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A mathematical model to predict the heating-up of large-scale wood piles

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ABSTRACT

A mathematical model to predict the heating-up in open air wood chip piles has been developed. This model includes the heat production from chemical, physical and microbial exothermal processes. In the manuscript the laboratory experiments needed to develop and validate the model are described. In addition, temperature and gas concentrations were measured in two large-scale wood piles (volumes bigger than 1000 m^3), in order to provide the applicability of the model to large-scale scenarios. The predictions of the model and the large-scale experimental data showed good agreement concerning the maximum temperature reached inside an open air wood pile. Special attention has been devoted to the microbial processes, since they proved to be the most important cause of heat production in the early stages of storage. This work is intended to help in predicting and thus avoiding possible self-ignition scenarios for this type of wood storage.

1. Introduction

The storage of wood chips in large open air piles with thousands of tons of material is susceptible to the self-ignition of the bulk material, as it has already been frequently reported, for example in Rothenburg (2000) and in Traunreut (2005). Being nowadays scrap or rest wood from the forest industry one of the main sources of renewable fuels and in the perspective of the prognosticated increase in the use of renewable energies in the near future by Nitsch (2007), the number of open air wood storages and thus the possibility of their self-ignition seems destined to grow in the next years.

Undesired fires from self-ignition bring important economical losses and cause emission of carbon dioxide and of toxic gases, like carbon monoxide through incomplete combustion. Furthermore, since the energy production must be guaranteed, the losses in the renewable energy source would be possibly compensated with fossil fuels: this gives rise to additional carbon dioxide emissions. Prevention of the self-ignition in stored wood is therefore an economical and safety relevant issue. Nevertheless, only few studies, see Bergman and Nilsson (1971), Ernstson and Rasmuson (1993), Sampson and McBeath (1987) and Springer and Hajny (1970) dealt with the heating-up process inside open air wood piles. This work aims to improve the knowledge in the self-ignition of wood piles, in order to prevent possible fires.

The reasons for self-ignition have to be found in the exothermic reactions like slow oxidations, possible physical influences like coupled effects of condensation and wetting (mainly adsorption) of water molecules and microbial processes, which are occurring in these large wood heaps at common ambient temperatures. Due to the poor heat conductive properties of the bulk material, the heat produced inside the pile could not dissipate to the surroundings completely. Thus, a positive heat feedback loop would be initiated, which would finally turn in an extensive fire.

Among the factors influencing the possibility and frequency of occurrence of self-ignition, one of the most important is the storage geometry, since the heat production occurs in the whole bulked volume and the heat is dissipated only through the pile surface. Therefore, Steen (2000) described that an increase of the volume to surface (V/A) ratio results in a smaller self-ignition temperature (T_{SI}). The T_{SI} is defined as the highest surrounding temperature at which no ignition occurs: this means, for a surrounding temperature higher than the T_{SI}, the heat released by the reactions inside the material is larger than the heat transmission to the surroundings, making the process running into an ignition. The V/A dependence of the T_{SI} leads to the possibility of self-ignition at normal ambient temperatures, if the amount of stored material is large enough.

Standard laboratory scale investigation of the self-ignition in accordance to the European standard DIN EN 15188 (2007) was

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Nomenclature (SI units)

Quantity	Description, SI unit
A	Area, [m^2]
b	Biomass death rate constant, [s^{-1}]
C_k	Concentration of the species k, [kg/m^3]
CD	Pre-exponential factor condensation/adsorption, [s^{-1}]
c_p	Specific heat, [J/kg K]
D_k	Diffusion coefficient of the gas species k, [m^2/s]
E	Activation energy, [J/mol]
EV	Pre-exponential factor evaporation/desorption, [s^{-1}]
f	Fraction of dead biomass converted to inert, [-]
k_0	Pre-exponential factor, [s^{-1}]
K_b	Substrate saturation constant for MB, [kg/m^3]
K_h	Hydrolysis constant, [s^{-1}]
K_MH	Saturation constant for the group MH/X, [-]
M_k	Molecular weight of the species k, [kg/mol]
MB	Easy-biodegradable fraction concentration, [kg/m^3]
MH	Slowly-biodegradable fraction concentration, [kg/m^3]
q_{O_2}	Oxycaloric coefficient, [J/kg]
R	Gas Universal constant, [J/mol K]
S_{C_k}	Conversion rate of the species k, [kg/m^3 s]
S_T	Heat production, [W/m^3]
S_v	Evaporation/desorption rate of liquid water, [kg/m^3 s]
S_w	Condensation/adsorption rate of water vapor, [kg/m^3 s]
t	Time, [s]
T	Temperature, [K]
V	Volume, [m^3]
X	Biomass concentration, [kg/m^3]
Y	Biomass yield on MB, [-]
Y_{CO_2}	Biomass yield on CO$_2$, [-]
ΔH_R	Calorific value, [J/kg]
ΔH_v	Water evaporation enthalpy, [J/kg]
λ	Thermal conductivity, [W/m K]
μ_m	Biomass growth rate constant, [s^{-1}]
ν_k	Stoichiometric coefficient of the species k, [-]
ρ	Density, [kg/m^3]

performed in this work. Even though these experiments are necessary to determine the T_{SI} and the kinetic parameter of the combustion reaction, the extrapolation methods are valid only for simple defined geometries. Furthermore, hot storage experiments are usually performed at temperatures much higher than 100 °C, due to comparably small V/A ratios. Hence, the influences of moisture and of microbial processes on the course of self-ignition are reflected only in the initial phases of such experiments. Nevertheless, these aspects are important since moisture can increase the possibility of occurrence of a self-ignition, like shown by Lohrer, Schmidt, and Krause (2005) and affects the time to ignition, as already reported by Simms and Law (1967). In addition, a high microbial activity can bring important additional heat, see Weppen (2001).

In order to surmount these shortcomings, modeling of the coupled differential equations of heat and species transfer is needed. Therefore, a mathematical model has been developed to simulate the heating-up and possible self-ignition processes in wood storage. The model comprises three heat sources:

- A heat production rate, deriving from Arrhenius-type oxidation reactions inside the pile;
- A physical heat production/consumption rate, which reflects the transferred heat from endothermic evaporation/desorption and exothermic condensation/adsorption processes;
- A heat source arising from microbial processes, which is proportional to the oxygen consumption during aerobic respiration. In order to define proper oxygen consumption kinetics, respiratory experiments, coming from a modification of the so-called Sturm Test: ISO 14852 guideline (1999), have been performed.

The model has been solved numerically and has then been validated with laboratory experiments and finally compared to real scale experiments. For these experiments the temperature and concentrations of four different gases in two freshly established large pine wood piles have been measured.

This work presents experimental results of the hot storage tests as well as of the respiratory experiments and of the large scale measurements, which were used to generate the input parameter of the model. Furthermore, predictions of the developed model and comparison with experimental data are presented. This work aims for better understanding of the precursors of the self-ignition of large-scale wood piles and in achieving a safe and sustainable storage of this resource.

