Numerical Modeling of Fixed-Bed Cocombustion Processes through the Multiple Thermally Thick Particle Model

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ABSTRACT: Fixed-bed cocombustion provides opportunities for utilizing various low-quality solid residues, but there still remain obstacles for quantitative numerical modeling. The difficulties originate from the particles in the thermally thick regime and the diverse properties of different fuels. This work presents the multiple thermally thick particle (MTTP) model that considers detailed transport processes and chemical reactions in subparticle and interparticle scales, and different fuels can be assigned with distinctive physical and chemical properties. The model was validated by cocombustion experiments using wood and potato as representatives of low- and high-moisture fuels. The predicted results showed satisfactory agreement with measured values, and the characteristics of asynchronous conversion were clearly revealed. For thermally thick fuels with high moisture content, the drying process extends almost across the whole conversion zone and is highly overlapped with devolatilization process. Consequently, the structure of the in-bed conversion zone is beyond the expectation of conventional fixed-bed combustion theory.

1. INTRODUCTION

Combustion is one of the most attractive disposal methods of multiple biomass materials and solid wastes and can effectively reduce the massive waste volume, recover the potential energy, and eliminate harmful pathogens. Among various technologies, fixed-bed combustion is advantageous for its simple operation and low capital cost and therefore is suitable for disposing solid wastes in decentralized rural areas or communities. However, many organic solid wastes are not directly applicable in combustion systems because of their low calorific values and high tendency to cause slagging, since they commonly have high moisture content or high ash content. Co-combustion technology offers a promising solution to overcome these drawbacks. The stability and efficiency of the combustion process can be improved by properly blending low-quality organic wastes with high-quality fuels, which can also effectively increase the share of renewable solid fuels in the energy market.

Because of the diverse properties of solid wastes, blending different fuels in the combustion system may change the combustion characteristics compared to using individual fuels, which may have significant impacts on the operation of boilers and air pollutant control devices. Recently, the cocombustion characteristics of various solid fuels have attracted considerable attention, and many researchers have investigated the thermal behaviors and kinetics of cocombustion processes for various fuel blends mainly through thermogravimetric analysis. These investigations have provided insightful results for fundamental aspects of cocombustion processes, but for industrial-sized combustion equipment, the complexity of cocombustion also originates from the inhomogeneity of reactions and transport processes both on subparticle and interparticle scales.

In practice, different feedstocks may have different sizes depending on their sources and physical properties, ranging from millimeter- to centimeter-sized. The particle size directly determines the thermal history of fuel particles, consequently influencing the onset of ignition and duration of different conversion processes, such as drying and burn-out. Particularly, centimeter-sized fuel particles are often used for fixed-bed combustion considering the economic efficiency of pretreatment and convenience in operation, and using feedstocks with different particle sizes will present challenges in analyzing the combustion behaviors inside the fuel bed. Meanwhile, the physical and chemical properties of various solid residues may significantly differ from each other, such as the elemental composition, devolatilization kinetics, and char reactivities. In addition to the experimental validation of cocombustion
processes in lab-scale fixed-bed reactors, advanced numerical modeling through CFD methods offers a promising approach to thoroughly investigate the in-bed combustion processes as well as predict the overall efficiency and emissions.11

The Eulerian–Eulerian method is widely adopted for the CFD modeling of fixed-bed combustion process because of its high computational efficiency,12 especially for large-scale industrial combustion equipment. In this model framework, the solid phase is regarded as a pseudofluid so that the equations of mass and energy conservation could share the same form as the gas phase. However, in much of the literature, the fuel particles are simply regarded as in a thermally thin regime.13,14 For the thermally thin particle, the conversion stages (such as drying, devolatilization, etc.) will proceed consecutively, and inside the fuel bed the boundaries of each reaction zone are legible. When a thermally thick particle is used as in industrial practice, the heat resistance will cause a significant intraparticle temperature gradient and the overlapping of different conversion stages.15 The importance of the intraparticle gradient has been highlighted in many recent modeling works, and some researchers also attempted to develop subgrid particle models.6,16,17 The superiority of the thermally thick model over the thermally thin model has been proved in predicting the in-bed reactions and heat transfer.18 For the fixed-bed cocombustion process, using solid fuels with large particle size and high moisture content can notably alter the onset of ignition and propagation of the ignition front,19 which confirmed the necessity to use thermally thick model when modeling the fixed-bed cocombustion processes.

The difficulties of modeling the fixed-bed cocombustion process originate not only from the particles in the thermally thick regime but also from the diverse properties of different fuels. The fixed-bed cocombustion process has been numerically studied in some investigations, but the models were often largely simplified. The fuel bed was often considered as a homogeneous continuous porous medium, in which the fuel properties of the solid phase were averaged according to the mixing ratios of different fuels.20 For feedstocks with different moisture contents, particle sizes, and pyrolysis kinetics, their combustion behaviors may be quite distinct from one another. Clearly, this can result in remarkable deviations from the realities of modelling an “averaged fuel” rather than individually calculating their conversion processes. Recently, Zhou et al.21 developed a numerical model for cocombustion of the blended solid waste fuel in the grate boiler. In their innovative work, individual fuel physical and chemical properties were successfully considered based on the Eulerian–Eulerian approach, but the intraparticle gradient was still neglected. It is the general situation in industrial practice to use solid fuels with large particle sizes and different fuel properties. So far, there has been no report on developing numerical models to simulate the fixed-bed cocombustion processes considering individual fuel properties and the effects of intraparticle temperature gradients.

