

Modelling the Coupled Heat and Mass Transfer during Fires in Stored Biomass, Coal and Recycling Deposits

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Abstract: In this paper the advances in the development of a numerical model for predicting the possibility of occurrence of the self-ignition in stored biomass, coal heaps or underground seams and dump deposits are presented.

Furthermore, the determination of the kinetics/stoichiometric parameters of the combustion reaction are presented. Then, the results of some simulation performed are compared with experimental data.

Finally, some conclusions and the possibility of future work are drawn.

Keywords: self-ignition, fire prevention, storage, biomass, bulk materials.

1. Introduction

The self-ignition of stored bulk-materials, coal heaps or underground seams is a problem, with which BAM has been long dealing with (Steen, 2000, Schmidt, 2001, Krause *et al.*, 2006). Recently, due to the exponentially increase of the use of alternative energy sources, the storage of big amounts of biomass has become frequent, generating new possible fire sources.

Self-ignition is caused by the low-temperature and low-rate exothermic reactions within the deposit of material. These processes release small portions of heat but, if this heat cannot be dissipated to the surroundings completely, the temperature inside the deposit rises. This leads to an enhancement of the exothermic reactions and to a positive heat feed-back loop, which, at circumstances can end in an extensive fire.

Additional heat sources that may be precursors of self-ignition are physical processes like adsorption of water and, in the case of biomass or landfills, the biological processes like fermentation. Recent studies (Hogland and Marques, 2003, Kindlein *et al.*, 2006) remarked the importance of the biological processes in the heating-up of landfills.

In order to avoid emissions from undesired fires and hazardous cost-intensive and time

consuming fire fighting, a reliable assessment of the fire hazard is necessary. The normal procedure of such a hazard assessment requires four steps:

- experimental investigation of the relevant processes on lab-scale,
- providing the output results of the lab-scale experiments as input parameters to a validated fire model,
- applying the fire model to the on-site geometry, initial and boundary conditions,
- performing multi-dimensional, time-dependent calculations of fire scenarios on real scale.

Simplified reaction models reflecting the chemical conversion of the different materials suspected to undergo self-ignition were developed based on the lab-scale experiments. Transport coefficients were determined experimentally as well. The set of balance equations used covered conductive heat transfer and diffusional transport of up to 6 reactants and products. In order to account for contribution of the convection inside the porous material, the diffusional coefficients have been increased by two orders of magnitude, with respect to a simply diffusional flow.

The following practical applications of the model were considered:

- prediction of permissible dimensions and permissible storage times of heaps of biomass in thermal power stations,
- computation of hot spot formation and fire propagation in coal seams in a real geological structure (Wuda coal field, Inner Mongolia, P.R. China)
- self-ignition in a deposit of combustible recycling material mixed with non-reacting matter.

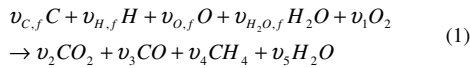
Results obtained are the evolutions with time of the temperature and species concentrations.

2. Numerical Model

2.1 Chemistry/Physics

The model presented in this section, based on the works of Schmidt (2001), Schulze (2005) and Krause *et al.* (2006), covers the effects of self-heating, ignition and fire propagation through combustible bulk materials.

The combustion process can be described by a general equation, in the form of equation (1). Chemical species included are fuel (formed by C, H, O and moisture), oxygen, carbon monoxide, carbon dioxide, methane, water (as vapour). The following expressions describe the chemistry used in the model:



The following assumptions were made:

- diffusive transport mechanism inside the bulk phase,
- convective currents were considered by modifying the diffusion coefficient,
- bulk material is homogeneous and isotropic,
- materials properties are independent of time and location.

The temperature and concentration fields were solved with a Fourier-type equation (2) and with Fick-type equations (3), respectively :

$$\frac{\partial T}{\partial t} = \frac{\lambda}{\rho \cdot c_p} \cdot \text{div grad } T + S_T \quad (2)$$

$$\frac{\partial C_k}{\partial t} = D_k \cdot \text{div grad } C_k + S_{C_k} \quad (3)$$

Each species considered is converted at its specific rate during the combustion reaction. For the decomposition of the solid fuel, an Arrhenius-type reaction rate as given in equation (4) applies:

$$\frac{dC_f}{dt} = -C_f \cdot k_0 \cdot \exp\left(-\frac{E}{RT}\right) \quad (4)$$

where k_0 is the pre-exponential factor, E the apparent activation energy specific for each reaction and R is the universal gas constant. The reaction rate is of first order, as it is assumed that the decomposition reaction depends, besides the

temperature, on the concentration of the fuel only.