2. Experiment

2.1. Hot storage tests

The European standard DIN EN 15188 (2007) establishes that the so-called hot storage test should be used for the laboratory scale investigation of the self-ignition processes. In Fig. 1 the set-up of this test is schematically drawn: the specimen to study is exposed to high temperature surroundings and the temperature in its center is measured. At first, the temperature in the sample will reach the surrounding temperature. Subsequently, if the heat released inside the probe is greater than heat dissipation, the material will reach self-ignition. By varying the surrounding temperature, the minimum T_{SI} and the induction time to self-ignition – i.e. the time from the beginning of the experiment to the exponential increase in the temperature – are determined. The experiments are repeated for samples with different V/A ratios: then the values of T_{SI} and induction time to self-ignition (t_{SI}) can be extrapolated to bigger V/A ratios for the same geometry type, as shown in Figs. 2 and 3 for pine sawdust and pine wood chips. The two graphs show also that a reduction in the particle size increases the possibility of occurrence of a self-ignition, since both values of self-ignition temperature and of induction time to self-ignition are smaller for pine sawdust (average particle size 0.25 mm) than for pine wood chips (average particle size 10 mm).

2.2. Respirometric tests

In order to estimate the activity during the microbial respiration, experiments were performed at a laboratory scale. A schematic drawing of the experimental set-up, which comes from a modification of the ISO 14852 guideline (1999), is shown in Fig. 4.

In these experiments, the microbial activity is determined through the monitoring of the production of carbon dioxide, which under aerobic conditions is linked to the oxygen consumption. The heart of the set-up is a 4-L sealed glass recipient in which the substance to be incubated is inserted. The walls of the reactor are tempered, as to maintain the desired temperature, which is

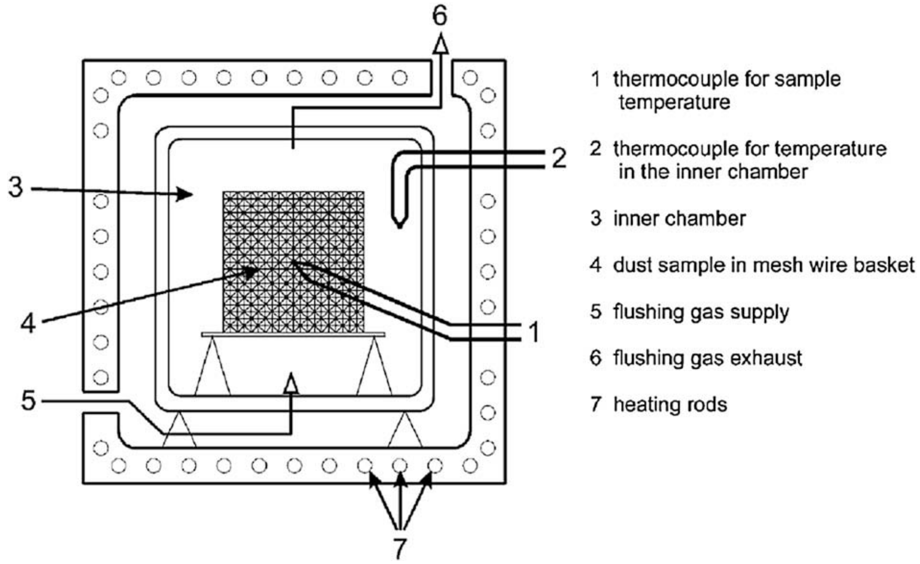


Fig. 1. Hot storage test set-up.

continuously measured in the center of the reactor and acquired by means of a Keithley USB-Box (model KUSB-3108) connected to a portable PC. In order to keep fully aerobic conditions and thus optimal microbial growth, air is continuously flushed into the recipient at a flow rate of approximately 0.02 Nm^3/h. Before coming in the reactor, the air, which is pumped from the surroundings, passes through an active coal bed and a high concentrated potassium hydroxide solution, in order to remove the carbon dioxide present in the atmosphere. Furthermore, the air has to be sterilized by flowing through a sterile filter and to be humidified by bubbling in a washing bottle filled with distilled sterile water.

The outgoing air is led consecutively through three washing bottles, each one filled with 300 mL of a 0.2 molar aqueous barium hydroxide solution. As the air comes in contact with this solution, the carbon dioxide formed during the respiration precipitates as barium carbonate and forms a suspension. The washing bottles are substituted with bottles containing fresh solution at regular time periods: during the change the pump is stopped and the reactor output is closed. This process is very fast and the fully aerobic conditions are still guaranteed.

After removing the precipitate by filtration, the concentration of the consumed solution is checked via titration, using aqueous hydrochloric acid 0.2 molar as titrant and bromothymol blue as pH indicator. From these measurements the amount of carbon dioxide produced by respiration can be easily calculated.

2.3. Large-scale experiments

To provide large-scale experimental data, the evolution of temperature and gas concentrations of oxygen, carbon dioxide, carbon monoxide and methane at different locations of two newly established wood debris piles were monitored:

- The first wood pile (20 × 15 × 6 m in dimensions) was build-up on July 2007 and was analyzed during 10 months. The material consisted of pine wood chips with an average particle size of ~10 mm (broad distribution) and an initial water content of about 35% (Fig. 5, Wood Pile 1).
- To investigate the effect of the particle size, a second pine wood pile (20 × 15 × 5 m) was constructed on May 2008 and was analyzed during 6 months. The material had an average particle size of ~2 mm (narrow distribution) and an initial water content of about 46% (Fig. 5, Wood Pile 2).

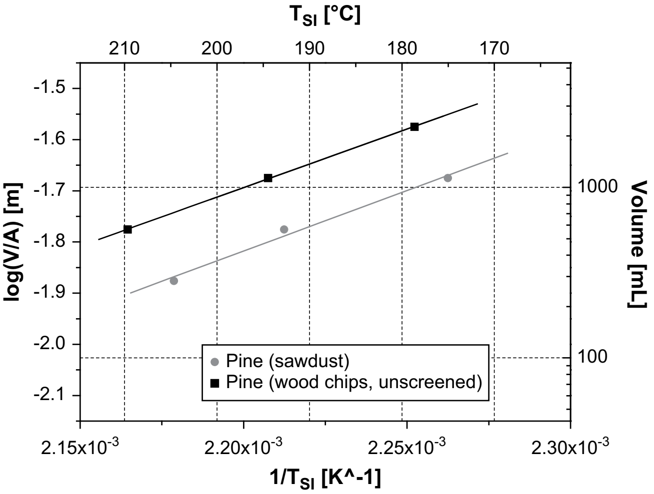


Fig. 2. V/A dependence of the self-ignition temperature for pine wood.