In this work, we present the multiple thermally thick particle (MTTP) model for quantitative analysis of the fixed-bed cocombustion process. The MTTP model extended the Eulerian–Eulerian type multiphase model with high computational efficiency, further dividing the solid phase into several subphases, representing the different layers of the thermally thick fuel particle. The governing equations are formulated based on the intraparticle transport and conversion processes, which could reveal the conversion process of different fuels independently. The model is validated based on fixed-bed cocombustion experiments of conventional biomass and high-moisture fuels under different mixing ratios, and the in-bed conversion processes are demonstrated in detail. The framework of the MTTP model is easily extensible, making it also suitable for the fixed-bed cogasification and copyrolysis process.

2. EXPERIMENTAL SECTION

2.1. Fuel Properties. To simulate the cocombustion process of thermally thick solid fuels with different properties, poplar wood and fresh potato were selected as representative fuels with low and high moisture contents. In this work, the poplar wood was harvested in Zhejiang province, China, and the raw materials were cut, lathed, and shaped into spheres with diameters of 1.50 cm. The fresh potato was also peeled and cut into small spheres with a diameter of 1.50 cm (±0.2 cm) before each experiment. The proximate analysis of wood and potato was based on the standard methods (CEN/TS 14774-3:2004 for moisture content, CEN/TS 14775:2004 for ash content, CEN/TS 15148:2005 for volatile matter (VM) content, and fixed carbon (FC) content by difference). The ultimate analysis was conducted by using a Vario El cube elemental analyzer (Germany). The results of the proximate and ultimate analyses of the biomass sample are shown in Table 1. Apparently, the compositions of these two fuels are largely distinct from one another, which requires separate setting of the fuel properties in the numerical model rather than simply using averaged values.

2.2. Fixed-Bed Combustion Experiment. Figure 1 shows a schematic of the fix-bed test rig for the cocombustion experiments of wood and potato. The test rig consists of a cylindrical combustion chamber with a diameter of 12.0 cm. Primary air is provided from the bottom of the chamber. A porous ceramic plate is placed under the grate of the chamber to ensure the uniformity of the air flow. Electrically heated silicon carbide rods are inserted on top of the chamber as a radiation heater and can be heated to 1173 K to ignite the fuel bed. Four thermocouples are located in the fuel bed, and the temperature can be recorded continuously. The distances of the four thermocouples (T1–T4) from the bottom of the fuel bed are 17.0, 12.0, 7.0, and 2.0 cm, respectively. The flow rate of the primary air was kept at 0.10 kg/(m²·s) at room temperature in each experiment.

| Table 1. Results of Proximate and Ultimate Analysis |
|-----------------------------------------------|
| proximate analysis (wt %, as received) | ultimate analysis (wt %, daf basis) |
| M | V | FC | A | C | H | O* | N |
|---|---|---|---|---|---|---|---|
| poplar wood | 13.42 | 71.40 | 14.77 | 0.41 | 53.72 | 7.44 | 38.84 | <0.1 |
| potato | 71.50 | 22.03 | 5.51 | 0.96 | 43.86 | 7.15 | 47.57 | 1.42 |

*By difference.
Three different mass ratios of wood and potato (\(M_{\text{wood}}:M_{\text{potato}} = 2:1, 1:1, \text{ and } 1:1.5\)) were used in this study, and the major focus was on the influence of different fuel compositions, especially moisture content. In pre-experiments, the mixing ratio of 1:2 (\(M_{\text{wood}}:M_{\text{potato}}\)) was also performed, but the combustion process could not be sustained because of the overly high moisture content. The wood spheres and potato spheres were preweighed before each experiment and uniformly mixed before being placed in the combustion chamber. For each mixing ratio, the experiments were repeated at least three times to ensure the repeatability. In each experiment, the fuel mixture was put into the chamber to form a fuel bed of 20 cm, and then the conversion of the fuel bed will be initiated by radiation.

3. NUMERICAL MODEL

3.1. Framework of the MTTP Model. The MTTP model is an extension of classic Eulerian–Eulerian model coupling with a detailed subgrid model to treat the intra- and interparticle interactions during cocombustion processes. The classic Eulerian–Eulerian model treats the fuel bed as a uniform and continuous porous medium, in which the solid phase is regarded as a homogeneous pseudofluid. In the MTTP model, the solid phase is further split into multiple subphases, representing different layers of thermally thick fuel particles. Figure 2 shows the schematic diagram of the fixed-bed cocombustion processes and the formulation of the subgrid model.