Equation (5) defines then the conversion rates of the species produced/consumed in this reaction:

$$\frac{dC_i}{dt} = \frac{v_i}{v_f} \cdot \frac{M_i}{M_f} \cdot \frac{dC_f}{dt} \quad (5)$$

where v_i is the stoichiometric coefficient of the corresponding reaction equation and M_i is the molecular weight. Note that the stoichiometric coefficients are always negative for reactants and positive for products.

The moisture transport affects the self-ignition and combustion process. In Lohrer *et al.* (2005) the source terms for vaporization or condensation have been proven to be of the same type of eq. (4) and are going to be included in the model in further calculations.

The heat source term is the reaction enthalpy, as shown in the following equation:

$$S_T = \frac{1}{\rho \cdot c_p} \Delta H_R \frac{dC_f}{dt} \quad (6)$$

Resuming, the model consists of 7 coupled time dependent PDEs solving the temperature field and 6 concentration fields (fuel, oxygen, carbon monoxide, carbon dioxide, methane, water vapour). For solving the system of equations numerically in our case, the commercial Finite-Element-Code COMSOL Multiphysics was used.

2.2 Biology

In the case study of biomass piles or landfills, the biological processes occurring in the pile bring an additional heat source (Hogland and Marques, 2003, Kindlein *et al.*, 2006). The model presented in 2.1 can then underestimate the temperature in the pile and the induction time to the self-ignition.

Therefore, a study of the disposable literature about microbiological activity in stored bulk materials has been performed. It has been found that the most important heat source in this scenario has to be found in the aerobic processes, i.e. processes in which micro-organism need oxygen to grow. Among the models to predict the aerobic metabolism, the one proposed by Tremier *et al* (2005) was chosen to be

implemented in Finite-Element-Code COMSOL for an approximation of this additional heat source.

This model is based on oxygen consumption kinetics and assumes that the organic matter is composed by three fractions: easily-biodegradable, slowly-biodegradable and non-biodegradable organic matter. The easy-biodegradable matter can be directly used by the micro-organism to grow, while the slowly-biodegradable must before being hydrolyzed, since the degradation processes occur in the aqueous phase. It is known that approximately 450 kJ/mol O₂ are produced during aerobic process (Weppen, 2002): then, if the oxygen consumption is known or good modelled, the additional heat source due to biology can be estimated. For further information about the model by Tremier *et al.* (2005) we remit to the original paper.

Even if the model by Tremier *et al.* (2005) was developed for composting, also wood (or every partially organic/biodegradable material in general) can be seen as formed by the three described fractions, obviously in a different percent. The micro-organism growth rate can be in the present study slower than during the composting process, since the optimum conditions are not present (especially lack of nitrogen can limit the process in the case of biomass piles).

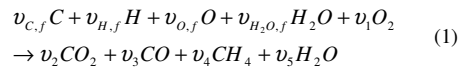
Thus, the input parameters of the model, which for preliminary calculations were taken from literature, are currently being proved with lab-scale respirometric experiments. These experiments, which come from an adaptation of the so-called Sturm Test (ISO 14852), allow following the microbiological activity through the monitoring of the CO₂ production during the micro-organism respiration.

To implement the model in the Finite-Element-Code COMSOL Multiphysics, four additional concentration fields and the additional heat source were introduced and solved.

3. Experimental Results

3.1 Combustion Reaction Coefficients

As said in the introduction, the combustion process can be described by a general equation, in the form of equation (1):



The stoichiometric coefficient for the fuel can be determined if the mass composition and moisture of the sample are known. Therefore, CHN-analyses, determinations of moisture content according to Karl Fischer and the ashes determinations according to DIN 51719-A were performed.

Then, for every one of the elementary components a balance equation can be written –equations (7), (8) and (9). If at least two of the four ratios between the amounts of the gas products are known –equations (10) and (11)– a solvable system is obtained.

$$v_{C,f} = v_2 + v_3 + v_4 \quad (7)$$

$$v_{H,f} = 4v_4 + 2v_5 - 2n_{H_2O,Br} \quad (8)$$

$$v_{O,f} = 2v_2 + v_3 + v_5 - 2v_1 - v_{H_2O,f} \quad (9)$$

$$\frac{v_2}{v_3} = \frac{\sum_k c_{CO_2} * \Delta t}{\sum_k c_{CO} * \Delta t} = M \quad (10)$$

$$\frac{v_4}{v_5} = \frac{\sum_k c_{CH_4} * \Delta t}{\sum_k c_{H_2O} * \Delta t} = L \quad (11)$$

The system of equations can be reduced as follows and can be finally written as a 3x3-matrix.