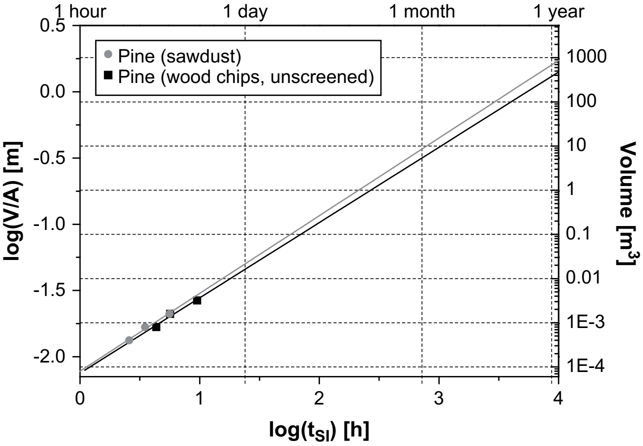


Fig. 3. Extrapolation of the induction time to self-ignition for pine wood.

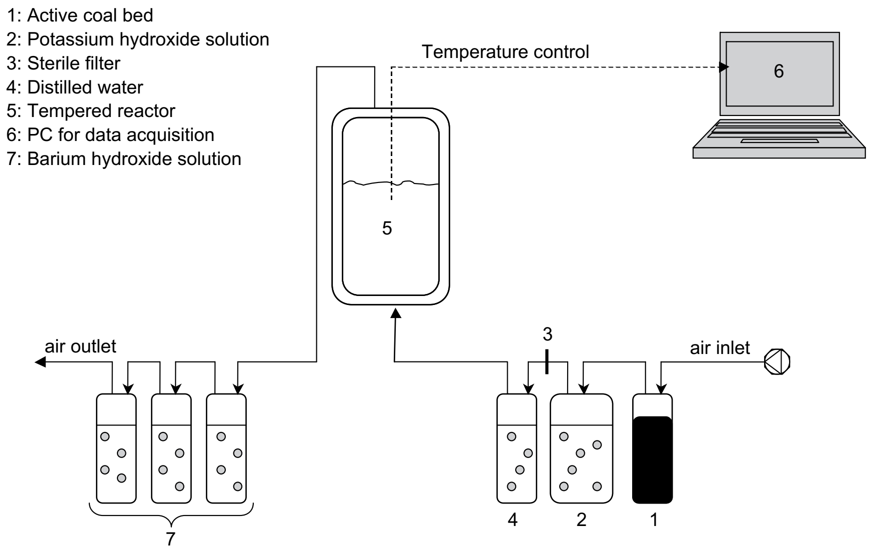
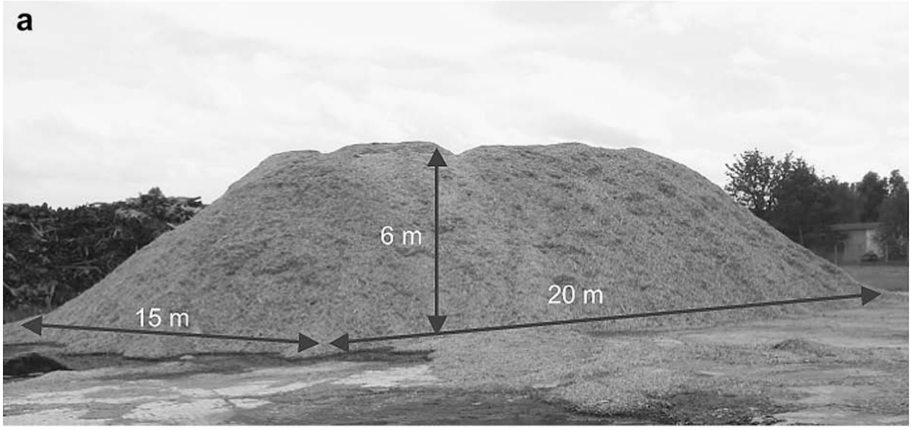


Fig. 4. Schematic drawing of the respiratory test.

Temperature was continuously measured inside the pile by means of up to 18 K-Type thermocouples. Two further sensors were arranged outside the heap to detect the ambient temperature (one for the temperature in the sun and one for the temperature in the shadows). The thermocouples were connected with three 4-Channels data-loggers model TL309, PCE Group, and two 4-Channels model SP-1700, Veriteq, which allowed storing a value every 30 min for each sensor. Solar cells provided the necessary energy

Wood Pile 1: Pine wood (average particle size ~10 mm)



Wood Pile 2: Pine wood (average particle size ~2 mm)

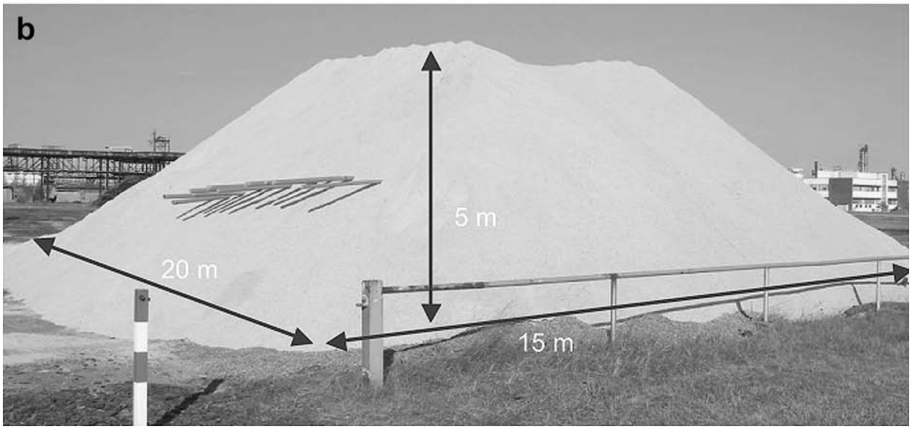


Fig. 5. Photographs of the established wood piles.

for the data-loggers to work for the entire storage period. In order to protect them from rain/adverse weather conditions, the data-loggers were stored inside a sealed-box.

Gas measurements were taken discontinuously by means of an oxygen analyzer (Servomex Gasanalysator 5200) and of a mobile FTIR-Spectrometer (Gasmet Model Dx4000N) for carbon dioxide, carbon monoxide and methane. In order to reach the inner part of the pile, steel tubes were inserted in the material during its piling. These tubes remained closed at the outer end when no data were taken. During the measurements, the outer ends were opened and connected to the oxygen analyzer and to the spectrometer. Gas transfer to the measuring devices was guaranteed by the internal pump of the spectrometer.

3. Modeling

The model used in the calculations covers the effects of self-heating and ignition through the combustible bulk material and makes the following assumptions:

- Conductive heat transfer and diffusive transport mechanism inside the bulk phase occur,
- Convective currents are considered by increasing the diffusion coefficient,
- Bulk material is homogeneous and isotropic,
- Material properties are independent of time and temperature.

