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A numerical simulation of spontaneous ignition of bagasse

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Abstract

This paper presents a numerical study of spontaneous ignition of a bagasse cube basket inside a convective oven. The study considered a cubic bagasse mass as a porous medium allowing oxygen from the surroundings to diffuse into and react with the interior of the bagasse matrix. A set of coupled partial differential equations of heat and mass transfer was solved numerically with a well-known CFD software package, ANSYS FLUENT. The simulated results were then compared with experimental measurements. In general, good agreement between the simulated and measured centre temperatures of a cubic bagasse basket was obtained. Simulation results demonstrated that as the cubic bagasse basket size and its initial moisture content increased the spontaneous ignition time increased. Alternatively, decreasing the porosity increased the spontaneous ignition time. The differences between 2D and 3D simulation results were also investigated. It was found that the simulated centre temperature in the 3D simulation was slightly higher than that obtained from 2D calculations.

Keywords: Ignition simulation, Spontaneous ignition, Bagasse, Fire safety

1. Introduction

Spontaneous ignition of a bagasse stockpile arises when oxygen is present to maintain a low temperature reaction of bagasse, but the heat generated by the exothermic process of bagasse decomposition is not adequately dissipated by conduction or convection. This causes a temperature increase inside the bagasse mass. The bagasse oxidation rate depends on a local temperature and oxygen concentration within the bagasse matrix. An increase in temperature leads to a higher oxidation rate and eventually thermal runaway occurs resulting in a self-ignition.

Bagasse is the residue from sugar extraction and it is the principal fuel used at sugar mills. In the 2017-2018 crop year, Thailand was the worlds' second-largest sugar exporter following Brazil [1]. The sugar production in that crop year was more than 14.7 million metric tons. Spontaneous ignition of large bagasse stockpiles with a potential to transition into endogenous fires can cause large economic losses. It represents a direct hazard to sugar factories and the surrounding environment. There have been many instances in which spontaneous ignition inside large bagasse stockpiles developed into fires. There are several examples of this in sugar factories in Khon Kaen [2] and in Nakhon Ratchasima provinces[3]. From a concern of fire safety, it is interesting to examine how the relevant parameters and conditions can affect spontaneous ignition so that fire safety engineers may be able to determine under which conditions spontaneous ignition can occur and how to avoid it.

Previously, theoretical and experimental work was done by Boonmee and Pongsamana [4]. They demonstrated a method to determine a safe bagasse stockpile size based on the classic spontaneous ignition theory developed by Frank-Kamenetskii [5]. The bagasse kinetic parameters were obtained using two methods, the Frank-Kamenetskii [5] and the crossing-point methods[6-9]. Unfortunately, the Frank-Kamenetskii spontaneous ignition theory is based on a quasi-steady heat conduction equation. Thus, the time for spontaneous ignition to occur cannot be obtained. Moreover, a bagasse stockpile is a porous medium. Thus, diffusion of oxygen from surroundings to react with bagasse inside the stockpile is present. It is practically impossible to include the transient and oxygen diffusion effects into the problem to determine a closed form solution of a safe bagasse stockpile size. Therefore, a numerical modeling of the problem comes into play. Such modeling has the capability to solve a set of coupled partial differential equations. Thus, it offers the great advantage of high flexibility to simultaneously account for various coupled processes, including transient and oxygen diffusion effects.

Some numerical simulations of spontaneous ignition of coal storage facilities have been done by Handa et al. [10], Ejlali et al. [11], Zhu et al. [12], and Akgun and Essenhigh [13]. Yuan and Smith [14-15] coupled transient heat and mass transfer equations that were numerically solved by a well-known commercial CFD (Computational Fluid Dynamics) software package, FLUENT. Other researchers performed numerical simulations considering biomass fuel. For instance, Yan et al. [16] did numerical simulations of

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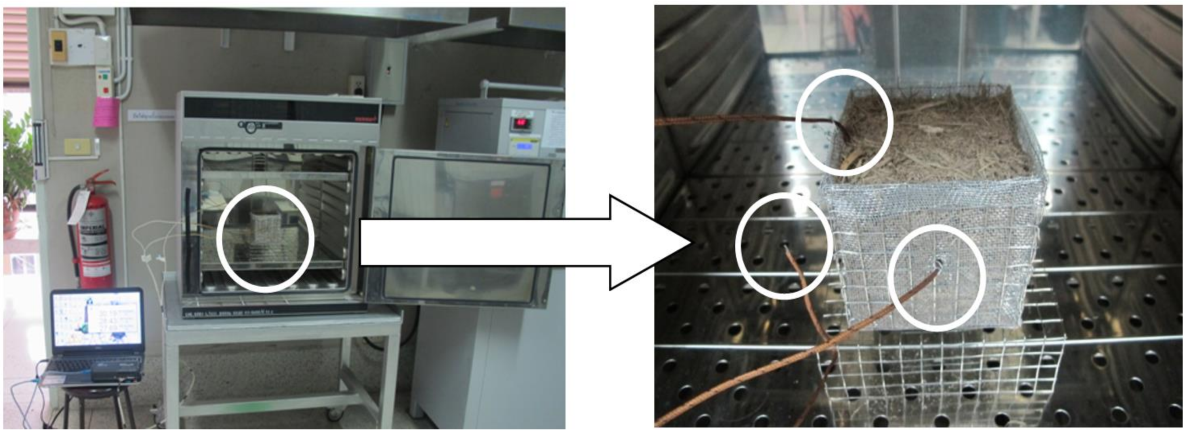

Three thermocouples are used to measure the oven and sample temperatures.