The layer-based particle model is commonly adopted for simulating the conversion processes of the large fuel particle for its high computational efficiency. In the current work, the particle is assumed to be spherical, and the particles of different fuels are all divided into four connected layers, including the wet layer, dry layer, char layer, and ash layer. In each layer, the material properties are constant. The wet layer of each fuel is composed of moisture, volatile, char, and ash following the relative content from proximate analysis. Similarly, the dry layer contains volatile, char, and ash, and the char layer is composed of char and ash. The outermost layer is purely ash. Initially the fuel particle is almost all wet layer, and 0.1% of initial mass is assigned to other layers for the stability of numerical calculation.

The particle structure is purely conceptual, and in the numerical model the particles are modeled by multiple subphases. For the porous fuel bed, the void fraction \(\varepsilon\) is assumed to be constant and the shrinking of solid is accounted as a result of mass loss. It is further assumed that the particles are identical for the same fuel in each computational cell, and the ratio of numbers of different fuel particles is constant. Therefore, the \(k\)th layers of all the particles of \(N\)th fuel in a certain computational cell are lumped as the \(k\)th subphase of the fuel particle.
Nth fuel, and the volume fraction of the kth subphase of the Nth fuel in the solid phase follows these relationships:

$$\alpha_{k,N} = \frac{V_{k,N}\cdot n_{N}}{\sum_{N} V_{N}\cdot n_{N}}$$  \hspace{1cm} (1)

$$\sum_{N} \sum_{k} \alpha_{k,N} = 1$$  \hspace{1cm} (2)

in which $\alpha_{k,N}$ is the volume ratio of the kth layer of Nth fuel, $V_{k,N}$ is the volume of the kth layer of the Nth fuel, and $n_{N}$ is the number of fuel particles in a unit volume.

Although the total void fraction $\varepsilon$ is a constant, the volume fraction of each solid subphases will continuously change during the conversion process. For instance, when the drying process of the Nth fuel begins, $\alpha_{\text{wet},N}$ will decrease as the wet fuel is converted to dry fuel, and correspondingly $\alpha_{\text{dry},N}$ will increase following the relationship of mass conservation. In the present model, it is assumed that the fuel particles will not break up or merge together.

For the conceptual fuel particle, drying is assumed to occur at the boundary of the wet layer, and the pyrolysis process occurs inside the dry layer. Char heterogeneous reactions occur at the boundary of the char layer, which causes the accumulation of the ash layer. Inside the fuel particle the heat is transferred by conduction between different layers. For the ash layer, the convective and radiative heat transfer with the surrounding environment is also considered. These relationships determine the rules of mass and energy exchange between different phases in the fuel bed.

### 3.2. Governing Equations and Numerical Methods.

The governing equations for the gas phase and solid subphases, including mass, momentum, energy, and species conservations, are summarized in Table 2. The conservation equations of the gas phases have been extensively discussed in many studies in the literature, and in this section the details of the conservation equations of the solid subphases will be illustrated.

The present work divides the solid phase into multiple subphases, and the solid species is distributed in each subphase following certain mass ratios. With the onset of different conversion processes, the value of $\alpha_{k,N}$ for each subphase would continuously change. It is worth noting that in many modeling works the species conservation equations of the solid phase, including moisture, volatile (or dry fuel), and char, were solved. In the present work, the continuity equations for solid subphases are solved as an alternative. Solving the mass conservation equations of subphases is mathematically equivalent with solving those of the solid phase species, but the equations of mass conservation of each subphase (i.e., each layer of fuel particle) are conceptually more natural considering the shrinkage of the solid fuel particles. The particle structure can be calculated with the following relationships:

$$\alpha_{\text{wet},N} = n_{N}d_{\text{wet},N}^{3}/\sum_{i} n_{i}d_{i}^{3}$$  \hspace{1cm} (3)

$$\alpha_{\text{dry},N} = n_{N}(d_{\text{dry},N}^{3} - d_{\text{wet},N}^{3})/\sum_{i} n_{i}d_{i}^{3}$$  \hspace{1cm} (4)

$$\alpha_{\text{char},N} = n_{N}(d_{\text{char,},N}^{3} - d_{\text{dry},N}^{3})/\sum_{i} n_{i}d_{i}^{3}$$  \hspace{1cm} (5)

$$\alpha_{\text{ash},N} = n_{N}(d_{\text{ash},N}^{3} - d_{\text{char},,N}^{3})/\sum_{i} d_{i}^{3}$$  \hspace{1cm} (6)

| Governing equations | Phase | Expression |
|---------------------|-------|------------|
| Mass conservation   | Solid | $\frac{\partial}{\partial t}(\rho_{g}u_{g}) + \frac{\partial}{\partial x_{j}}(\rho_{g}u_{g}u_{j}) = -\sum_{k} \xi_{k}^{N}$ |
| Momentum conservation | Gas   | $\frac{\partial}{\partial t}(\rho_{g}u_{g}) + \frac{\partial}{\partial x_{j}}(\rho_{g}u_{g}u_{j} - \mu \frac{\partial u_{g}}{\partial x_{j}}) = S_{k,N} + S_{i,N}$ |
| Energy conservation | Solid | $\frac{\partial}{\partial t}(\rho_{g}u_{g}) + \frac{\partial}{\partial x_{j}}(\rho_{g}u_{g}u_{j} + S_{g,N})$ |

where $S_{x_{m},a}$ is the heat of gas-phase reactions, and $S_{v,a}$ is the convective heat transfer between gas and solid phase.