The temperature (T) and concentration (C_k) fields were solved with a Fourier-type Eq. (1) and with Fick-type Eq. (2), respectively.

$$\frac{\partial T}{\partial t} = \frac{\lambda}{\rho \cdot c_P} \cdot \text{div grad } T + S_T \tag{1}$$

$$\frac{\partial C_k}{\partial t} = D_k \cdot \text{div grad } C_k + S_{C_k} \tag{2}$$

In Eq. (1) S_T represents the sum of heat productions arising from chemical S_{T_chem}, physical S_{T_phys} and microbial processes S_{T_bio}, as expressed in Eq. (3). In Eq. (2) each substance k considered is converted at its specific rate S_{C_k} during the three parallel thermal processes.

$$S_T = S_{T_\text{chem}} + S_{T_\text{phys}} + S_{T_\text{bio}} \tag{3}$$

Resuming, the model consists of 11 coupled time dependent partial differential equations (PDE) solving the temperature field and 10 concentration fields (fuel, oxygen, carbon monoxide, carbon dioxide, methane, water, water vapor, easy-biodegradable substrate, slowly-biodegradable substrate and biomass). For solving the system of equations numerically, the commercial Finite-Element-Code COMSOL Multiphysics was used.

In the following paragraphs it will be separately described how the three energy sources (chemical, physical and microbial heat) contributing to the warming-up of a wood pile have been determined.

3.1. Chemistry

For the simulation of the oxidation/combustion reactions a model based on the works of Krause, Schmidt, and Lohrer (2006) and Schulze (2005) was used. The combustion process of biomass can be described by a general equation, in the form of Eq. (4). Chemical species included are fuel (formed by C, H, O and moisture), oxygen, carbon monoxide, carbon dioxide, methane, and water (as vapor). The stoichiometric coefficients of the combustion are determined experimentally, as described by Schulze (2005).

$$\nu_\text{fuel} C_x H_y O_z + \nu_1 O_2 \rightarrow \nu_2 CO_2 + \nu_3 CO + \nu_4 CH_4 + \nu_5 H_2O \tag{4}$$

For the decomposition of the solid fuel an Arrhenius-type reaction rate, as given in Eq. (5), applies:

$$S_{C_\text{fuel}} = -C_\text{fuel} \cdot k_0 \cdot \exp\left(-\frac{E}{R \cdot T}\right) \tag{5}$$

Here, C_fuel is the fuel concentration, k_0 is the pre-exponential factor, E the apparent activation energy specific for the combustion 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 on the temperature, on the concentration of the fuel only: a first order kinetic for the wood decomposition has been assumed in many studies (Nunn, Howard, Longwell, & Peters, 1985 as well as Rostami, Murthy, & Hajaligol, 2004, among others).

Eq. (6) defines then the conversion rates of the substances produced/consumed in this reaction:

$$S_{C_k} = \frac{\nu_k}{\nu_\text{fuel}} \cdot \frac{M_k}{M_\text{fuel}} S_{C_\text{fuel}} \tag{6}$$

where ν_k is the stoichiometric coefficient of the species k for the combustion reaction equation and M_k is its molecular weight. Note that the stoichiometric coefficients are always negative for reactants and positive for products.

The chemical heat source term S_{T_chem} is the reaction enthalpy, as shown in the following equation:

$$S_{T_\text{chem}} = -\frac{1}{\rho \cdot c_P} \Delta H_R S_{C_\text{fuel}} \tag{7}$$

As boundary settings a Neumann condition for the temperature field and a Dirichelet condition on the concentration for the gas species was given. This means, for the heat transfer a condition on the heat flux was defined, while for the mass transfer constant concentrations at the bounduary were set.

3.2. Physics

The combustion process and thus the self-ignition are also affected by the moisture transport, since vaporization/desorption and condensation/adsorption of water can subtract or produce heat, respectively. According to Lohrer et al. (2005), the source terms of the transport species liquid water and vapor (not reacting) can be calculated by Eqs. (8) and (9), respectively. The heat source term related to physical processes can be then calculated by Eq. (10).

$$S_w = -\text{EV} \cdot C_w \cdot \exp\left(-\frac{\Delta H_v \cdot M_{H_2O,\text{liq}}/1000}{R \cdot T}\right) + \text{CD} \cdot C_v \tag{8}$$

$$S_v = -S_w \tag{9}$$

$$S_{T_\text{phys}} = S_w \cdot \Delta H_v \tag{10}$$

The first part of Eq. (8) represents the evaporation/desorption of liquid water (index w) while the second part denotes the condensation/adsorption of water vapor (index v). Eq. (8) is an empirical equation, since the coefficients EV and CD are V/A-dependent constants, which have to be determined experimentally for every substance. The initial water concentration is determined from the moisture content and the initial water vapor concentration from the air relative humidity and temperature.

3.3. Microbiology

As mentioned, microbial activity occurring in stored organic material like compost or wood chips are highly exothermal and can bring an important additional heat source (Weppen, 2001). The most important heat sources in wood chip piles have to be found in the aerobic processes, i.e. processes in which microorganisms consume oxygen for their metabolism (Springer and Hajny, 1970).

To predict the aerobic metabolism, a model based on the one proposed by Tremier, de Guardia, Massiani, Paul, and Martel (2005) was chosen. This model determines the oxygen consumption kinetics, which can be related to the microbial heat production and introduces three new modeling variables, which actively contribute to the oxygen consumption:

- The microorganisms, referred to as biomass (X);
- The easily-biodegradable fraction (MB), which can be immediately consumed by microorganisms (for example free sugars) and which is already in the aqueous phase;
- The slowly-biodegradable fraction (MH), which is composed of solid or soluble macromolecules (in the case of wood mainly cellulose, lignin and hemicelluloses), that have to be hydrolyzed, before being metabolized.

A fourth fraction (the inert or non-biodegradable fraction MI) which appears in the publication of Tremier et al. (2005) is not concerned by biological reactions and has been therefore not included in our model. Eqs. (11)–(14) describe the reaction rates for the microorganisms, the easy and the slowly-biodegradable fraction and the related oxygen consumption from respiration, respectively:

$$S_X = \mu_m \frac{\mathrm{MB}}{K_\mathrm{b} + \mathrm{MB}} X - bX \tag{11}$$

$$S_\mathrm{MH} = -K_\mathrm{h} \frac{\mathrm{MH}/X}{K_\mathrm{MH} + \mathrm{MH}/X} X \tag{12}$$

$$S_\mathrm{MB} = -\frac{1}{Y} \mu_m \frac{\mathrm{MB}}{K_\mathrm{b} + \mathrm{MB}} X + K_\mathrm{h} \frac{\mathrm{MH}/X}{K_\mathrm{MH} + \mathrm{MH}/X} X \tag{13}$$

$$S_{\mathrm{O}_2} = \frac{1 - Y}{Y} \mu_m \frac{\mathrm{MB}}{K_\mathrm{b} + \mathrm{MB}} X + b(1 - f)X \tag{14}$$

