air and exhaust gas (including the underlying chemical reaction) and one for heat-transport and -exchange. Boundary conditions are set for air at a constant incoming flow rate of 297 mg/l at 26.85 °C; for the exhaust gases of 0 mg/l were anticipated. Both conditions are constrained to implement normal conditions for outpouring gas. The model as presented in this paper and its results show good agreements with respect to quality when compared with international literature. For the chosen special case, chemical reactions amongst the solid and the gas phase as well as heat- and mass-transport of products are proving to be sufficiently accurate. However, future work has to be done to verify and validate FEFLOW for the purpose of simulating smouldering combustion in porous media.

INTRODUCTION AND MOTIVATION

Industrial combustion processes require large amounts of fuel. Coal and lignite as well as crude oil and its distillates are the favored sorts of combustion material due to their high caloric values. In the last years especially the use of regenerative materials like wooden pellets, strands or biogases is promoted and enforced.

The class of solid fuels, which include oxygen by nature, due to geometric shape or due to transport processes like filling, mining or crushing, may be subsumed in the class of porous media. Normally the gas included in the space between the solids is air, containing about 21 % oxygen. Resulting from the natural process of generating coal and lignite, particularly these solids have additionally small pores, which are filled with air due to the mining process.

Coal and lignite are often transported over large distances by train or ship. Then coal is stored in stockpiles. The storage time may last from a few days to several weeks, depending on the total storage amount and the energy demand.

While coal is transported or even stored in stockpiles, an oxidation process occurs. The oxidation starts with the mining process, because freshly mined coals are immediately exposed to air. Due to oxidation heat is generated and absorbed. This circulation may lead to local hot spots, inducing natural convection processes inside the pile. Oxidation processes supplied by natural or forced convection (wind) can be classified as smouldering fires.

Oxidation of fuel by smouldering fires in solids is a direct loss of caloric value. Additionally large amounts of gaseous exhausts are set free. Especially in the current times with new calculated scenarios about the progressing climate change presented every week it is necessary to force scientific research in energy use. Getting insight into chemical and physical processes in stored porous media may help to avoid smouldering fires as well as to develop new extinguishing methods.

The finite element system FEFLOW is specialized to simulate flow as well as heat and mass transport in porous media. Therefore the present paper shows a first approach to implement a model of a self-heating coal stockpile into FEFLOW.

STATE OF THE ART

Modeling chemical reaction or combustion in porous media is often done by referring to coal or lignite. Mainly two-dimensional models are used.

One-Dimensional Model

The dissertation published by Schmal in 1987 presented a one-dimensional model for simulating smouldering in coal piles. The model was set up with the chemical reaction of coal and oxygen, generation of reaction enthalpy by chemisorption, evaporation and condensation of water, transport of water and oxygen by diffusion and convection and heat transport by conduction and convection. Essential properties and parameters are determined by experiments with different coal types. Flow velocities and flow behaviour are measured with tracer gas injection. The model was verified and validated by three stockpiles of 2,500 tons of Australian coal.

Two-Dimensional Models

Simulation setups for two-dimensional models are often found in international literature. Only few are validated and verified by in situ measurements at real scale.

Lohrer analysed material values and self-heating temperatures for different coal and lignite. The specific properties are used to simulate the experimental setups. Numerical calculations are made to predict smouldering fires in coal stockpiles. Diffusion was implemented as temperature-dependent, but convection was neglected.

Weßling presented a model developed in Rockflow for simulating smouldering and combustion processes in coal seams in 2007. Diffusion, dispersion and convection were implemented for oxygen transport. Heat was exchanged by conduction, convection and radiation. The single-level chemical reaction was adapted from experiments made by Krause and Schmidt (2001) and Schmidt et al. in 2003. Combustion temperatures are simulated between 900-1300 K, the velocities of the combustion front ranged from 3 to 50 m per year.

The same simulator and chemical reaction type was used by Li in 2005 for predictions on self-heating in coal stockpiles. In situ measurements in a coal stockpile are used for comparison to simulation data. Oxygen is transported by diffusion and convection, heat by conduction and convection.