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Table 3. Source Terms for the Solid Phase Conservation Equations

| Source Term | Wet Subphase | Dry Subphase | Char Subphase | Ash Subphase |
|-------------|--------------|--------------|---------------|--------------|
| $S^E_{k,N}$ | $- \frac{R_{\text{drying}}}{Y_{\text{water}}}$ | $R_{\text{drying}} - Y_{\text{water}} \ln \frac{1}{1 - Y_{\text{water}}}$ | $- \frac{R_{\text{py}}}{Y_{\text{vol,wf}}}$ | $R_{\text{char}} - Y_{\text{char,wf}} \ln \frac{1}{1 - Y_{\text{char,wf}}}$ |
| $S_{\text{Evap},k,N}$ | $- \frac{R_{\text{drying}} \cdot L_{\text{H}_{\text{evap}}}}{Y_{\text{water}}}$ | $R_{\text{py}} \cdot \Delta H_{\text{devol}}$ | $- \Delta H_{\text{char}} \frac{\rho_{\text{char}}}{\rho_{\text{char,vol}}}$ | $- \Delta H_{\text{char}} \frac{\rho_{\text{char}}}{\rho_{\text{char,vol}}}$ |
| $S_{\text{Cond},k,N}$ | $A_k K_\text{a} \left( \frac{T_{k+1} - T_k}{\frac{R_k}{R_k + R_k}} - A_k K_{\text{a,1}} \frac{T_k - T_{k-1}}{R_k - R_{k-1}} \right)$ | $A_k K_\text{a} \left( \frac{T_{k+1} - T_k}{\frac{R_k}{R_k + R_k}} - A_k K_{\text{a,1}} \frac{T_k - T_{k-1}}{R_k - R_{k-1}} \right)$ | $- \Delta H_{\text{char}} \frac{\rho_{\text{char}}}{\rho_{\text{char,vol}}}$ | $- \Delta H_{\text{char}} \frac{\rho_{\text{char}}}{\rho_{\text{char,vol}}}$ |
| $S_{\text{Vol},k,N}$ | $Q_{\text{rad}} \cdot \frac{\omega_k}{\omega_i} + A_k K_\text{a} (T_k - T_e)$ when $k$ is ash subphases; $0$ in other cases; $Q_{\text{rad}}$ is calculated based on flux model for each computational cell. | $- \Delta H_{\text{char}} \frac{\rho_{\text{char}}}{\rho_{\text{char,vol}}}$ | $- \Delta H_{\text{char}} \frac{\rho_{\text{char}}}{\rho_{\text{char,vol}}}$ | $- \Delta H_{\text{char}} \frac{\rho_{\text{char}}}{\rho_{\text{char,vol}}}$ |
| $S_{\text{Evolution},k,N}$ | $\sum_{j} \omega_j^k \int_{T_{ref}}^{T_k} C_p j dT - \omega_j^k \int_{T_{ref}}^{T_k} C_p j dT$ | $\sum_{j} \omega_j^k \int_{T_{ref}}^{T_k} C_p j dT - \omega_j^k \int_{T_{ref}}^{T_k} C_p j dT$ | $\sum_{j} \omega_j^k \int_{T_{ref}}^{T_k} C_p j dT - \omega_j^k \int_{T_{ref}}^{T_k} C_p j dT$ | $\sum_{j} \omega_j^k \int_{T_{ref}}^{T_k} C_p j dT - \omega_j^k \int_{T_{ref}}^{T_k} C_p j dT$ |

in which $d_{\text{wet},N}, d_{\text{dry},N}, d_{\text{char},N}$, and $d_{\text{dry},N}$ are the diameters of the wet layer, dry layer, char layer, and the whole fuel particle of the $N$th fuel.

For the $k$th subphase of the $N$th fuel, the source terms of mass conservation equations $S_{k,N}$ depend on the reaction process of the $k$th subphase and the neighboring subphases, as summarized in Table 3. For instance, when the drying process occurs in the wet layer and the devolatilization process also occurs in the dry layer, the dry layer will receive mass from the wet layer and simultaneously give out mass to the char layer. It should be noted that the exchange of mass between solid subphases will only occur between the adjacent layers of the same kind of fuel particles in each computational cell.