Figure 1 Experimental setup for a study of spontaneous ignition of bagasse from [4].

bulk bio-mass fuel (sawdust and small wood pellets) with an in-house CFD code called SMAFS (Smoke Movement and Flame Spread). The effects of temperature distribution within the bulk fuel and the initial moisture content of the sample were discussed in their work.

Nevertheless, no previous work has been done for bagasse. Therefore a computational simulation of spontaneous ignition of bagasse was carried out in the current work. The purpose of this paper is to numerically study a self-ignition process of a cubic bagasse bulk inside a convective oven and compare the results with previous experimental work [4]. The study considered a cubic bagasse bulk as a porous medium allowing oxygen from the surroundings to diffuse into and react inside a bagasse matrix. A set of coupled partial differential equations of heat and mass transfer was solved numerically with a well-known CFD software ANSYS FLUENT. The simulation was based on the solution of a set of transient conservation equations. They included the mass equation, the momentum equations with Darcy's law in porous media, the energy equations for both gas and solid phases and the species equations with chemical reactions. The effects of 2D and 3D governing equations, cubic sample size, initial moisture content and porosity were investigated in this work.

2. The experiments

Spontaneous ignition experiments of bagasse were performed previously by [4]. Here, a brief description of the experimental setup is provided to facilitate understanding of the development of the current CFD model. Figure 1 shows the experimental setup to study spontaneous ignition of bagasse in a convective oven. The surroundings (oven), sample surface and sample centre temperatures were continuously recorded using type K thermocouples. The bagasse samples were collected from stockpiles in the field and kept in a conditioned bag to preserve their original state as much as possible. The tests were carried out with three cubic basket sizes which with edge lengths 8, 9 and 10 cm. The bulk bagasse density in the basket for each test was kept constant at approximately 100 kg/m^3. Heating experiments were carried out until the spontaneous ignition temperatures were reached for all the samples. The time required to reach spontaneous ignition was determined. Further details of this experimental work have been published [4].

3. Theoretical model

3.1 Numerical model

A well-known CFD software package, FLUENT, from Fluent, Inc., was utilized in this study to simulate the spontaneous ignition of bagasse in a cubic basket. FLUENT is a general purpose CFD solver for fluid flow, heat transfer and chemical reaction modeling applications. It can model the transport and reactions of chemical species by solving the conservation equations for mass, species, momentum and energy. Multiple chemical reactions can be simultaneously modeled with reactions occurring in the bulk phase (volumetric reactions) and/or on wall or particle surfaces, and in a porous region.

Figure 2 illustrates computational domains used for the bagasse samples in this study. A square domain was employed for 2D simulations while a cubic domain was used for 3D simulations. The coupled partial differential equations for mass conservation, species conservation, momentum conservation with Darcy's law in porous media, and energy conservation equations were numerically solved. A local thermal equilibrium between gas and solid phases was assumed. Thus, only one energy equation was required. Assuming isotropic porosity, the relevant governing equations can be written as follows.

The continuity equation:

$$\frac{\partial(\gamma\rho)}{\partial t}+\nabla.(\gamma\rho\vec{v})=0 \tag{1}$$

where ρ is gas density, γ is porosity and $\vec{v}$ is a gas velocity vector.

The momentum equation with Darcy's law is:

$$\frac{\partial(\gamma\rho\vec{v})}{\partial t}+\nabla.(\gamma\rho\vec{v}.\vec{v})=-\gamma\nabla p+\nabla.(\gamma\bar{\tau})+\gamma\rho\vec{g}-\frac{\gamma^{2}\mu}{K}\vec{v} \tag{2}$$

where p is the pressure, $\bar{\tau}$ is the stress tensor, $\vec{g}$ is the gravitational vector, μ is the molecular viscosity that was assumed to be constant in the calculations, and K is the permeability.

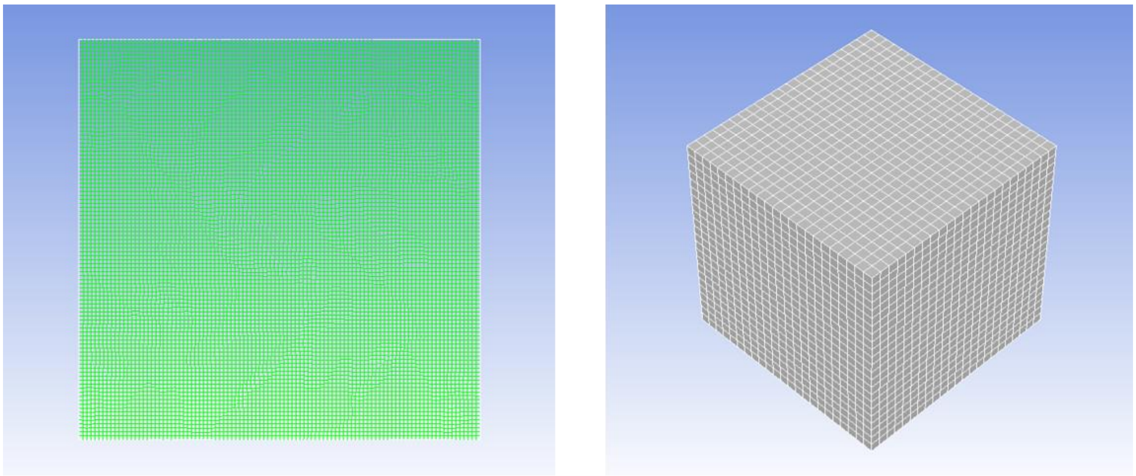
(a) 2D simulation (b) 3D simulation

Figure 2 A computational domain setup in the study (a) 2D simulation and (b) 3D simulation