Brooks and Glasser simulated self-heating in coal stockpiles focusing on the particle diameter in 1988. They were able to prove increasing temperatures being proportional to decreasing diameter. Oxygen was only transferred by natural convection. Hot spots are observed in all locations near incoming oxygen.

In 1993 Salinger et al. reconfigured the model used by Brooks and Glasser. Instead of direct interaction between coal and oxygen via boundary conditions, the area beside and above the stockpile was extended to simulate and analyse airflow and the influence of forced convection on chemical reactions inside the pile. Oxygen was transported by diffusion and convection, heat was exchanged by conduction and convection. Salinger et al. proved that forced convection has no or little influence on transport of heat and oxygen.

Three-Dimensional Models

Krause and Schmidt measured self-heating temperatures of different dust types in 2001. The chemical kinetics formulation is used in the present paper as well as in published literature. An overview about the chemical reactions in coal and lignite can be found in Wang et al (2003).

Schmidt, Lohrer and Krause used the same model to determine the coherence between self-heating temperature and fraction of air oxygen in 2003. For lignite a proportional relation could be proved.

In 1979 Nordon developed a one-dimensional model. The setup was raised to three dimensions. A good summary was published by Carras and Young in 1994. The simplifications and mathematical formulations made by Nordon are used by Li, Weßling and Schmal.
Further models can be found in literature, e. g. Akgun and Essenhigh (2001), Fierro et al (2001), Moghtaderi et al (2000) and Smith and Glasser (2005).

MATHEMATICAL EQUATION SYSTEM

As a basis for implementation in FEFLOW the model developed by Li (2005) is adapted in the present paper. The six equations for motion, heat and mass transfer have been derived from the FEFLOW reference manual. For a detailed derivation refer to the work of Kohl et al. (2008) and Plagge (2008).

Simplifications and Assumptions

The following simplifications are adapted from Li and Weßling:

- temperature dependencies of conduction, heat capacity, diffusion and dynamic viscosity are neglected,
- exothermal oxidation energy is released only in the solid phase,
- coal is a homogenous, isotropic material; tensors of diffusion, dispersion, thermodispersion and permeability are simplified to scalars,
- influence of air moisture and moisture-fraction of coal are neglected,
- distribution of particle and pore diameter are neglected,
- chemical components of the oxidation process like H, N, S, are unrecognized,
- incoming and outpouring gases are ideal and incompressible as well as transported together,
- mixture of exhaust gas fractures is not regarded.

Equation system

The continuity equation with the vectorial DARCY-velocity is derived as:

$$S_0 \frac{\partial h}{\partial t} + \frac{\partial q_i^f}{\partial x_i} = -q_i^f \left(\frac{1}{\rho^f} \frac{\partial \rho^f}{\partial x_i} \right) \quad with \quad q_i^f = -K_{ij} \frac{\mu_0^f}{\mu^f} \left(\frac{\partial h}{\partial x_i} + \frac{\rho^f - \rho_0^f}{\rho_0^f} e_j \right)$$

Generation and degradation of coal and ash:

$$\frac{\partial C_k^{\alpha}}{\partial t} = R_k \quad with \quad R_k = -\frac{v_k}{v_{Coal}} \frac{m_k}{m_{Coal}} C_{Coal} C_{O_2} k_0 e^{-\frac{E}{RT}}$$

Transport of oxygen and exhaust gas:

$$\varepsilon_{\alpha} R_k = \varepsilon \frac{\partial C_k^{\alpha}}{\partial t} + q_i^f \frac{\partial C_k^{\alpha}}{\partial x_i} - \frac{\partial}{\partial x_i} \left[\left(D_d^f + \beta_T V^{\alpha} \right) \delta_{ij} \frac{\partial C_k^{\alpha}}{\partial x_j} \right]$$

Transport of heat by conduction and convection:

$$c^b \frac{\partial T}{\partial t} + \rho^f c^f q_i^f \frac{\partial T}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\left[\lambda_{ij}^{fs,cond} + \rho^f c^f \alpha_T V_q^f \delta_{ij}\right]\frac{\partial T}{\partial x_j}\right) = Q_T$$

With the tensor of conduction $\lambda_{ij}^{fs,cond}$, the heat capacity c^b and the energy-source Q_T:

$$\lambda_{ij}^{fs,cond} = \left(\varepsilon\lambda^f + (1-\varepsilon)\lambda^s\right)\delta_{ij} \qquad c^b = \left[\varepsilon\rho^f c^f + (1-\varepsilon)\rho^s c^s\right] \qquad Q_T = -R_{Coal}\Delta H$$

For a detailed explanation of the nomenclature see the FEFLOW Reference Manual – Part I (2005).

