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CFD Simulations of Packed-Bed Combustion: Accounting for Irregularities in Particle Orientation in the Estimation of Bed Radiative Properties

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Modelling of packed-bed combustion includes the problem of modelling the radiative heat transfer. Thermal radiation significantly contributes to heat transfer both across the bed and from the hot gases to the top of the fuel layer. Several methods can be utilized aside from the so-called effective bed conductivity, such as the P1 or the Discrete Ordinates Model. When using the porous media for the fuel representation, its effective radiative properties must be determined, namely the extinction coefficient Gómez et al. (2014). It is often determined by assuming regularly oriented and mono-sized particles Shin and Choi (2000). Expressions for its estimation differ in the quantity representing the fuel and bed properties, for example, the bed porosity or particle emissivity. However, the absorption and scattering are influenced not only by how densely the particles are packed but also by their mutual position and orientation. The estimated radiative properties can significantly influence the combustion simulation, both quantitatively (e.g., the thickness of the reaction front, and ratios of the produced gases) and qualitatively (ignition of the fuel or the flame extinction). This work compares expressions of the radiative properties, that are modified by introducing irregularities in the positions or orientation of the fuel particles. The model for the radiative properties is implemented as a part of the radiation model based on the Discrete Ordinates method, modified for the case of two Eulerian phases representing the fuel and gas phase. In the presented work, these models for radiative properties are compared in a case of a fixed-bed reactor described by Zhou et al. (2005) and compared to the reported experimental results. The case is modelled in two dimensions. The radiation model is also described, including its implementation in ANSYS Fluent.

1. Introduction

CFD based modelling of the packed-bed combustion provides valuable insight into related processes, including the thermal decomposition of the fuel or for example, the development of solid and gaseous pollutants. In the recent review of Hoang et al. (2021), focusing on modelling techniques for municipal solid waste combustion, all three basic heat transfer mechanisms are reported to be included in packed-bed combustion models. The emphasis is put on models using the so-called effective thermal conductivity. This was widely used by authors of earlier works in the packed-bed combustion modelling (Zhou et al., 2005). Effective conductivity provided by Yagi and Kunii (1957) combines conduction in both the gas and the fuel, radiation between surfaces and inter-particle voids and the effect of convection and lateral mixing gas. An important note on including the radiative heat transfer using effective conductivity was made highlighted by Strieder (1997). One of the basic assumptions is relatively large interparticle distances and extension to the densely packed beds are not reliable using only the basic theory of the radiative heat transfer. This extension requires empirical validation and possibly evaluation of the radiative properties of the bulk.

Other approaches can be however used to model radiation inside densely packed beds. If a continuum phase is used to represent the fuel, it presents a second participating medium in the radiative heat transfer, which's radiative properties must be defined. The continuum representation of the fuel was used in the presented work. During the implementation of the radiation model, the choice of the model for the radiative properties – namely

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the extinction coefficient – was found to influence, if for given conditions fuel can be ignited. Calculation of the extinction coefficient according to Shin and Choi (2000), usually used in packed-bed combustion modelling (Gómez et al., 2014), was implemented in our model. However, as the authors themselves point out, the model is derived from an ideal arrangement of fuel particles. In the study presented here, the original expression given by Shin and Choi (2000) is compared to two modifications aiming to better capture the particles' shape and arrangement. Comparison is made in the case of an experimental fixed-bed reactor (Zhou et al., 2005).

2. Mathematical model

The fuel is represented as a porous medium defined over the whole computational domain. The bed location is then specified by choosing a non-zero volume fraction of the solid phase. In this work, particles are modelled as hollow cylinders (representing straw). The shape and size of particles are introduced via parameters of the porous media, e.g., specific surface and mass and heat transfer coefficient. Particles are assumed to be thermally thin. Transport equations for the mass conservation of both phases were adopted mainly from the work of Zhou et al. (2005), among others including the heterogeneous reactions such as moisture evaporation, devolatilization and fixed carbon oxidation. Mass conservation was solved for each of the four main fuel components – moisture, volatiles, fixed carbon, and ash. Permeability and inertial loss coefficient for modelling the Pressure loss in the bed were estimated using Ergun's equation.
The heat transport in the solid phase is modelled using a modified version of the model of Fjellerup et al. (2003), which calculates the effective heat conductivity of the bed. The original effective conductivity included effects of the flow and radiation, which in this work were excluded from the effective conductivity and included via the convective heat exchange between solid and gas and by solving the radiative heat transfer separately.