The gas species transport equation in a porous medium is:

$$\frac{\partial(\gamma\rho Y_i)}{\partial t}+\nabla.(\gamma\rho\vec{v}Y_i)=\nabla.(\gamma\Gamma_i\nabla Y_i)+\gamma\dot{S}_{Y_i} \tag{3}$$

where Γ_i is the diffusion coefficient of the i^{th} species. Y_i is the mass fraction of the i^{th} species.

The species considered in the simulation were oxygen (Y_{O_2}), carbon dioxide (Y_{CO_2}), water vapor (Y_{H_2O}) and nitrogen (Y_{N_2}). $\dot{S}_{Y_i}$ is the rate of production or destruction of the i^{th} species due to bagasse decomposition.

Thermal equilibrium between the solid and gas phases within a porous medium was assumed and thus the energy equation is:

$$\frac{\partial}{\partial t}(\gamma\rho H+(1-\gamma)\rho_S H_S)+\nabla.(\vec{v}(\rho H)) = \nabla.(k_{eff}\nabla T)+\dot{S}_H+\dot{S}_W \tag{4}$$

where H is the enthalpy of gas, H_S is the enthalpy of solid, ρ_S is the solid density, T is the temperature, $\dot{S}_H$ is the enthalpy heat source from bagasse oxidation, $\dot{S}_W$ is the enthalpy heat sink from moisture evaporation, and k_{eff} is the effective thermal conductivity of the porous medium.

The effective thermal conductivity in the porous medium was estimated as the following:

$$k_{eff}=\gamma k+(1-\gamma)k_S \tag{5}$$

where k is gas phase thermal conductivity and k_S is solid medium thermal conductivity.

The porosity parameter γ can range from 0 to 1, where 0 means the computational domain is all solid and 1 is when the computational domain is entirely gas. The porosity of the bagasse γ was defined as:

$$\gamma=1-\frac{\rho_{bulk}}{\rho_{bagasse}} \tag{6}$$

where ρ_{bulk} is the bagasse bulk density and, $\rho_{bagasse}$ is the bagasse solid density.

The permeability was assumed to follow an empirical correlation after [16] as:

$$K=\frac{\gamma^3 d_{bagasse}^2}{150(1-\gamma)^2} \tag{7}$$

where $d_{bagasse}$ is the bagasse particle diameter.

3.2 Bagasse oxidation

The source terms in the species $\dot{S}_{Y_i}$ and energy $\dot{S}_H$ equations require information from the reaction of bagasse with oxygen. The study assumed the bagasse oxidation took place at pore surfaces inside the porous bagasse matrix. Oxygen was allowed to diffuse into the bagasse matrix from the sample surface where the oxygen concentration was at the surrounding value ($Y_{O_2,\infty}$=0.233). The primary products of bagasse oxidation were carbon dioxide (CO_2) and water (H_2O).The chemical reaction was simplified as:

$$\text{Bagasse}+\text{a}O_2\rightarrow \text{b}CO_2+\text{c}H_2O \tag{8}$$

where a, b and c are the stoichiometric coefficients of the reaction.

A chemical formula of bagasse must be provided to determine the stoichiometric coefficients in equation (8). Based on an extensive literature review [17-21] chemical structure from ultimate analysis of bagasse samples, the bagasse chemical composition was obtained and summarized in Table 1.

Table 1 shows that the main components of bagasse are carbon (C), hydrogen (H), and oxygen (O) with very small amounts of nitrogen (N) and sulfur (S). Neglecting nitrogen and sulfur, the average percent by mass of C:H:O was 48:6:46, yielding a chemical formula for bagasse as $C_4H_6O_{2.875}$. Accordingly, the balanced chemical reaction for bagasse oxidation employed in this study was:

$$C_4H_6O_{2.875}+4.0625O_2\rightarrow 4CO_2+3H_2O \tag{9}$$

The production or destruction rates of the i^{th} species ($\dot{S}_{Y_i}$) were based on equation (9) as one mole of bagasse reacts with 4.0625 moles of oxygen to form 4 moles of carbon

Table 1 Summary of bagasse chemical composition from ultimate analysis

C % by mass	H % by mass	O % by mass	N % by mass	S % by mass	Higher Heating Value (Δh_C, MJ/kg)	References
46.95	6.06	46.78	0.13	0.08	-	[17, 18]
43.79	5.96	43.36	1.69	-	17.70	[19]
38.30	6.04	41.35	1.71	-	15.90	[19]
45.48	5.96	45.21	0.15	-	17.33	[20]
51.70	6.30	42.00	-	-	-	[21]