IMPLEMENTATION IN FEFLOW AND MODEL SETUP

As far as possible, properties and values are taken from Li (2005) and Weßling (2007). Specific Values for FEFLOW such as hydraulic air head, thermodispersion or storage coefficients are assumed or calculated. The chemical reaction and the equations needed are stated briefly. For detailed description refer to work of Plagge (2008).

Model geometry and mesh generation

A typical raised coal stockpile can be modeled as a frustum. To simplify simulation, a two-dimensional section has to be taken. This was done by an 40 meter wide, 10 meter high cut through the middle of an 80 meter long stockpile with a slope of 45 degree. FEFLOW has automatically set an aquifer depth of one meter. Simulation has been run with a mesh size of 4040 elements (2127 nodes) as shown in figure 1.
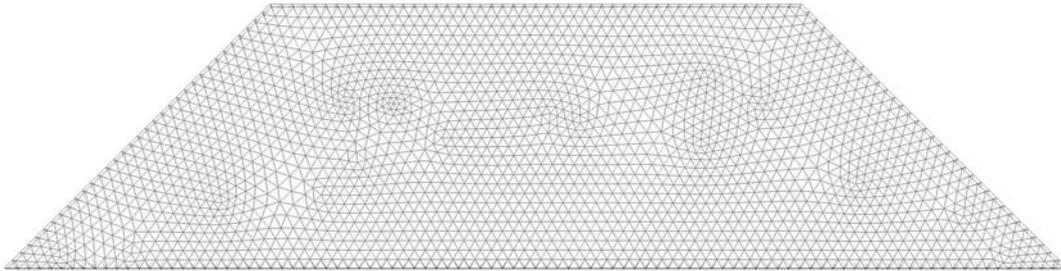

Figure 1: Mesh generated with 4040 elements.

Classification and temporal properties

The phenomenon was defined as a saturated, transient, thermohaline multi-species-transport-problem. Chemical reactions are simulated with four chemical species: coal, ash, oxygen and exhaust gas. Coal and ash are solid, oxygen and exhaust gas are described as fluid material. The final simulation time was set to 75 days.

Initial conditions

For coal and oxygen included in the pores a homogenous system temperature T=26.85 °C is set. The reference temperature T_0 is assumed with 0 °C. Initial concentrations for the four chemical species are set as given in table 1.

$C_{coal}^s = 501000 \; mg/l$	$C_{oxygen}^f = 297 \; mg/l$	$C_0 = 297 \; mg/l$
$C_{ash}^s = 0 \; mg/l$	$C_{exhaust\;gas}^f = 0 \; mg/l$	

Table 1: Initial and reference concentrations.

Boundary conditions

At the left and right flanks as well as the top 1st kind Dirichlet boundary conditions have been set for temperature and concentrations for oxygen and coal as shown below.

$$T(x_i,t)=T_1^R(t)=300\,K=26{,}85\,°C$$
$$C(x_i,t)=C_2^R(t)=297\,mg/l$$
$$C(x_i,t)=C_3^R(t)=0\,mg/l$$

The bottom boundary has unchanged conditions. Thereby the second kind boundary condition prevents heat and mass exchange.

Calculation of necessary material properties

Some properties have been calculated in other ways than usual for FEFLOW. Especially the hydraulic head h was calculated to express meter air head instead of water. Furthermore the specific storage coefficient S_0 and the tensor of hydraulic conductivity of fluid phase K_{ij} were determined. Material properties from calculations and literature are shown in table 2.