The source terms of the energy conservation equations for the $k$th subphase of the $N$th fuel $S^E_{k,N}$ are formed by the addition of five different energy sources:

$$S^E_{k,N} = S_{\text{Rec},k,N} + S_{\text{Cond},k,N} + S_{\text{Env},k,N} + S_{\text{Blowing},k,N} + S_{\text{Evolution},k,N}$$

These five energy sources cover the change of sensible enthalpy because of the heat transfer and solid-phase conversion processes. For the $k$th subphase of the $N$th fuel, $S_{\text{Rec},k,N}$ represents the heat generation and consumption due to the solid reactions, such as the latent heat of vaporization and the thermal effect of pyrolysis. $S_{\text{Cond},k,N}$ represents the heat conduction with neighboring subphases in the current computational cell calculated based on Fourier’s rule. $S_{\text{Env},k,N}$ represents the heat exchanged between the particle and the environment through solid-solid radiative and gas-solid convective heat transfer, and only the subphases representing the ash layer would receive this source term. The XDEM/CFD modeling of the fixed-bed combustion process in ref 23 has revealed that both interparticle radiation and gas-to-particle convection play essential roles in the heat transfer inside the fuel bed, while the interparticle heat conduction can be neglected. Therefore, in this work only interparticle radiation and gas-to-particle convection were considered in $S_{\text{Env},k,N}$. The overall radiation heat transfer is calculated by the widely used

$$u_i = - \frac{1}{1 - \epsilon} \int_0^T \sum_N \left( R_{\text{drying},N} \theta_{\text{drying},N} + R_{\text{devol},N} \theta_{\text{devol},N} \right. \right. \left. + R_{\text{char},N} \theta_{\text{char},N} \right) \ dy$$

in which $\theta_{\text{drying},N}, \theta_{\text{devol},N}$, and $\theta_{\text{char},N}$ are the coefficient of shrinkage caused by drying, devolatilization, and char reactions:

$$\theta_{\text{drying},N} = \frac{1}{Y_{\text{water}}} - \frac{(1 - Y_{\text{water}})/Y_{\text{water}}}{\rho_{\text{dry,N}}}$$

$$\theta_{\text{devol},N} = \frac{1}{Y_{\text{vol,wf}}} - \frac{(1 - Y_{\text{vol,wf}})/Y_{\text{vol,wf}}}{\rho_{\text{dry,N}}}$$

$\theta_{\text{char},N}$ is given by the reaction rate of the endothermic pyrolysis, and consequently the volume of the particle can be regarded as the summation of all these layers. During conversion processes, with the mass loss of the solid phase, the volume will correspondingly change. In this work, the shrinking of the solid phase is related to the mass loss, and therefore the velocity of the solid phase $u_i$ parallel to the direction of fuel bed (denoted as the $y$ direction) could be solved based on the following relationship:

flux model, which is reallocated to each solid subphase based on the volume fraction of each fuel. $S_{\text{Blowing},k,N}$ is caused by the expulsion of the gases from the inner layers, which is calculated based on the assumption that the gases leaving the $k$th subphase have the same temperature as the solid phase. Finally, $S_{\text{Evolution},k,N}$ stands for the enthalpy exchange with the interior and exterior layers because of the conversion of solid phase materials. The detailed expressions of source terms are summarized in Table 3.

Because the fuel bed is fundamentally composed of a large number of particles, by assuming that the porosity is constant in the fuel bed, the bed shrinkage is solely dependent on the variation of particle size. The particle is assumed to be composed of a wet layer, dry layer, char layer, and ash layer, and consequently the volume of the particle can be regarded as the summation of all these layers. During conversion processes, with the mass loss of the solid phase, the volume will correspondingly change.
$$\begin{align*}
&H_2 + \frac{1}{2}O_2 \rightarrow H_2O \\
&CH_4 + \frac{3}{2}O_2 \rightarrow 2H_2O + CO \\
&CH_4 + H_2O \xrightarrow{\text{Re}} 3H_2 + CO \\
&CO + \frac{1}{2}O_2 \rightarrow CO_2 \\
&C + \frac{1}{2}O_2 \rightarrow 2(1 - \xi)CO + (2\xi - 1)CO_2 \\
&C + CO_2 \rightarrow 2CO \\
&C + H_2O \rightarrow CO + H_2
\end{align*}$$

Figure 3. Reactions in the solid and gas phases in the present model.

Table 4. Rate Expressions and Kinetic Data of Reactions, where the General Expression of Kinetic Constants Is $k = A \exp(-E/RT)^{2,22}$

| Rate expressions | $A$ (s$^{-1}$) | $E$ (J/kmol) |
|------------------|--------------|--------------|
| $R_{\text{drying,N}}$ | \( \frac{A_h(T_{\text{dry}} - T_{\text{dry}})}{Q_{\text{evap}}/H_{\text{evap}}} \) if $T_{\text{dry}} < 373K$ | \( \frac{A_h(T_{\text{dry}} - T_{\text{dry}})}{Q_{\text{evap}}/H_{\text{evap}}} \) if $T_{\text{dry}} \geq 373K$ |
| $R_{\text{py,N}}$ | $k_{\text{py}}a_{\text{dry,N}}\rho_{\text{dry,N}}$ | $3.4 \times 10^6$ | $6.9 \times 10^7$ |
| $R_{\text{char,N}}^i$ | $P_i S_{\text{char,N}}$ | $k_{\text{char}} = 0.08 - 0.0001(T - 273)$ | $1.715$ | $8.56 \times 10^7$ |
| $k_{\text{char}} = 0.08 - 0.0001(T - 273)$ | $k_{\text{char}} = 0.08 - 0.0001(T - 273)$ | $3.42$ | $1.48 \times 10^8$ |
| $k_{\text{char}} = 0.08 - 0.0001(T - 273)$ | $k_{\text{char}} = 0.08 - 0.0001(T - 273)$ | $3.42$ | $1.10 \times 10^8$ |