Table 2 Summary of input parameters in the CFD simulation

Bagasse properties	Defined value	References
Bulk density	100 kg/m^3	[4]
Particle density	600 kg/m^3	[4]
Porosity	0.83	Calculated based on data from [4]
Permeability	1.857 x 10^{-8} m^2	Calculated based on data from [4]
Thermal conductivity	0.043 W/m-K	[23]
Pre-exponential factor	1 x 10^7 kg/s-m^3	[4]
Activation energy	89 kJ/mol	[4]

dioxide and 3 moles of water. Bagasse oxidation is an exothermic chemical reaction. The heat generated per mass of bagasse reacted is basically the heating value (Δh_c). The average heating value of bagasse obtained from the literature [19-20], 17 MJ/kg, was employed in this study. The bagasse oxidation rate was assumed to follow the Arrhenius reaction rate. The dependence of the rate of oxidation on temperature and oxygen concentration can be expressed in the form:

$$\dot{R}_{bagasse} = A\left[Y_{O_2}\right]^n e^{\frac{-E}{\bar{R}T}} \tag{10}$$

where $\dot{R}_{bagasse}$ is the bagasse oxidation rate, A, is the pre-exponential factor, n is the apparent order of reaction (n = 0.325 was used in the calculation), E is the activation energy and $\bar{R}$ is the universal gas constant.

The enthalpy heat source of the bagasse oxidation, $\dot{S}_H$, was then estimated as:

$$\dot{S}_H = \dot{R}_{bagasse}\Delta h_C \tag{11}$$

3.3 Moisture evaporation

The effect of moisture evaporation was taken into account in this study. Evaporation is an endothermic process and thus it acts as a heat sink in the energy conservation equation. There are various ways to include the moisture evaporation effect during biomass combustion. In this study, it was assumed that the drying of bagasse was constrained by the heat transfer inside the bagasse matrix and thus the moisture evaporation rate was approximated after [22] as:

$$\dot{R}_M \begin{cases} = f_M \dfrac{\left(T_S - T_{evap}\right)\rho_M C_{PM}}{\Delta h_{evap}\delta t} & \text{if } T_S \geq T_{evap} \\ = 0 & \text{if } T_S < T_{evap} \end{cases} \tag{12}$$

where $\dot{R}_M$ is the moisture evaporation rate, f_M is the initial moisture fraction, ρ_M is the moisture density, C_{PM} is the moisture specific heat, δt is the simulation time step, T_S is the bagasse solid phase temperature, T_{evap} is the moisture evaporation temperature and Δh_{evap} is the moisture heat of evaporation.

The enthalpy heat sink from moisture evaporation, $\dot{S}_W$, was then calculated as:

$$\dot{S}_W = \dot{R}_M \Delta h_{evap} \tag{13}$$

4. Model input parameters

4.1 Initial and boundary conditions

In this study, bagasse was filled into a basket in a manner that was assumed to be homogeneous and isotropic. The initial moisture content was approximately 5% as it was measured in the experiments of [4]. When the bagasse filled basket was placed in a convective oven, it was subjected to both convective and radiative heat transfer from all six sides. The net heat flux imposed upon the bagasse sample surface was the summation of the radiative and convective heat fluxes. The radiative heat flux was calculated as $\varepsilon\sigma(T_\infty^4 - T_{surf}^4)$, where ε is the emissivity (assumed to be unity), σ is the Stefan Boltzmann constant, T_∞ is the surrounding temperature (oven temperature) and T_{surf} is the bagasse surface temperature. The convective heat flux was estimated as $h(T_\infty - T_{surf})$, where h is the convective heat transfer coefficient. As the environment inside the oven was well circulated [16], a constant convective heat transfer coefficient of 15 W/m^2 K was employed.

The boundary conditions for the species equations were assumed to be zero flux except for the oxygen concentration, which was assumed to be constant at the ambient oxygen concentration ($Y_{O_2,\infty}$= 0.233).

4.2 Model input parameters

The relevant model input parameters are summarized in Table 2. The bagasse properties are its bulk density, particle density and activation energy. Values from previous work were used in the current study [4]. The porosity and permeability were calculated based on the input information from [4]. The thermal conductivity of solid bagasse was adopted from [23]. The pre-exponential factor used in the study was the value that gave the best fit of the simulated temperature to the measured temperature from the experiments of [4].