Chemical equations and heat generation

A common chemical approach to describe the oxidation of coal by oxygen as a one-step irreversible reaction can be derived as (Schmidt 2001):

$$\nu_{fuel}F + \nu_{oxidizer}O = \nu_{solid\,products}SP + \nu_{gaseous\,products}GP + \Delta H$$

The integrated Reaction-Kinetics-Editor is used with user-defined equations to incorporate chemical reaction and heat generation into the simulation as noted above. The Arrhenius-expression was calculated and assumed to be constant ($Rate_1$). Four reaction equations are determined after stoichiometric data was inserted (table 2):

$$R_1 = -1 \cdot Rate_1 \cdot C_1 \cdot C_2 \qquad R_2 = -0{,}764 \cdot Rate_1 \cdot C_1 \cdot C_2$$
$$R_3 = 1{,}316 \cdot Rate_1 \cdot C_1 \cdot C_2 \qquad R_4 = 0{,}449 \cdot Rate_1 \cdot C_1 \cdot C_2$$

The generation of heat is expressed by

$$Q_T = 2{,}268 \cdot 10^{-3} \cdot C_1 \cdot C_2$$

$c^b = 3{,}06 \cdot 10^5\,J/m^3/K$	$\alpha_L = 0{,}5\,m$
$c_p^f = 1000\,J/kg/K$	$\alpha_T = 0{,}5\,m$
$D_{d,O_2}^f = 10^{-6}\,m$	$\beta_L = 0{,}5\,m$
$D_{d,exhaus\,gas}^f = 10^{-9}\,m$	$\beta_T = 0{,}5\,m$
$E/R = 12368\,K$	$\bar{\beta} = 31{,}318 \cdot 10^{-4}\,1/K$
$h_0 = 8069{,}33\,m$	$\Delta H = 2{,}1 \cdot 10^7\,J/kg$
$K_{ij} = 0{,}6976 \cdot 10^{-3}\,m/s$	$\varepsilon = 0{,}4$
$k_{ij}^s = 10^{-10}\,m^2$	$\varepsilon_s = 0{,}6$
$k_0 = 10^9\,m^3/kg/s$	$\lambda^f = 24{,}36 \cdot 10^{-3}\,W/m/K$
$m_{coal} = 1089\,g/mol$	$\lambda^s = 0{,}1\,W/m/K$
$m_{ash} = 489\,g/mol$	$\mu_0 = 1{,}81 \cdot 10^{-5}\,Pa\,s$
$m_{oxygen} = 32\,g/mol$	$\nu_{coal} = -1$
$m_{exhaust\,gas} = 30{,}5\,g/mol$	$\nu_{ash} = 1$
$p_0 = 101{,}325\,kPa$	$\nu_{oxygen} = -26$
$S_0 = 4{,}957 \cdot 10^{-5}\,1/m$	$\nu_{exhaus\,gas} = 47$
	$\rho_0^f = 1{,}28\,kg/m^3$

Table 2: Material properties and stoichiometric data.

RESULTS

The following figures are generated from the model presented in this paper. The results will be discussed in detail for heat, mass and velocity distribution. The head differs only about two meters and is therefore assumed as a constant.
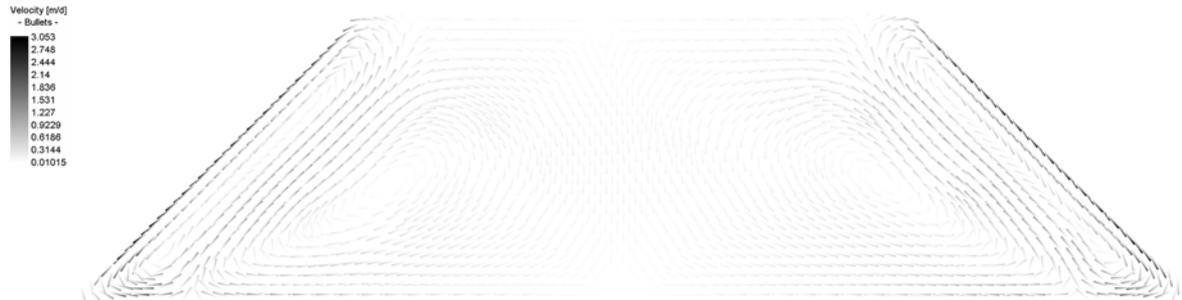

Figure 2: Velocity distribution of self-heating coal stockpile.