where $k_{\text{char}} = k_{\text{char}}^{\text{dry,N}} + k_{\text{char}}^{\text{g,N}}k_{\text{char}}^{\text{dry,N}} + k_{\text{char}}^{\text{g,N}}$ and $k_{\text{char}}^{\text{dry,N}}$ and $k_{\text{char}}^{\text{g,N}}$ are the real densities of the wet, dry, char, and ash layers, respectively.

Table 5. Physical Properties Used in the Model$^{2,22}$

| parameter | wood | potato | wet fuel | dry fuel | char | ash |
|-----------|------|--------|----------|----------|------|-----|
| density (kg/m$^3$) | 651.90 | 586.69 | 291.14 | 381.64 | 342.76 |
| bed porosity | 0.4 | | | | |
| thermal conductivity (W/m K) | $k_{\text{char,N}} = 0.13 + 0.0003(T - 273)$ | | | | |
| heat capacity (kJ/kg K) | $\gamma_{\text{char,N}} = 0.44 + 0.001 \times T \cdot 7 \times 10^{-4}T^2$ | | | | |
| diffusion coefficient | $D_p = 0.8$ | | | | |
| emissivity | | | | | | 0.8

in which $Y_{\text{water}}$ is the mass fraction of water, $Y_{\text{vol,WF}}$ is the mass fraction of volatile free of water, $Y_{\text{char,WF}}$ is the mass fraction of char free of water and volatile, and $\rho_{\text{water,N}}$, $\rho_{\text{dry,N}}$, $\rho_{\text{char,N}}$, and $\rho_{\text{ash,N}}$ are the real densities of the wet, dry, char, and ash layers, respectively. The real densities of each layer for wood and potato particles have been experimentally measured, and the results are listed in Table 5.

3.3. Reaction Models. Figure 3 gives the overview of reactions considered in the solid and gas phases in the present model. The rate expressions and kinetic data are presented in Table 4. The physical properties used in this model are shown in Table 5. In the solid phase, the conversion processes include the drying, pyrolysis, and char reactions. For the drying process, both the equilibrium model and the thermal model...
were considered. The pyrolysis process of each fuel is modeled with a one-step global reaction. The volatile is released to the gas phase immediately after pyrolysis, and a volatile breakup approach is adopted to calculate the specific composition of the volatiles. The elemental composition of the volatile is \( C_6H_{9.89}O_{6.46} \) for wood and \( C_6H_{9.61}O_{5.65} \) for potato, and the results of the volatile breakup approach are listed as follows:

\[
C_6H_{9.89}O_{6.46} \quad (\text{For wood}) \rightarrow 3.64CO + 1.4CO_2 + 3.035H_2 + 0.952CH_4 + 0.012H_2O \quad (12)
\]

\[
C_6H_{9.61}O_{5.65} \quad (\text{For potato})
\rightarrow 2.74CO + 1.45CO_2 + 1.18H_2 + 1.81CH_4 + 0.01H_2O \quad (13)
\]

The releases of volatiles of wood and potato follows their local devolatilization rates, and the volatile breakup approach is simply intended to calculate the stoichiometric coefficients for the resultant species. For a detailed algorithm for calculating the volatile composition, the reader is referred to the work of Gu et al.\(^2\). For the overall reaction rate of heterogeneous char reactions, the kinetics reaction rate \( R_{\text{char}} \), gas film diffusion \( R_{\text{diff}} \), and ash-film diffusion \( R_{\text{diff}} \) were all considered at the gas—solid interface.

3.4. Numerical Methods. For simplicity of calculation, the calculation field was treated as one-dimensional only considering the combustion chamber of the test rig. When the radial inhomogeneity of porosity or the heat loss from the wall is considered in the model, a higher dimensional computational grid could also be adopted. All the conservation equations were integrated over these bed cells to obtain corresponding algebraic linear equations using the finite volume method. The flux term was discretized by the second order upwind scheme, whereas central differencing scheme was used for the diffusive term. The implicit method was used to ensure stability when dealing with the unsteady term. The SIMPLE method was implemented to solve the velocity—pressure coupling problem.

The finite volume method is used to solve the governing equations. To obtain time and grid independent solutions, all the calculations in this study were carried out with a time step of \( 1.0 \times 10^{-3} \) s and a space step of 0.10 mm. The use of fine enough mesh in the model can secure the boundedness of the central differencing scheme, thus improving the accuracy and robustness of the calculation.\(^2\) The detailed structures in the fuel bed can be better resolved, such as the ignition front where temperature gradient is very large. For the boundary conditions at the surface of the fuel bed, the gradients of the gaseous concentration and temperature were set as zero, and the gradients of the particle compositions and temperature for the solid phase were also set as zero.