Two additional equations are introduced. Eq. (15) describes the carbon dioxide production, which is related to the growing microorganisms and Eq. (16) calculates the microbial heat production by multiplying the oxygen consumption rate by the oxycaloric coefficient, i.e. the amount of heat produced pro-mole oxygen during aerobic respiration.

$$S_{\mathrm{CO}_2} = Y_{\mathrm{CO}_2} \mu_m \frac{\mathrm{MB}}{K_\mathrm{b} + \mathrm{MB}} X \tag{15}$$

$$S_{T_\mathrm{bio}} = S_{\mathrm{O}_2} \cdot q_{\mathrm{O}_2} \tag{16}$$

Since the original model was developed for aerobic processes during composting, its parameters have been adapted to the case of wood decomposition. In particular microorganism growth kinetics on pine wood have been determined experimentally (see Section 2.2 for the set-up and Section 4.2 for the results).

4. Results and discussions

4.1. Hot storage tests

In Fig. 6 the experimental values of the self-ignition temperature obtained by means of the hot storage test are compared with the results of the simulation for different wood chips species. Since during the hot storage tests the temperature surrounding the sample is higher than 80 °C – temperature at which it can be considered that the microbial activity ceases – and since the sample reaches fast this temperature, the microbial heat production is not relevant. Therefore, in the calculation referring to Fig. 6 only the chemical and physical heat source (Eqs. (7) and (10), respectively) were implemented in the calculation.

The values of the numerically simulated and the experimentally determined T_SI are in good agreement for all tested wood samples. Furthermore, in all cases the simulated values were somewhat lower than in the experiments, yielding to a conservative estimation. The results shown in Fig. 6 validate the model for what concerns the prediction of the chemical and physical heat source.

4.2. Respirometric tests

Figs. 7 and 8 show the microbial carbon dioxide production along time for the respirometric tests performed with pine wood chips with an average particle size of 10 mm, at 30 and 40 °C, respectively. In both cases, the reactor was filled with 1.2 kg wet weight of material, with an initial moisture content of 50%, which is an optimal value for the growth of microorganisms (Fengel and Wegener, 1984).

Independent of the incubation temperature, the carbon dioxide production increased intensively to its maximum value within the first 30–40 h after the start of the test. This high respirometric activity reflects a high metabolic activity and a very intense growth rate of the microorganisms present in the wood. Fengel and Wegener (1984) reported the use of the easiest-biodegradable und highly-energetic components of wood, e.g. sugars and amino acids, as substrate in the first stages. This high microbial activity is the principal cause of the intense heat production, which normally occurs after the building-up of wood piles (Springer and Hajny, 1970). According to our experiments, carbon dioxide production rate is higher for incubation temperatures of 40 °C rather than 30 °C.

In the isothermal experiments at 30 °C a second peak in the carbon dioxide production was observed after 1450 h. This second

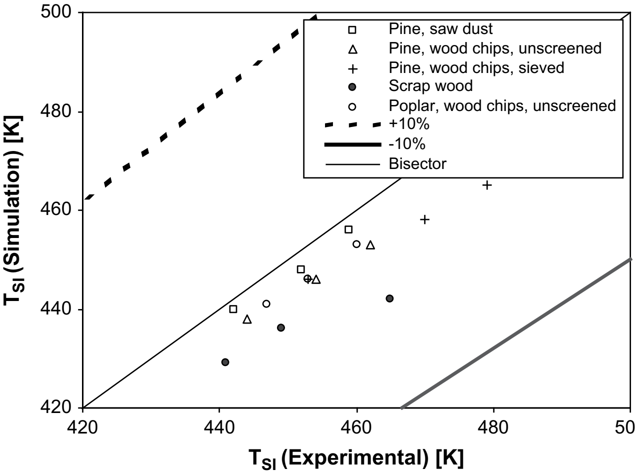


Fig. 6. Comparison of the numerically simulated and experimentally determined self-ignition temperatures for the investigated woods.

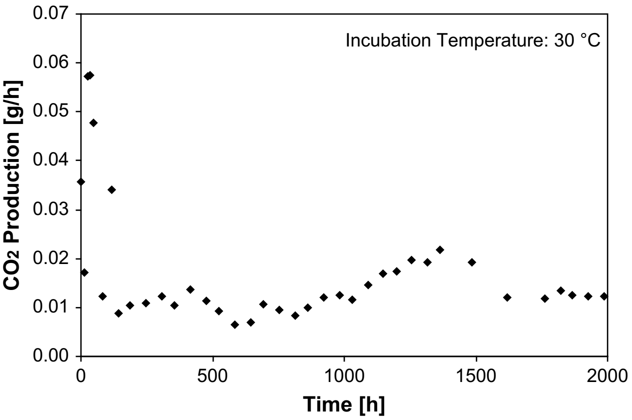


Fig. 7. Carbon dioxide production over time during the incubation of pine wood chips at a temperature of 30 °C.

peak was less intense and therefore the resulting heat production would be much more contained. The appearance of the second carbon dioxide production maximum results probably from a different typology of wood decomposition: after the successful establishment of habitat-specific microorganisms also less biodegradable wood components (e.g. cellulose) can be metabolized and/or the availability of easy-biodegradable fractions is temporarily increased due to the establishment of successional microbial communities, see De Boer, Folman, Summerbell, and Boddy (2005).

The experimental curves of the carbon dioxide production were used to determine the microorganisms growth rate (μ_m) on pine wood: the best fit of the simulated to the experimental values was obtained for μ_m of 0.22 and 0.28 h^{-1} for incubation temperatures of 30 and 40 °C, respectively. Since only a microbial community is included in the model, the second peak in the carbon dioxide production curves by 30 °C cannot be identified. As the most of the heat is released during the first stages (up to the first peak in the experimental curves), this does not affect the prediction of the temperature inside the pile, which is the main objective of this work.

It has to be noticed, that the stochastic properties of the wood affection brought to a large data dispersion in the absolute value of the carbon dioxide production peaks in replicated experiments. The calculated growth rates contain therefore a certain imprecision. The effect of these and other variables on the model predictions was considered in a sensitivity analysis performed when applying the model to large-scale scenarios and will be discussed later.