As shown in figure 2 the velocity profile develops two vortexes near the flank sides. These vortexes are generated by natural convection due to self-heating. The minimal velocities are about zero in the inner centre and increasing to a maximum of three meter per day at the flanks.
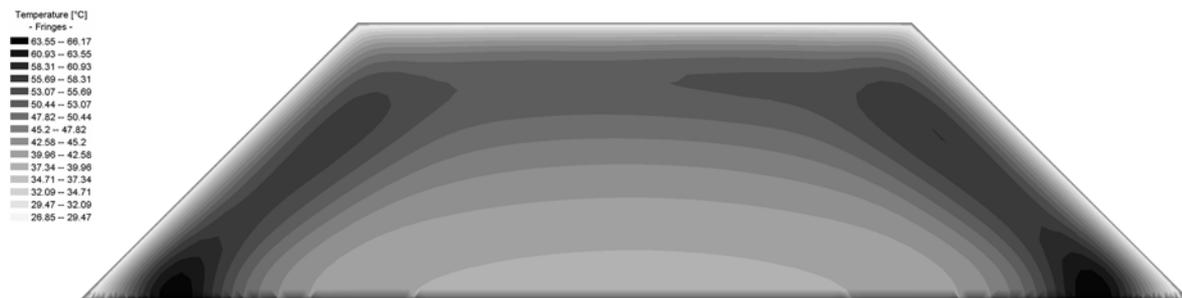

Figure 4: Temperature distribution of self-heating stockpile.

Comparing the left and right side of the pile in figure 4, self-heating of coal shows an approximately symmetric heat generation. The maximum temperature is about 66,17 °C and is only reached by two hot spots in the lower flanks. Around the air side the influence of fresh air is visible through a colder area of about one meter in depth from surface.
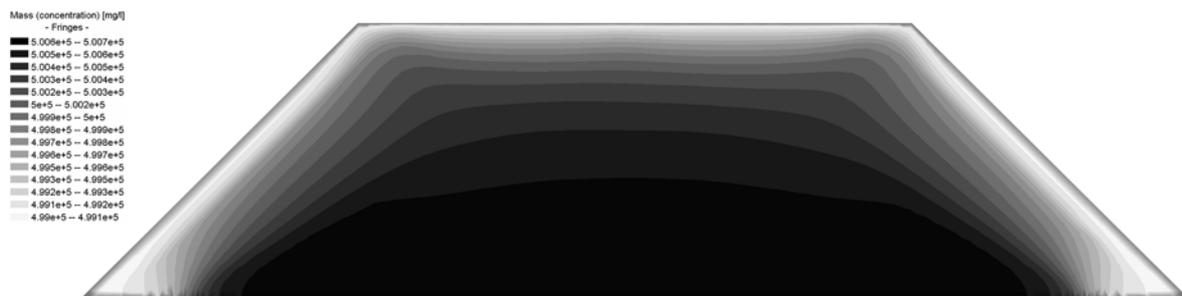

Figure 5: Mass distribution of coal in the coal stockpile.

The degradation of coal is shown in figure 5. Around the border coal is oxidized by about 2000 mg/l. Constantly inflowing oxygen enhances the process. In the inner areas the rate of oxidation is slower, because oxygen is initially only available by the amounts stored in the pores.
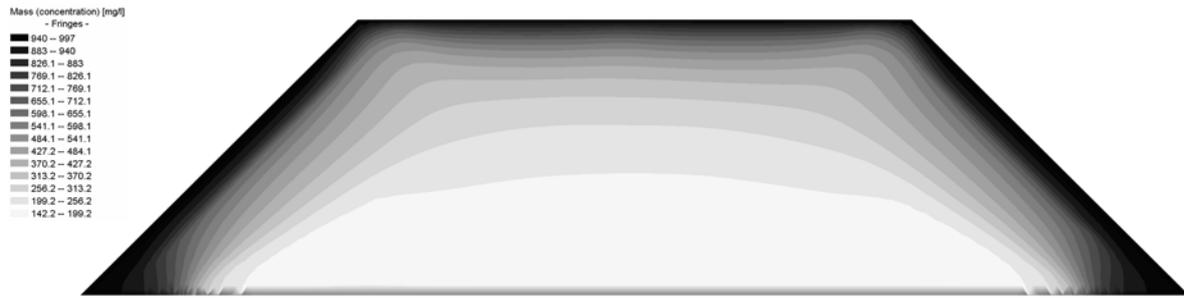
Figure 6: Mass distribution of ash in the coal stockpile.