4. RESULTS AND DISCUSSIONS

4.1. Model Validation. Validation of the MTTP model was performed based on the comparisons between the measured and predicted temperatures in the fuel bed under different mixing ratios, as shown in Figure 4. The average temperature of the outermost layers of each fuel particle was adopted as the simulated temperature inside the fuel bed, and a more detailed comparison of the temperature distributions between gas phase and different solid phases will be presented in the following sections. In general, the calculated temperature profiles are in good agreement with the measured data. The increase of the modeled temperature is slightly faster than in the experimental results, which is probably because of the adiabatic assumption of the furnace wall in the numerical model.

When exposed to the radiative heat from the freeboard, the temperature would slowly increase at first because of the drying process, after which the temperature would rise rapidly because of the ignition of volatiles and char. After ignition at the bed surface, the ignition front will propagate downward steadily inside the fuel bed until the char residue is burned out. As shown in Figure 4, when changing the mixing ratio of wood and potato, the maximum flame temperature decreased from about 950 °C (\( M_{\text{wood}}=M_{\text{potato}}=2:1 \)) to 900 °C (\( M_{\text{wood}}=M_{\text{potato}}=1:1 \)) and 650 °C (\( M_{\text{wood}}=M_{\text{potato}}=1:1.5 \)), mainly caused by the increase of the moisture content.

Meanwhile, it is also worth noting that the maximum temperature inside the fuel bed at the mixing ratio of 2:1 rose to around 1200 °C in the final stage of combustion. This is a characteristic behavior of the final char combustion stage in fixed-bed combustion,\(^2\) and the numerical results have well reproduced this phenomenon. Generally, at the final stage all the moisture of the solid fuel has evaporated, and the heating value of the residue (mostly char) is much higher than that of the raw fuel; thereby the temperature will be higher than that during the previous ignition front propagation stage. However, such a “final high-temperature stage” seemed to be missing at the mixing ratios of 1:1 and 1:1.5. When the thermally thick fuel particle with high moisture content was used, drying of the inner fresh fuel layer and pyrolysis of the dry fuel layer could coexist almost along the whole conversion process.\(^2\)

Consequently, it can be anticipated that the maximum flame
temperature will not be significantly changed even at the final combustion stage.

The comparison of experimental and numerical results of the ignition front velocity and ignition delay time at different mixing ratios is shown in Figure 5. The average ignition front velocity was calculated based on the distance between two adjacent thermocouples and the time interval when the temperatures of two thermocouples rose to 400 °C, and the ignition delay time was determined from the start to the moment that the highest thermocouple rose to 400 °C. When changing the mixing ratio of wood and potato from 2:1 to 1:1 and 1:1.5, the average moisture contents of the mixed fuel were 32.78, 42.46, and 52.14 wt %, respectively. With the increase of the moisture content, the ignition front velocity decreased from around 0.0053 m/min and 0.0012 m/min, while the ignition delay time increased from 11.2 and 26.2 min. The modeling results are very close to the measured values, which proved the applicability of the MTTP model for predicting the combustion behaviors of solid fuel mixtures in a thermally thick regime with diverse properties.

4.2. In-Bed Conversion Processes. After validation of the numerical model, in this section the detailed structure of the in-bed conversion zone will be demonstrated based on the modeling results, i.e., the distribution of drying, devolatilization, and char reactions inside the fuel bed.

In classic fixed-bed combustion theory, it is widely accepted that the combustion stages inside the fuel bed can be identified according to temperature with four sequential zones: namely, the (1) preheating and drying zone, (2) volatile devolatilization and combustion zone, (3) char combustion zone, and (4) ash residue burning-out zone. However, when thermally thick fuel particles with high moisture content were used, the boundaries of different conversion zones could not be clearly defined. Figure 6 shows the modeling results of reaction rates for drying, devolatilization, and char reactions of two different fuels inside the fuel bed when the bed height decreased to 10.0 cm.

The devolatilization rate of wood and drying rate of potato contribute the majority of the weight loss for the two fuels. With the increasing mass fraction of the potato, the central peak position of devolatilization gradually moved upward for both fuels, and the overall conversion rate gradually decreased. The width of the conversion zone was first enlarged when changing the mixing ratio of wood and potato from 2:1 to 1:1, and especially the devolatilization process was prolonged both for wood and for potato. However, the conversion zone was then narrowed at the mixing ratio of 1:1.5, and the devolatilization rate even did not reach the peak value inside the fuel bed. In all three cases, the distribution of the drying rate of wood was limited near the bottom of the fuel bed, but the drying rate of potato almost expanded throughout the whole conversion zone, which is not within the expectation of classic theory for fixed-bed combustion.