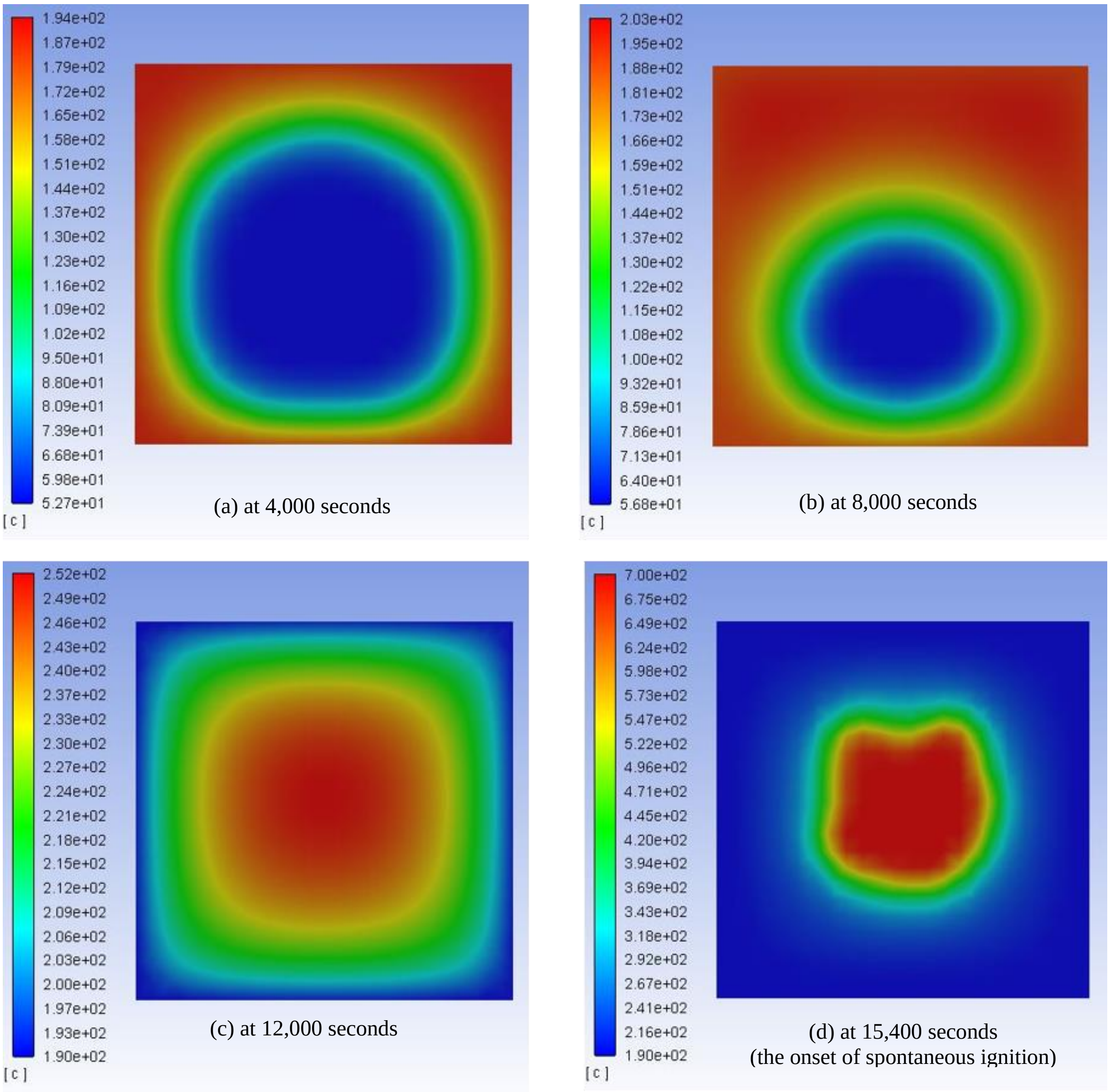

Figure 3 Temperature distribution time history in degrees Celsius at the centre plane of a 10 cm cubic 3D domain at (a) 4,000 seconds, (b) 8,000 seconds, (c) 12,000 seconds and (d) 15,400 seconds. (For color, the reader is referred to the web version of this paper.)

4.3 Numerical aspects

Computational simulations were performed in both 2D and 3D domains with a well-known CFD program, FLUENT from Fluent Inc. A grid refinement study was performed during the setup of the problem. The number of grid elements employed in the study is as follows. A square domain of 10,000 elements with uniform mesh was employed for 2D calculations. A cubic domain of 12,167 elements with uniform mesh was used in 3D simulations. The pressure-implicit with splitting of operators (PISO) scheme was used to integrate the time evolution of the relevant variables. The simulations were carried out until spontaneous ignition occurred. The computations were run on a personal computer (PC) of Intel® Core™ i7-7700HQ CPU @2.80 GHz processor with total CPU times of approximately 2 to 3 hours for 2D calculations and 9 to 10 hours for 3D calculations.

5. Results and discussion

5.1 General observations

Figure 3 shows a simulated temperature distribution time history at the centre plane of a 10 cm cubic 3D domain at four times,4,000, 8,000, 12,000, and 15,400 seconds. The surrounding (boundary) temperature here was 190 °C and the initial temperature of the sample was about 30 °C. In Figure 3(a) at 4,000 seconds and Figure 3(b) at 8,000 seconds, the temperature around the domain centre was still lower than the outer edge boundaries. Heat transfer takes place as time progresses. The temperature at the centre rose to reach the boundary temperature. After that, due to the exothermic reaction of bagasse oxidation, the temperature around the centre area surpassed the boundary temperature as can be seen in Figure 3(c) at 12,000 seconds. At this time, the temperature at the centre was about 250 °C, while the