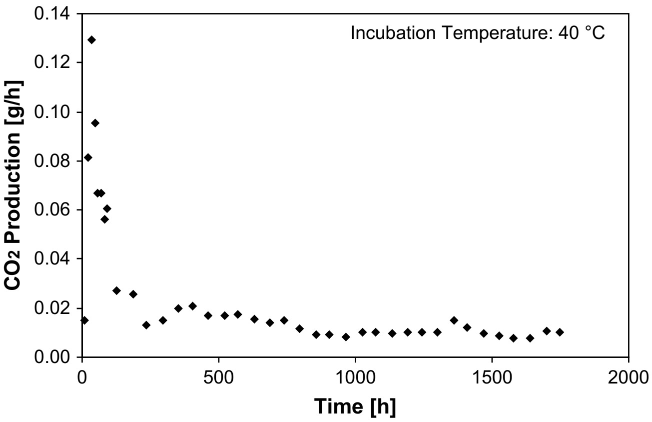


Fig. 8. Carbon dioxide production over time during the incubation of pine wood chips at a temperature of 40 °C.

4.3. Large scale

In order to validate the developed mathematical model in its complete form (chemical, physical and microbial heat production), simulations of the heating-up of large-scale wood piles were performed. In Fig. 9 the model predictions of the temperature in the pile center are compared with the experimental results of the two measured wood piles. The parameters used in the calculations are shown in Table 1. The very high value for the oxycaloric coefficient (2000 kJ/mol oxygen) has been taken from the work of Von Stockar and Birou (1989), under the consideration that the microbial investment of energy for oxidative processes increases strongly under non-optimal aerobic conditions, which are common in the inner parts of a large wood pile.

The best predictions of the model were obtained for the pine wood pile with material of smaller particle size: as it can be seen from Fig. 9b, the temperature in the center of the pile is predicted well during almost all the storage time. Particularly, the maximum value generated by the simulation is in very good agreement with the experimental data (67 °C).

Fig. 9a shows that the model predictions for the pile with pine wood with a bigger particle size are poorer. Probably, this is caused by considering the convection with increased diffusion factors and not with real velocity fields: due to the bigger particle size of the Wood Pile 1 (average of 10 mm) these velocity fields could

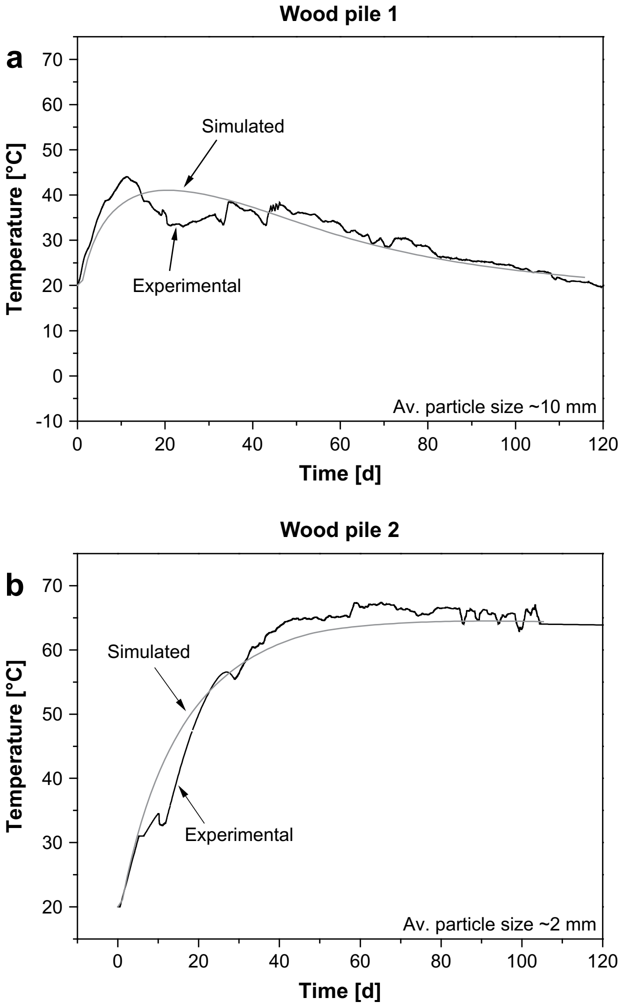


Fig. 9. Temperature evolution in the center of the Wood Piles 1 (a) and 2 (b): model predictions vs. experiments.

Table 1
Summary of the default values of the coefficients and parameters used in the calculations for Wood Pile 1 and Wood Pile 2 (Fig. 9).

Parameter	Wood Pile 1	Wood Pile 2	Description	Unit	Source
b	2.775E-5	2.775E-5	Biomass death rate constant	[s^{-1}]	Literature, Tremier et al., 2005
C_{fuel}	136	225	Fuel initial concentration	[kg/m^3]	Experimental, wood density
C_{O_2}	0.252	0.252	O_2 initial concentration	[kg/m^3]	Experimental
C_{CO_2}	0	0	CO_2 initial concentration	[kg/m^3]	Assumed
C_{CO}	0	0	CO initial concentration	[kg/m^3]	Assumed
C_{CH_4}	0	0	CH_4 initial concentration	[kg/m^3]	Assumed
CD	0.000027	0.00004	Pre-exponential factor condensation/adsorption	[s^{-1}]	Experimental, hot storage test
c_p	1350	1500	Specific heat of wood	[J/kg K]	Experimental
D_k	8.00E-3	8.00E-3	Gas species diffusion coefficient	[m^2/s]	Increased diffusion coefficients
E/R	11,667	12,509	Activation energy/R	[K]	Experimental
EV	0.015	0.001	Pre-exponential factor evaporation/desorption	[s^{-1}]	Experimental, hot storage test
f	0.2	0.2	Fraction of dead biomass converted to inert	[-]	Literature, Tremier et al., 2005
k_0	9.64E + 4	8.15E + 5	Pre-exponential factor	[s^{-1}]	Experimental
K_b	0.009317	0.009317	Substrate saturation constant for MB	[kg/m^3]	Literature, Tremier et al., 2005
K_h	4.244E-5	4.495E-5	Hydrolysis constant	[s^{-1}]	Estimated
K_{MH}	6.5	6.5	Saturation constant for the group MH/X	[-]	Literature, Tremier et al., 2005
M_{fuel}	0.030	0.030	Fuel molecular weight	[kg/mol]	Experimental
M_{O_2}	0.032	0.032	O_2 molecular weight	[kg/mol]	
M_{CO_2}	0.044	0.044	CO_2 molecular weight	[kg/mol]	
M_{CO}	0.028	0.028	CO molecular weight	[kg/mol]	
M_{CH_4}	0.016	0.016	CH_4 molecular weight	[kg/mol]	
$M_{H_2O,\mathrm{vap}}$	0.018	0.018	H_2O (vap) molecular weight	[kg/mol]	
$M_{H_2O,\mathrm{liq}}$	0.018	0.018	H_2O (liq) molecular weight	[kg/mol]	
MB_0	6.8	8.1	MB initial concentration	[kg/m^3]	Estimated
MC_0	0.35	0.46	Initial moisture content	[-]	Measured, Karl-Fischer
MH_0	130	218	MH initial concentration	[kg/m^3]	Estimated
q_{O_2}	62.5	62.5	Oxycaloric coefficient	[kJ/kg]	Literature, Von Stockar & Birou, 1989
R	8.314	8.314	Gas Universal constant	[J/mol K]	Constant
RH_0	0.94	0.76	Relative humidity (initial, assumed constant)	[-]	Measured, weather station
T_0	293	293	Initial temperature of wood	[K]	Experimental
$T_{0,\ \mathrm{air}}$	286	286	Air temperature (initial)	[K]	Measured, weather station
X_0	2.76E-2	3.45E-2	Biomass initial concentration	[kg/m^3]	Estimated
Y	0.68	0.68	Biomass yield on MB	[-]	Literature, Tremier et al., 2005
Y_{CO_2}	1.79	1.79	Biomass yield on CO_2	[-]	Literature, Koutinas, Wang, & Webb, 2003
α	8	8	Heat transfer coefficient	[$W/m^2\,K$]	Calculated, natural convection
ΔH_R	2.01E + 7	2.01E + 7	Calorific value	[J/kg]	Experimental
ΔH_v	2.1e6	2.1e6	Water evaporation enthalpy	[J/kg]	
λ	0.188	0.069	Wood thermal conductivity	[W/m K]	Experimental
μ_m	7.094E-5	7.094E-5	Biomass growth rate constant	[s^{-1}]	Experimental, respirometric tests
ν_{fuel}	−1	−1	Fuel stoichiometric coefficient	[-]	Experimental
ν_1	−0.961	−0.961	O_2 stoichiometric coefficient	[-]	Experimental
ν_2	0.79	0.79	CO_2 stoichiometric coefficient	[-]	Experimental
ν_3	0.189	0.189	CO stoichiometric coefficient	[-]	Experimental
ν_4	0.021	0.021	CH_4 stoichiometric coefficient	[-]	Experimental
ν_5	0.812	0.812	H_2O (vap) stoichiometric coefficient	[-]	Experimental
ρ	210	300	Average wood density	[kg/m^3]	Experimental