2.1. Model description

At a large scale, the fuel bed acts like an optically thick medium. As the combustion is simulated in two or three dimensions, the Discrete Ordinates Model (DOM) is selected as appropriate for modelling the radiative heat transfer across the bed with an arbitrary directional resolution. The radiative heat transfer is solved for a defined set of discrete directions spanning the total solid angle, each represented by a vector $\vec{s}_i$ and weight w_i and solving a radiative transport equation (RTE), as expressed with Eq(1) (Modest, 2003).

$$\vec{s}_i \cdot \nabla I(\vec{s}_i) + \left(\eta\, \alpha_g + (1-\eta)\beta_s\right) I(\vec{s}_i) = \frac{\sigma_R}{\pi}\left[\alpha_g \eta\, T_g^4 + \alpha_s(1-\eta)\, T_s^4\right] + \frac{\sigma_s}{4\,\pi}\sum_j w_j\, I(\vec{s}_j')\, \Phi_s(\vec{s}_i \cdot \vec{s}_j') \quad (1)$$

β_s is the extinction coefficient of solid, σ_R is the Stefan-Boltzmann constant, α and σ are the absorption and scattering coefficients and Φ_s is the scattering function. η is the bed external porosity, i.e., the volume fraction of the gas outside the fuel particles. The absorption coefficient of the gas was modelled using the domain-based weighted-sum-of-grey-gases model. Scattering in the gas is assumed to be negligible.
The extinction coefficient β_s represents the ratio of the radiative intensity I of the radiation transmitted through a medium by a distance Δx. and the initial intensity I_0 (Modest, 2003). The ratio I/I_0 can be also interpreted as a probability P of finding an unobstructed path of length Δx, passing through the porous for the given direction. Then, β_s can be expressed with Eq(2).

$$\beta_s = -ln\, P/\Delta x \quad (2)$$

Using the same approach as in the work of Gómez et al. (2014), the absorption and scattering coefficients can be estimated using the surface emissivity, as expressed with Eq(3) and Eq(4), assuming opaque particles.

$$\alpha_S = \varepsilon_p\, \beta_s \quad (3)$$

$$\sigma_S = \left(1 - \varepsilon_p\right) \beta_s \quad (4)$$

A simple model of the extinction coefficient was proposed by Shin and Choi (2000). They assumed, that the radiation in each direction is partially blocked by a layer of ideally arranged particles. Although it is not directly mentioned, the spherical shape of particles was assumed, as explicitly stated in other parts of their combustion model. Eq(5) is the proposed expression for the extinction coefficient.

$$\beta_s = -2 \ln \eta\, / r_p \quad (5)$$

Assuming that the particles were arranged as assumed by the authors, the actual attenuation of radiation (in the direction normal to the particle layer) would be given by the surface area of the particles' shadow instead of the volumetric fraction, leading to the expression for β_s to be $-\ln(4\eta/\pi)/d_p$ for cylindrical and $-\ln(1.5\,\eta)/d_p$

for spherical particles, as illustrated in Figure 1. Assuming more particles than just a single layer leads to a further increase in the value of β_s.

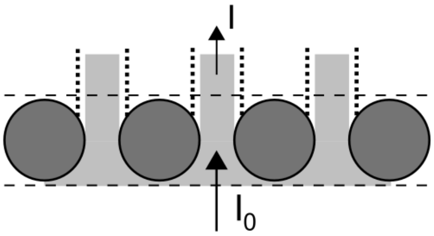

Figure 1: Particles' arrangement assumed by Shin and Choi (2000) for estimation of β_s. The grey area represents the actual transmitted radiation, dotted lines illustrate the amount of radiation as given by the proposed expression for β_s.

Strieder (1997) in his work focused on solving radiative heat transfer inside a bed consisting of mono-sized cylinders. The probability of finding an unobstructed path is expressed with Eq(6). Each particle is assigned to a certain plane with a given orientation in space, to which the particle's axis is perpendicular. The summation goes over all these particle groups, denoted by index j. n_j is the number of particles in the group per unit area and θ_j is the angle between the plane and the direction of radiation. Mutual overlap of the particles is allowed.

$$\ln P = \sum_j - d_p n_j \Delta x \cos(\theta_j) \tag{6}$$

Note, the original expression for P used by Strieder (1997) contains a second term under the summation, related to a probability that the starting point of the path does not lie inside any particle. In our case, we investigate the absorption of radiation starting only from points inside voids between particles. The second term (probability of choosing the starting point inside some particle) is then zero by definition.
The porosity η can be viewed as the probability of randomly choosing a point lying inside bed voids. As such, η can be expressed with Eq(7).

$$\ln \eta = \sum_j -\pi\, d_p^2/4\, n_j \tag{7}$$

For a continuous variation in the particles' orientation, the summation used in Eq(5) and Eq(6) is replaced by integration from 0 to $\pi/2$ and n_j has to be substituted with $\xi(\theta)\sin\theta$. For two cases of particle orientation, the expressions for the extinction coefficient are listed in Table 1.

Table 1: Three expressions for the extinction coefficient: fully random orientation (RP); original model of Shin and Choi (2000) (SC); all particles perpendicular to the radiation direction (PP).