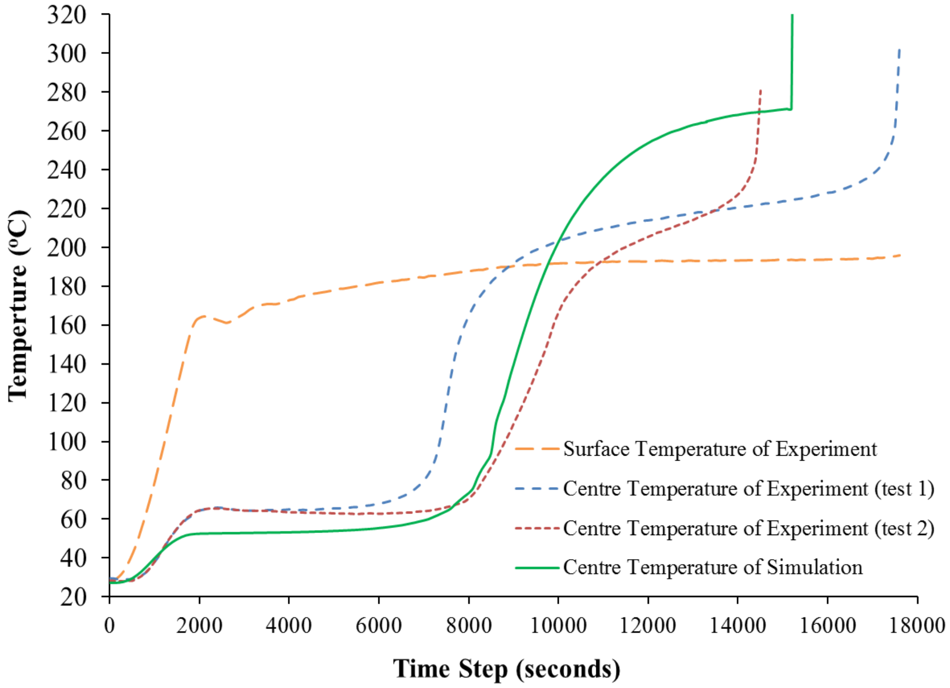

Figure 4 Simulated and measured temperature time history of a cubic sample size of 10 cm

temperature of the outer edge remained at the boundary temperature,190 °C. At 15,400 seconds (approximately four and a half hours) spontaneous ignition was observed. The heat generated from the bagasse oxidation is much higher than the losses from conduction and convection. Thermal runaway occurs and the temperature at the centre increases rapidly. The temperature at the vicinity of the domain centre increased to as high as 700 °C.

Figure 4 plots the simulated temperature and measured temperature at the sample centre taken from the experiments of [4]. As expected, when the cubic bagasse sample is subjected to external heating, the temperature at the bagasse basket edge (surfaced temperature) immediately starts to increase. With the penetration of a heat wave into the sample, the centre temperature increases. Due to the lag of the heat wave arrival, the increase of the centre temperature is correspondingly delayed. As can be seen in Figure 4, there is a significant difference in temperature rise pattern between the surface and the centre at around 2,000 seconds. At the surface, the temperature increases steadily with time. However, at the centre the temperature increases and then levels off to a flat plateau at about 60 °C. This flat plateau indicates moisture evaporation taking place inside the bagasse porous matrix. The heat propagation from the surface and the heat generated from bagasse oxidation are balanced by the heat required to evaporate the moisture. Accordingly, the centre temperature remains relatively constant. This observation was also reported by [16]. It can been seen in Figure 4 that this evaporation phenomena inside the sample from the experiments is well captured by the current simulations. After approximately 8,000 seconds, all the moisture has evaporated and the centre temperature starts to steadily increase with time. At approximately 15,400 seconds, the simulated centre temperature rapidly increases, indicating spontaneous ignition. A small discrepancy is obtained from the simulated and experimental ignition times. This difference may due to the uncertainty in the kinetic reaction of the porous bagasse.

5.2 Effect of 2D and 3D on the numerical simulation

The effect of 2D and 3D simulations is portrayed in Figure 5. In general, good agreement between 2D and 3D simulations is obtained up until approximately 7,000 seconds. During this period the heat generated from the bagasse oxidation and the heat wave penetration from the surface are balanced by the heat used for moisture evaporation. Once all the moisture has evaporated, some discrepancy between the 2D and 3D simulations is noticed. The simulated temperature from the 3D is slightly higher than that obtained in 2D. This may be explained as the generated heat from bagasse oxidation in 3D is slightly higher than in 2D because the oxidation heat in 3D is generated based on a bulk volume where in 2D simulation, the oxidation heat is generated based on a 2D plane area.

5.3 Effect of sample size

Figure 6 illustrates the effect of sample size upon spontaneous ignition. With decreased sample size from 10 cm to 8 cm, the ignition time decreases as expected from 15,400 seconds for a 10 cm sample size to 7,300 seconds for an 8 cm sample. The smaller the sample, the faster the heat wave penetration into the sample centre, yielding a faster bagasse oxidation rate. Accordingly, spontaneous ignition occurs faster in a small sample. It is interesting to note that the sample centre temperature at ignition for all sizes remains approximately constant at about 270 °C. This indicates that spontaneous ignition is mainly controlled by the kinetics of bagasse oxidation.