contribute to enhance the cooling-down of the pile registered after the 10th day of storage. Nevertheless, the most important parameter, i.e. the absolute maximum temperature experimentally achieved (45 °C) could be represented by the model with an error smaller than 10%.

For both wood piles the microbial heat production was responsible for the fast initial temperature increase, since it was much higher than the other two heat sources. This result is in agreement with the experiments of (Springer and Hajny, 1970). Anyway, microbial activity and the related heat production ceases as soon as the easy-biodegradable fractions of wood are consumed, i.e. a few days after the start of storage. Since for the investigated pile geometries the achieved temperatures were not critical, no self-ignition was observed.

In order to demonstrate the possibility of occurrence of a self-ignition, a simulation of a larger wood pile (height = 12 m, width = 60 m, material: pine wood with particle size smaller than 4 mm) was performed. Assuming a pile length much higher than its width, a 2D calculation could be performed. Furthermore, due to symmetry in the geometry, only one half of the pile was computed. The material was considered to be stored at an ambient temperature of 15 °C. Due to the fact that the pile dimensions are larger than those of the investigated real piles, criticality was reached, whereas most parameters were held constant (some parameters, like EV und CD decrease with the pile volume, like shown by Lohrer et al. (2005) and had to be adapted). According to the calculations a self-ignition would be registered after about 310 days, as it can be seen in Fig. 10 (in this picture the results of the calculations in the computed half of the pile were mirrored, to give a clearer illustration). It has to be noticed that, if no microbial heat source would be implemented in the model, no self-ignition would be observed. Even if microbial activity ceases for temperatures higher than 80 °C, these processes do accelerate the other heat release rates and can turn a non-critical pile into criticality.

In Table 2 the results of the sensitivity analysis of the model applied to large-scale scenarios are shown. The effects of variations of ±25% and ±75% of the most important model parameters on the maximum temperature, minimum oxygen concentration, as well as on the carbon dioxide and biomass maximum concentrations were studied:

- Effect of growth rate (μ_m): a variation −75% of this parameter had strong effects on all output parameters, while variations of

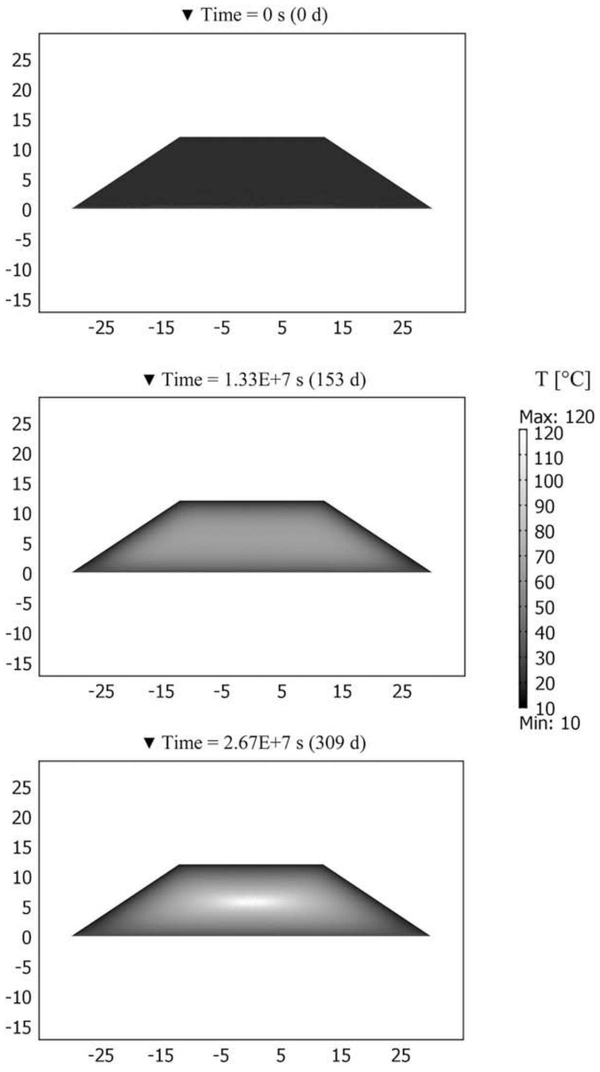


Fig. 10. Study of the self-ignition of a pine wood pile (height = 12 m, width = 60 m, material stored at an ambient temperature of 15 °C).

±25% and of +75% did only influence slightly the carbon dioxide and oxygen concentration peaks, but not the biomass concentration peak and maximum temperature.