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The structure of the conversion zone is further depicted in Figure 7 based on the distribution of different reaction rates at
the mixing ratio of 2:1. For a wood particle with relatively lower moisture content, the overlapping of the drying zone, devolatilization zone, and char reaction zone is not significant, and the three conversion processes could be regarded to proceed consecutively. However, for potato the drying process lasted almost until the end of its devolatilization. When the potato was still drying, the devolatilization of wood almost terminated and the char combustion process had started. Therefore, the conversion processes of different kinds of fuels are asynchronous inside the fuel bed. The dryer fuel may have

Figure 7. Structure of the conversion zone based on distribution of different reaction rates when the mixing ratio is 1:1 and the bed height decreased to 10.0 cm.

Figure 8. Modeling results of in-bed temperature distribution of gas and solid phase when the bed height decreased to 10.0 cm. (a–c) Temperatures of the gas phase and the surface of two solid fuel particles; (d–f) differences of temperatures between the gas phase and the surface of two solid fuel particles. The mass ratios of wood to potato are 2:1 (a, d), 1:1 (b, e), and 1:1.5 (e, f).
already been ignited, and the wet fuel was still preheating or drying. This may lead to a significant difference in particle surface temperature even at the same position, and different fuel particles may interact with each other, either directly through radiative heat transfer between one another or indirectly through convective heat transfer with the gas phase.

### 4.3. In-Bed Temperature Distribution of Different Phases

This section shows the ability of the MTTP model to separately simulate the temperatures of the gas phase and two different solid fuels inside the fuel bed, which is crucial for analyzing the asynchronous conversion behaviors during the co-combustion process. When solid fuels with different physical and chemical properties are used, the temperatures of the gas phase and the surface of the different solid particles may largely deviate from one another. The modeling results of in-bed temperature distribution of the gas and surface of different solid particles are shown in Figure 8 when the bed height decreased to 10.0 cm for each different mixing ratio. In general, the temperature of the gas phase rose smoothly as the fuels were ignited, but the temperature curve of the solid phases showed three different stages, i.e., a preheating stage under 100 °C, drying stage at around 100 °C, and afterward a fast-rising stage indicating the onset of combustion. It is worth noting that comparing Figure 6 and Figure 8, the fast rising of the surface temperature of fuel particles started before the moisture content was fully consumed, which is a characteristic behavior of a thermally thick particle. Because of the long duration of the intraparticle drying process for potato, the increase of the surface temperature of wood was earlier than that of the potato, and the surface temperature of the potato was lower than that of the wood until the fuel particles were dried out.

At the mixing ratio of 2:1, after ignition the temperature of the gas phase was slightly lower than that of wood but higher than that of potato. The difference between the temperatures of the gas phase and the fuel particles was within the range of ±200 °C, while the maximum difference between the surface temperatures of two solid phases was about 300 °C. However, at the mixing ratios of 1:1 and 1:1.5, the temperature of the gas phase was lower than the surface temperatures of both solid fuels, and the difference between the two the surface temperatures of solid fuels was reduced. Therefore, it can be anticipated that the higher proportion of potato in the fuel bed influenced the surface temperature of the wood, and the interactions between different solid phases weakened the overall conversion rate and mitigated the temperature difference between the two fuels. When the proportion of potato was higher than that of wood in the fuel bed ($M_{\text{wood}}:M_{\text{potato}} = 1:1.5$), the conversion process inside the fuel bed is quite similar to the self-sustaining oxidative pyrolysis process or smoldering combustion because of the low temperature, and in practice preheated primary air is often applied to accelerate the drying process.

The temperature distribution inside the fuel bed is intrinsically determined by the heat production and transfer. Figure 9 shows the modeling results of heat production and heat transfer over the fuel bed at the mixing ratio of 2:1 when the bed height decreased to 10.0 cm: (a) heat production from drying and char reactions; (b) heat transfer through radiation and convection.

![Figure 9. Modeling results of heat production and heat transfer over the fuel bed at the mixing ratio of 2:1 when the bed height decreased to 10.0 cm: (a) heat production from drying and char reactions; (b) heat transfer through radiation and convection.](image)

The multiple thermally thick particle (MTTP) model was developed to simulate the fixed-bed co-combustion process, in which the transport processes and chemical reactions both in subparticle and interparticle scales were considered, and different fuels could react independently based on their own properties. Model validation was conducted using mixtures of wood and potato spheres as representative fuels with low- and high-moisture content, which proved the applicability of the MTTP model. The modeling results further revealed that the conversion processes of different fuels were asynchronous, and the drying process could extend across the whole conversion zone and was highly overlapped with the devolatilization process.

### 5. CONCLUSIONS

The multiple thermally thick particle (MTTP) model was developed to simulate the fixed-bed co-combustion process, in which the transport processes and chemical reactions both in subparticle and interparticle scales were considered, and different fuels could react independently based on their own properties. Model validation was conducted using mixtures of wood and potato spheres as representative fuels with low- and high-moisture content, which proved the applicability of the MTTP model. The modeling results further revealed that the conversion processes of different fuels were asynchronous, and the drying process could extend across the whole conversion zone and was highly overlapped with the devolatilization process.

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