$$\begin{aligned} v_{C,f} &= (M+1)v_3 + (L)v_5 \\ v_{H,f} + 2v_{H_2O,f} &= (4L+2)v_3 \\ v_{O,f} + v_{H_2O,f} &= -2v_1 + (2M+1)v_3 + v_5 \end{aligned}$$

$$\begin{pmatrix} 0 & M+1 & L \\ 0 & 0 & 4L+2 \\ -2 & 2M+1 & 1 \end{pmatrix} \cdot \begin{pmatrix} v_1 \\ v_3 \\ v_5 \end{pmatrix} = \begin{pmatrix} v_{C,f} \\ v_{H,f} + 2v_{H_2O,f} \\ v_{O,f} + v_{H_2O,f} \end{pmatrix}$$

The values of the *M* and *L* ratios can be obtained from the FTIR analyse of the gas products of the combustion, if it is assumed that, during this phase the ratios remain constants. A more detailed description of the method is given in (Schulze, 2005).

3.2 Numerical Simulation

In Figure 1 a comparison of the simulated and the experimentally determined values of the so-called self-ignition temperature (SIT) for four different wood types is shown. More information

about the material properties can be found in (Schulze, 2005).

The experimental data were obtained by means of hot storage test, according to the German standards (VDI-guideline 2263, 1990). In this kind of experiments a sample of the substance to analyze is stored in a permeable container, in order to grant the access for oxygen. The substance is also exposed to a surrounding temperature at which the onset of a fire has to be expected.

Note that the SIT is defined to be the highest surrounding temperature at which no ignition occurs: this means, for a surrounding temperature higher than the SIT, the heat released by the reactions inside the probe is larger than the heat transmission to the surroundings, making the process running into a fire.

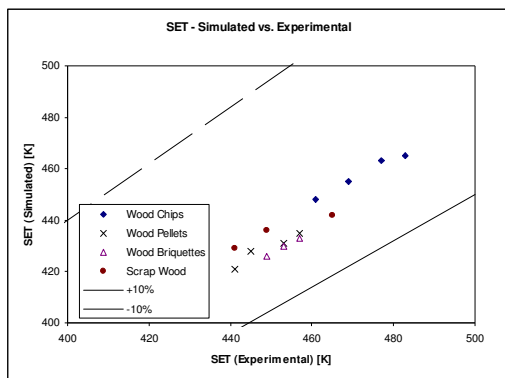


Figure 1: Comparison of the numerically simulated and experimentally determined self-ignition temperatures of the investigated woods

The values of the numerically simulated and the experimentally determined SIT of the wood samples are in good agreement. It can be seen that, in all cases the simulated values were somewhat lower than in the experiments. This yields to a conservative estimation.

It has to be noticed that, due to the fact that the surrounding temperature are higher than 70 °C –temperature at which it can be considered that the biology activity ceases, due to the death of micro-organism– the mere chemical/physical model described in 2.1 was implemented in the calculation.

Nevertheless, it is known (Steen, 2000) that the self-ignition temperature decreases with

increasing the volume of the bulk material, since the heat transfer to the surroundings is impeded. Thus, in real scale scenario, the biology has to be included, since it can accelerate the chemical/physical processes and increase the possibility of occurrence of a fire.

To give an example of the importance of the biology in a real-scale computation, a calculation of the self-ignition of a wood pile, with and without considering the heat produced by the micro-organisms have been performed. The pile considered was 6 meter high with a width of 30 m. The material is considered to lay on a concrete basement, which is a common praxis in wood storage.

In order to reduce the computational efforts, only a two-dimensional calculation was performed, assuming that the length of the pile was much bigger than the width. In addition, due to symmetry, only half of the cross section was considered. In the computations performed, the mesh used was made of about 4000 elements. As input parameters, the initial temperature of the wood pile and of the concrete basement was taken to be 15 °C while the ambient temperature was set to 15 °C, without consideration of the day and night cycles.

Figure 2 shows the computed temperature distribution in the pile after six month (a quite long but still possible storage period for wood in the practice), if the biological processes are not implemented. It can be seen that, according to this calculation, self-heating of the pile does not occur, since the temperature inside the pile does not increase appreciably.

Nevertheless, if the biological processes are considered, the pile reaches a self-ignition after a very short time (80 days approximately, as can be seen in Figure 3). Even if this example can overestimate the danger, since the biological processes have been considered to happen at the same speed of the composting processes, where the conditions for the growth of the micro-organisms are optimal, the computations show clearly that the biology in the wood pile has to be studied accurately, since it may be a cause for the occurrence of a fire.