In figure 6 the solid product of reaction – ash – is displayed. Ash generated by oxidation is about 150 to 1000 mg/l. Due to the theoretical reaction equation one mole of coal generates one mole of ash and one mole of gaseous products.
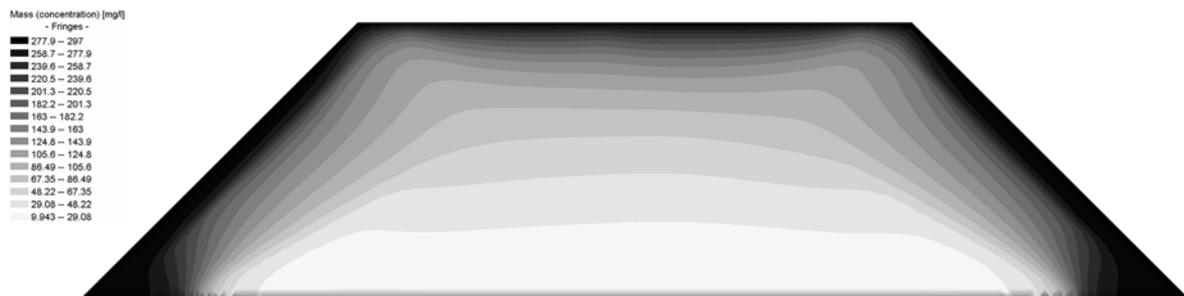

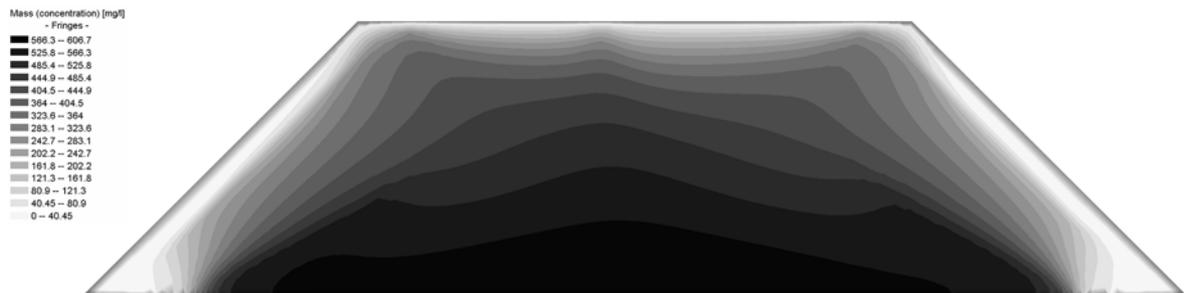**Figure 7: Oxygen distribution in the coal stockpile.**

Figure 8: Exhaust gas distribution in the coal stockpile.

The oxygen distribution as stated in figure 7 shows fresh oxygen entering the simulation domain as set by the boundary conditions. While the inner areas are low on oxygen, there are two accumulations visible in the lower corners. The constant supply of oxygen is one possible explanation for forming hot spots in this areas. Exhaust gases as shown in figure 8 are transported by convection in the inner centre of the pile. The exhaust gases fill the empty pores due to oxidation. Thus oxygen supply in the inner regions is obstructed.

SUMMARY

Chemical Reactions, flow, heat and mass transfer in porous media are a few key features provided by FEFLOW. The application is used to set up a model for simulating a self-heating coal stockpile in two dimensions. The equations system as well as the necessary data was derived from literature or calculated by the authors.

The results show good qualitative agreements with theoretical and experimental reviews in international literature. Furthermore the model is sufficiently accurate to calculate chemical reactions and the transport of heat and mass transfer in a coal pile.

Still additional work has to be done. For enhanced qualitative results and generation of quantitative series of measurements the model has to be verified. First attempts by varying material properties, mesh resolution and temporal settings have been made by Plagge (2008).

Furthermore exact comparisons between the mathematical equation system used by FEFLOW and analytical solutions have to be conducted to validate the model for common use.