- Death rate (b): increases of +25% and of +75% caused changes in all output parameters. Anyway, the highest variation was registered in the biomass maximum concentration for a decrease of b of −75%.
- Hydrolysis constant (K_h): the biggest effect of this parameter was to be found in the biomass concentration peaks and, in the case of a −75% variation, on the maximum temperature, which dropped strongly.
- Substrate saturation constant for the easy-biodegradable fraction (K_b): this was one of the less sensitive parameter, since only slight changes in the carbon dioxide maximum for variations of −75% were observed.
- Hydrolysis saturation constant (K_{MH}): variation of this variable had no influence on the output parameters.
- Biomass yield on easy-biodegradable fraction (Y): variations of this parameter had high influence on all concentration peaks. The maximum temperature was mostly affected by reductions of Y.
- Fraction of dead biomass converted to inert (f): variations of ±75% of this parameter showed a slight influence on the maximum temperature and on the oxygen concentrations. No other variations had relevant effects.
- Biomass, easy and slowly-biodegradable fractions initial concentrations (X_0, MB_0, MH_0): the least sensitive of these three parameters was the initial biomass concentration, which variations did not show any effect on any of the outputs. On the other hand, variations of MB_0 had big influence on all parameters except on the maximum temperature. Finally, changes in the slowly-biodegradable fraction initial concentration affected among all the maximum temperatures.
- The pre-exponential factors for evaporation/desorption (EV) and for condensation/adsorption (CD) had as expected no effect on the concentration peaks, but affected extremely the maximum temperature.
- The diffusional coefficients D_k did not influence the maximum temperature and the biomass concentration peaks, but changed strongly the oxygen concentration minimum and the carbon dioxide concentration maximum.

The analysis shows the high sensitivity towards the input parameters of the model and the difficulties encountered when

Table 2
Qualitative results of the sensitivity analysis.

Parameter ►	μ_m				b				K_h				K_b				K_{MH}			
▼Effect on:	+25%	−25%	+75%	−75%	+25%	−25%	+75%	−75%	+25%	−25%	+75%	−75%	+25%	−25%	+75%	−75%	+25%	−25%	+75%	−75%
T_{max}	–	–	–	↓↓↓	↓↓	–	↓↓↓	–	–	↓	–	↓↓↓	–	–	–	–	–	–	–	–
$C_{O_2,min}$	↓	↑	↓	↑↑↑	↑↑	↓	↑↑↑	–	–	–	↓↓	–	–	–	–	–	–	–	–	–
$C_{CO_2,max}$	↑	↓	↑	↓↓↓	↓↓	↑	↓↓↓	↑↑	↑	–	↑↑	↓↓	–	–	–	↑	–	–	–	–
X_{max}	–	–	–	↓↓↓	↓↓	↑↑	↓↓↓	↑↑↑	↑	–	↑↑↑	↓↓↓	–	–	–	–	–	–	–	–
Parameter ►	Y				f				X_0				MB_0				MH_0			
▼Effect on:	+25%	−25%	+75%	−75%	+25%	−25%	+75%	−75%	+25%	−25%	+75%	−75%	+25%	−25%	+75%	−75%	+25%	−25%	+75%	−75%
T_{max}	–	↓↓	↓	↓↓↓	–	–	↓	↑	–	–	–	–	–	–	–	–	↑	↓	↑	↓↓
$C_{O_2,min}$	↓	–	↓↓↓	↓	–	–	↑	↓	–	–	–	–	↓	↑	↓↓	↑↑↑	–	–	–	↑
$C_{CO_2,max}$	↑	↓	↑↑↑	↓↓↓	–	–	–	–	–	–	–	–	↑	↓	↑↑	↓↓↓	–	–	–	↓
X_{max}	↑↑	↓↓	↑↑↑	↓↓↓	–	–	–	–	–	–	–	–	↑	↓	↑↑	↓↓↓	–	–	–	↓
Parameter ►	EV				CD				D_k											
▼Effect on:	+25%	−25%	+75%	−75%	+25%	−25%	+75%	−75%	+25%	−25%	+75%	−75%								
T_{max}	↓	↑	↓	↑↑↑	↑↑	↓	↑↑↑	↓↓	–	–	–	–								
$C_{O_2,min}$	–	–	–	–	–	–	–	–	↑	↓	↑↑	↓↓↓								
$C_{CO_2,max}$	–	–	–	–	–	–	–	–	↓	↑	↓↓	↑↑↑								
X_{max}	–	–	–	–	–	–	–	–	–	–	–	–								

–, No appreciable variation of the output parameter; ↑, Increase of the output parameter; ↑↑, Strong increase of the output parameter; ↑↑↑, Extreme increase of the output parameter; ↓, Decrease of the output parameter; ↓↓, Strong decrease of the output parameter; ↓↓↓, Extreme decrease of the output parameter.

trying to simulate these kinds of coupled processes. In our case, among all the parameters studied the most sensitive were:

- The pre-exponential factors for evaporation/desorption (EV) and for condensation/adsorption (CD) on the maximum temperature;
- The diffusional coefficients D_k on the oxygen concentration minimum and carbon dioxide maximum;
- The death rate (b) and the biomass yield on easy-biodegradable fraction (Y) on the biomass concentration peak.

On the other hand, the less sensitive parameters were the substrate saturation constants (K_b and K_{MH}) and the biomass initial concentration (X_0).

5. Conclusions

In this paper a simplified model for predicting the heating-up and the possible self-ignition of large-scale wood piles is presented. The model includes three heat sources, which contribute to the temperature increase inside the pile: a chemical heat source from Arrhenius-type oxidations, a physical heat source, related to evaporation/adsorption and condensation/desorption processes and a heat source deriving from microbial exothermal reactions. The model, which consists of a system of coupled heat and mass transfer differential equations, has been solved with the Finite-Element-Code COMSOL Multiphysics.

Two types of laboratory tests have been performed. Firstly, the standard laboratory scale investigation of the self-ignition temperature has been performed, as to develop simplified reaction models for the chemical and physical processes. Furthermore, respirometric experiments have been carried out in order to investigate the microbial activity on wood and to adapt previous models to this material: the best model adaptation resulted in microorganism growth rates of 0.22 and 0.28 h^{-1} for incubation temperatures of 30 and 40 °C, respectively.

In order to provide large-scale experimental data to validate the global model, which computes simultaneously the chemical, physical and microbial heat sources, measurement in two newly established pine wood piles (volumes bigger than 1000 m^3) were performed. In these large-scale experiments, the evolution of temperature and gas concentrations of oxygen, carbon dioxide, carbon monoxide and methane at different locations were monitored. Simulations are in good agreement with experimental data, especially when predicting the maximum achieved temperature and the temperature rise in the center of the piles.

Examples of computations for larger geometries showed that the global model can predict the achievement of critical conditions and therefore help to identify possible self-ignition scenarios and avoid undesired fires.

A performed sensitivity analysis of the developed model showed the difficulties when simulating coupled heat and mass transfer processes with various heat sources. The maximum temperature in the pile center was very high sensitive to the evaporation/desorption and condensation/adsorption pre-exponential factors, while the gas concentration peaks were strongly affected by the diffusional coefficients. The biomass concentration maximum was strongly influenced by the microorganism death rate and the biomass yield on easy-biodegradable fraction.

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