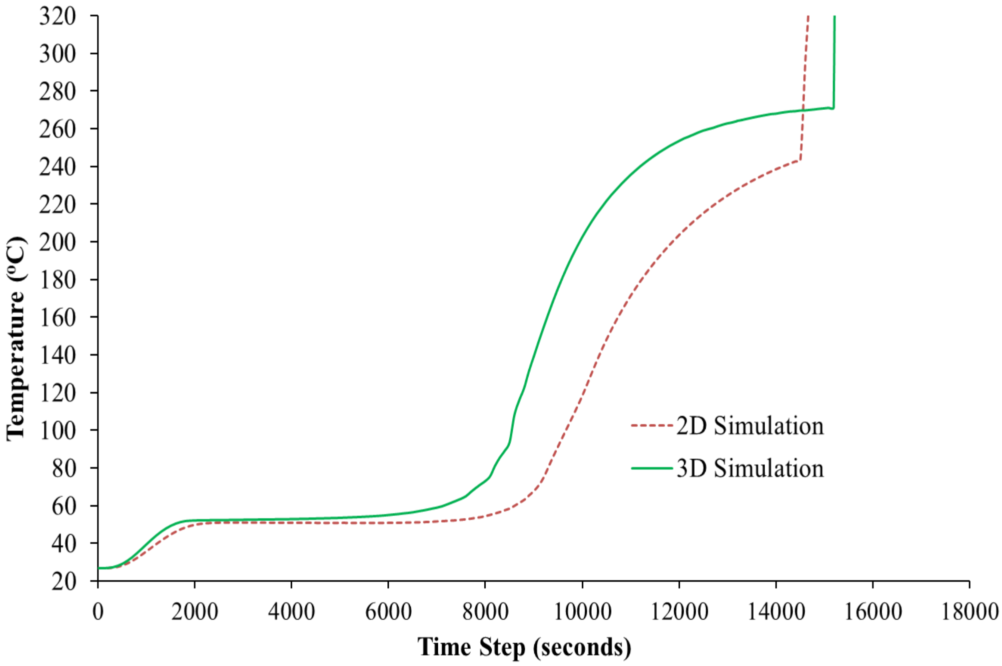

Figure 5 The simulated centre temperature based on 2D and 3D computational domains

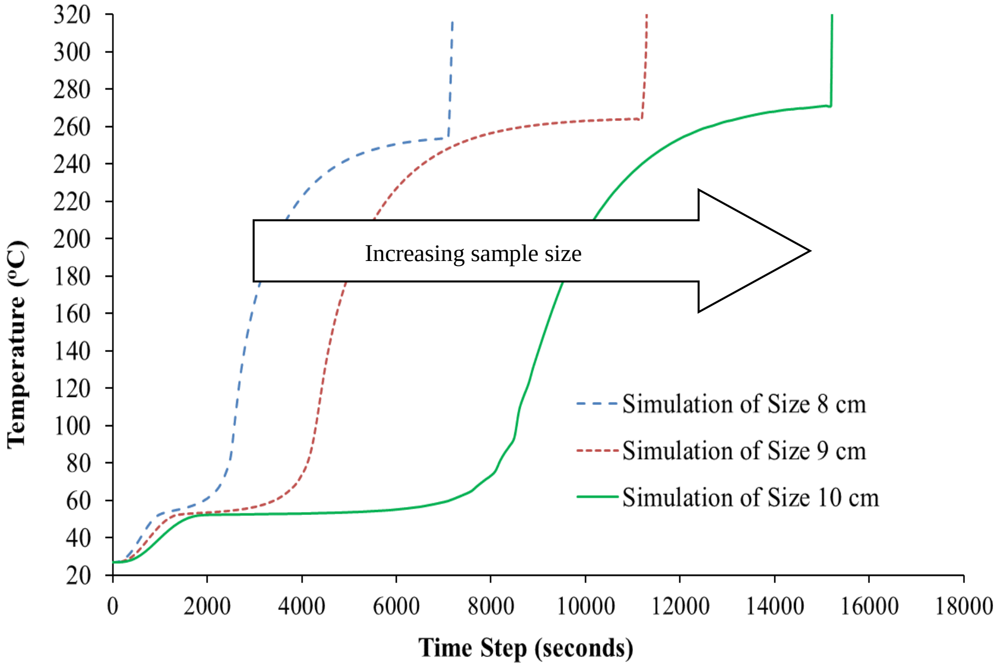

Figure 6 The effect of sample size to spontaneous ignition

5.4 Effect of initial moisture content

The initial moisture content effect for a sample size of 10 cm is examined in Figure 7. As the initial moisture content increases from 4.6% to 5.4%, the simulated time for spontaneous ignition to occur increases from 13,100 seconds (3.63 hours) to 18,600 seconds (5.17 hours). Generally, the spontaneous ignition of bagasse depends on several factors of which the initial moisture content is one. If we consider only the moisture content, it may be concluded that the higher the initial moisture content, the longer the time required to dry the sample and thus for simulated moisture contents ranging from 4.6 % to 5.4%, the time to spontaneous ignition increased with moisture content. The plot shows that before evaporation starts, the temperature rise patterns for all cases are almost identical. The evaporation process starts to take place at about 55 °C. Once all the moisture dries out, the temperature increases steadily with time again. As kinetic oxidation controls the spontaneous ignition process of porous bagasse, the calculated spontaneous ignition temperature for all initial moisture contents is constant at about 270 °C.