REFERENCES

Agun, F. and Essenhigh, R. H., Self-ignition characteristics of oal stockpiles: Theoretical predictions from a two-dimensional unsteady-state model, Fuel, 80:409-415, 2001

Brooks, K., Bradshaw, S. and Glasser, D., Sponataneous combustion of coal stockpiles – an unusual chemical reaction problem, Chemical Engineering Science, 43(8) (1988), 2139-2145

Carras, J. N. and Young, B. C., Self-heating of coal and related materials – models, application and test methods, Progress in Energy and Combustion Science, 20 (1994), 1-15

Diersch, H.-J., FEFLOW Reference Manual, WASY GmbH Institute for Water Resources Planing ans Systems Research, Berlin, (2005)

Fierro, V., Miranda, J. L., Romero, C.,Andrés, J. M., Arriaga, A., and Schmal, D., Model predictions and experimental results on self-heating prevention of stockpiled coals, Fuel, 80:125-134, 2001

Kohl, K.-J., Diersch, H.-J. and Plagge, M., Unveröffentlichte Arbeiten zur Herleitung von Schwelbrandmodellen, (2008)

Krause, U. and Schmidt, M., The influence of initial conditions on the propagation of smouldering fires in dust accumulations, Journal of Loss Prevention on the process industries, 14 (2001), 527-532

Li, X., Untersuchung zum Sauerstofftransport und zur Selbstentzündung in der Kohlenhalde Mehrum, Bachelor Thesis, Institut für Strömungstechnik und Elektronisches Rechnen im Bauwesen, Universität Hannover, (2005)

Lohrer, C. A., Einflussgrößen auf die Selbstentzündung von Schüttgütern und Stäuben – experimentelle Untersuchungen und numerische Simulation, PhD Thesis, Fakultät III – Prozesswissenschaften, Technische Universität Berlin, (2005)

Moghtaderi, B., Dlugogorski, B. Z. and Kennedy, E. M., Effects of wind low on self-heating characteristics of coal-stockpiles, Trans IChemE, 78(B):445-453, 2000

Plagge, M., Berechnung des Verlaufes von Schwelbränden unter Nutzung GIS-basierter Berechnungstools, Bachelor Thesis, Otto-von-Guericke University Magdeburg, (2008)

Salinger A., Aris, R. and Derby, J. J., Finite element formulations for large-scale coupled flows in adjacent porous and open fluid domains, International Journal for Numerical Methods in Fluids, 18 (1993), 1185-1209

Salinger A., Aris, R. and Derby, J. J., Modelling the spontaneous ignition of coal stockpiles, AIChE Journal, 40(6) (1994), 991-1004

Schmal, D., A model for the Spontaneous Heating of Stored Coal, PhD Thesis, Technische Universiteit Delft, (1987)

Schmidt, M., Untersuchungen zu Schwelbränden in Feststoffschüttungen verursacht durch Glimmnester und eigeschüttete heiße Gegenstände, PhD Thesis, Faculty of Process and Systems Engineering, 2001

Schmidt, M., Lohrer, C. and Krause, U., Self-ignition of dust at reduced volume fractions of ambient oxygen, Journal of Loss Prevention in the process industries, 16 (2003), 141-147

Smith, M. A. and Glasser, D., Spontaneous combustion of carbonaceous stockpiles. Part I. The relative importance of various intrinsic coal properties and properties of the reaction system, Fuel, 84:1151-1160, 2005

Smith, M. A. and Glasser, D., Spontaneous combustion of carbonaceous stockpiles. Part II. Factors affecting the rate of the low-temperature oxidation reaction, Fuel, 84:1161-1170, 2005

Wang, H., Dlugogorski, B. Z. and Kenndy E. M., Coal oxidation at low temperatures: oxygen consumption, oxidation products, reaction mechanism and kinetic modelling, Progress in Energy and Combustion Science, 29 (2003), 487-513

Weßling, S., The Investigation of Underground Coal Fires – Towards a Numerical Approach for Thermally, Hydraulically and Chemically Coupled Processes, PhD Thesis, Mathematisch-Naturwissenschaftliche Fakultät, Westfälische Wilhelms- Universität, 2007