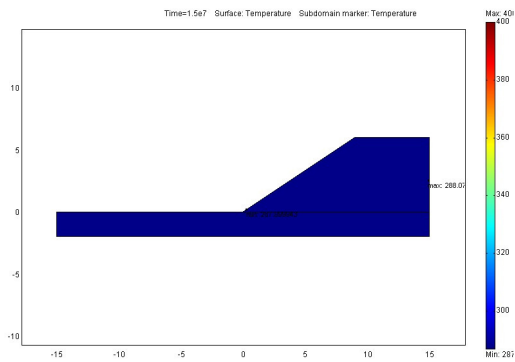


Figure 2: Study of the self-heating of a wood pile, without consideration of biology (material stored at an ambient temperature of 15 °C)

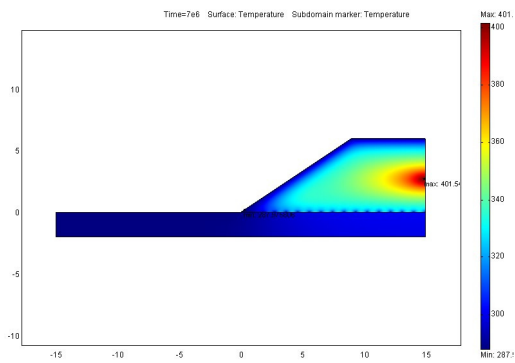


Figure 3: Study of the self-heating of a wood pile, with consideration of biology (material stored at an ambient temperature of 15 °C)

A second computational example dealt with self-ignition in a waste deposit of trapezoidal cross section. The bottom of the deposit had an extension of 30 m x 50 m the height was assumed to be 15 m. The top surface was 18 m in width and 50 m in length. The computational mesh was adopted to half of the deposit due to symmetry across the length axis.

In this example the fraction of combustible material was assumed to be 20 %, distributed homogeneously across the deposit. This can typically be found in deposits of construction wastes where inert matter like sand bristles from bricks or concrete are mixed with wood wastes, insulation materials, dyes etc. Thermophysical data and reaction kinetics were derived from the experiments using samples extracted from a MSW deposit.

A three-dimensional computation was performed supposing that the deposit was exposed to an

average ambient air temperature of 26°C which reflects climate conditions in a tropical environment. Further it was assumed that there is no heat transfer across the bottom of the deposit. Consequently, as a result of the computations the formation of a hot spot was observed in the symmetry axis of the deposit at the bottom after about 5.8 years.

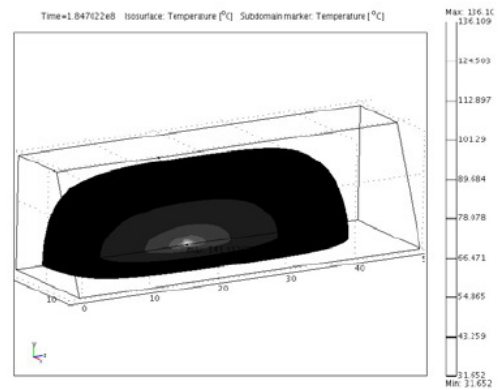


Figure 4: Formation of a hot spot in a waste deposit stored at an average temperature of 26 °C after 5.8 years of undistorted storage

5. Conclusions

The commercial Finite-Element-Code COMSOL Multiphysics was used to solve a system of coupled heat and mass transfer differential equations, which describe generation and propagation of fires in large-scale deposits of combustible bulk materials. The input parameters of the model have been determined experimentally with standardized tests and, as well, the model predictions were validated with lab-scale self-ignition tests.

The results encourage the authors to follow in the investigation and to put special attention to the simulation of the biological processes, which have been proven to be an important precursor of the self-ignition in the case of biodegradable materials.

6. References

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7. Appendix - Nomenclature

Symbols

| | |
|--------------|---|
| C | mass concentration, kg m ⁻³ |
| c_p | specific heat, J kg ⁻¹ K ⁻¹ |
| D | diffusion coefficient, m ² /s |
| E | activation energy, J/mol |
| k_0 | pre-exponential factor, s ⁻¹ |
| L, M | experimental ratios between gas products concentrations, - |
| R | universal gas constant, J mol ⁻¹ K ⁻¹ |
| S_T | heat production term, W/m ³ |
| S_c | production rate of the species k , kg m ⁻³ s ⁻¹ |
| T | temperature, K |
| t | time, s |
| ΔH_R | heat of reaction, J kg ⁻¹ |
| λ | thermal conductivity, W m ⁻¹ K ⁻¹ |
| ρ | bulk density, kg m ⁻³ |
| ν | stoichiometric coefficient, - |

Subscript

| | |
|--------|----------------|
| f | fuel |
| k, i | species k, i |