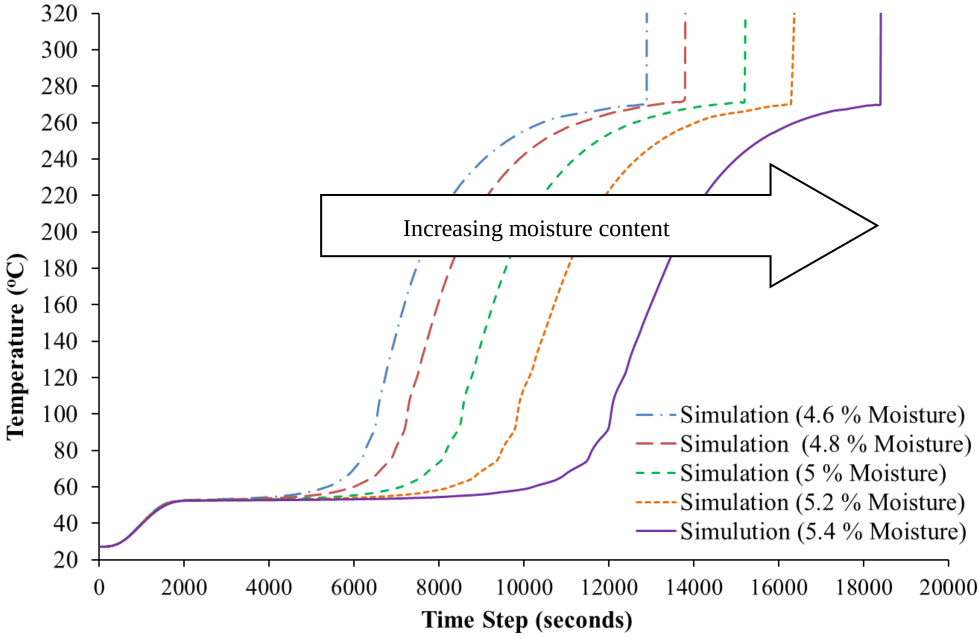

Figure 7 Simulated centre temperature time history for various initial moisture contents for a 10 cm sample

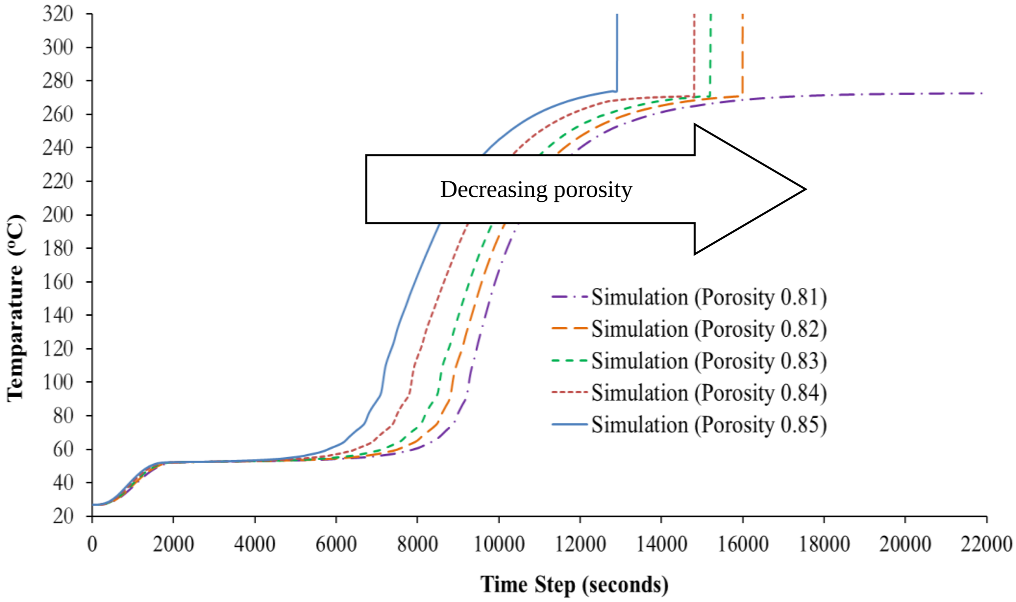

Figure 8 Simulated centre temperature time history for various porosity for a 10 cm sample

5.5 Effect of porosity

Figure 8 shows the effect of porosity on the spontaneous ignition of a 10 cm bagasse sample. In the calculations, the bagasse matrix was considered a porous medium. As can be seen in Figure 8, as the porosity was decreased from 0.85 to 0.81, the spontaneous ignition time increased and no spontaneous ignition occurs within 22,000 seconds (6.11 hours) for a porosity of 0.81. Decreasing the porosity means decreasing the gas volume inside the porous bagasse matrix. Thus, less oxygen can diffuse from the boundaries and react with bagasse solids at the pore surfaces. Accordingly, the bagasse oxidation rate decreases and the chance for spontaneous ignition to occur inside the computational domain is less likely.

It should be noted that in practice, the porosity of a bagasse pile would assume a range of values and not be limit to the porosity values of 0.81 to 0.85 used in this parametric study. Therefore, a field survey of bagasse pile porosity would be needed to simulate more accurate results.

6. Conclusions

A numerical simulation of spontaneous ignition of bagasse in a cubic basket has been conducted. The simulated results have been compared with experimental work. In general, good agreement between the simulated and measured centre temperatures was obtained. Some conclusions can be drawn as the follows.

1) As the cubic sample size increased, the time to spontaneous ignition increased.
2) The higher the initial moisture content, the longer the time required to dry out the moisture. Thus, for the simulated moisture contents ranging from 4.6 % to 5.4%, the spontaneous ignition time increases with moisture content.
3) Decreasing the porosity means decreasing the gas volumes inside the porous bagasse matrix. Thus, less oxygen can diffuse from the boundaries and react with bagasse solids at the pore surfaces. Accordingly the bagasse oxidation rate decreased and the spontaneous ignition time increased.
4) The simulated centre temperature from 3D simulation is slightly higher than that obtained from 2D simulation.

7. Acknowledgements

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