	RP	SC	PP
β_s [1/m]	$-\frac{2}{\pi}\frac{\ln\eta}{d_p}$	$-\frac{\ln\eta}{d_p}$	$-\frac{4}{\pi}\frac{\ln\eta}{d_p}$

2.2. Model implementation

The combustion model was implemented via ANSYS Fluent. The porous zone model with physical velocity formulation was used to model the pressure loss and increase of the flow velocity inside the bed. However, combining this model with the DOM does not allow for using the Non-Equilibrium Model for modelling the porous medium temperature. The fuel enthalpy along with several other quantities related to the fuel was included using the so-called User Defined Scalars (UDS), enabling to define of a new transport equation for an arbitrary physical quantity (ANSYS, Inc. 2021). The porous zone model was then used mainly for capturing the reduction of the gas phase volume fraction and the pressure loss and the porous media density, thermal conductivity and specific heat capacity were set to zero to avoid its influence on the energy balance. The effect of the porous solid on radiation is included by adjusting the transport equation during each iteration. Similar (but not identical) adjustments were used by Gómez et al. (2013).
First, the absorption coefficient of the gas is replaced by the volumetric average of α_g and α_s as expressed with Eq(8), using the macro DEFINE_WSGGM_ABS_COEFF. Also, the scattering coefficient is replaced with $(1-\eta)\,\sigma_s$.

$$\alpha = \eta \, \alpha_g + (1 - \eta) \, \alpha_s \tag{8}$$

After this adjustment, the emission term in Eq(1) is still not in the correct form. To account for the difference between the gas and fuel temperature, a source term given by Eq(13) is introduced into the RTE using macro DEFINE_DOM_SOURCE.

$$S_{RTE} = (1 - \eta) \, \alpha_s \, \frac{\sigma_R}{\pi} \left(T_s^4 - T_g^4 \right) \tag{13}$$

Fluent automatically assigns all the absorbed/emitted radiative energy (calculated by the modified DOM) to the gas phase. The last adjustments include a user-defined source term ΔS_{rad} , added to the solid and subtracted from the gas enthalpy transport equation. This source term is expressed in Eq(14).

$$\Delta S_{rad} = (1 - \eta) \, \alpha_s \left[\sum_i w_i \, I(\vec{s}_i) - 4 \, \sigma_R T_s^4 \right] \tag{14}$$

3. Simulation setup

The experimental reactor described by Zhou et al. (2005) was simulated. A two-dimensional section of the reactor was used as the model geometry. Only the main dimensions reported by the authors, the air inlet and the flue gas outlet were derived from the scheme of the reactor in the original publication. The schematic representation of the used geometry is shown in Figure 2. The domain was discretized using approximately 9,200 quadrilateral cells with a maximum size set to 5 mm. 12 prismatic layers were used near the walls, with the boundary cell height set to 0.5 mm.

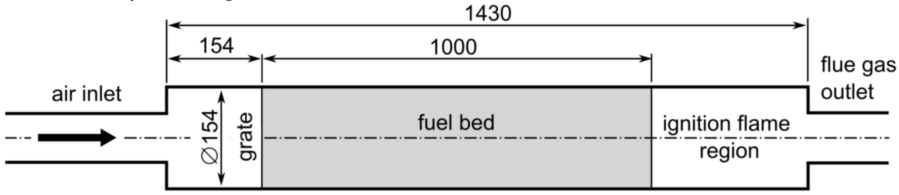

Figure 2: The model geometry, adapted from the description of the experimental reactor.

Bed dimensions and operating conditions were kept constant. Zhou et al. (2005) provided data on the fuel proximate and ultimate analysis. The LHV was estimated using a correlation provided by van Loo and Koppejan (2008). As in the work of Juřena and Hájek (2011), the composition of the devolatilization products was simplified using a representative compound, with properties derived from mass and energy balance, fuel composition and the LHV. According to the experimental observations of Zhou et al. (2005), the (external) porosity was kept at a constant value of 0.58 throughout the simulation, with straw particles having an outer diameter of 4.2 mm. The wall emissivity was set up according to Gómez et al. (2014), assuming a partially oxidized wall surface. Inlet boundary conditions and case initialization were set up according to the experiment described by Zhou et al. (2005). In their work, the straw emissivity is equal to the emissivity of straw char ($\varepsilon_p = 0.9$), which was used in our work. The authors mention that by decreasing the amount of char in the solid residuum, the emissivity may significantly decrease. Other values are used in works on packed-bed combustion modelling. A value of 0.8 was reported as a typical value for solid fuels by Yang et al. (2007) and used for simulations of MSW combustion. The inlet air temperature was set to 20°C, its mass flow rate $3.35 \cdot 10^{-3}$ kg/s, with a composition of 75.94 % N_2, 23 % O_2, 1.02 % H_2O and 0.04 % CO_2 (by mass).

4. Results and discussion

The data obtained from the simulated 200 s period are compared to those reported by Zhou et al. (2005). In the experiments, the straw was fed into the reactor and ignited with a gas burner. After the thermocouple below the bed top detected a temperature rise, the burner was removed. In the simulation done by the same authors, ignition was done by setting the temperature at the bed top to 800°C for 2 s. In the work presented here, the fixed temperature was set across the whole volume above the bed top and in the first layer of fuel containing cells. The temperature was kept at a minimum of 800°C for 6 s to keep the fuel burning after switching the ignition source off. The first observable results have shown, that in the case of randomly oriented particles (RO) the flame is extinguished very shortly after the ignition source is turned off, which can be seen on the graph of the maximum temperature during the calculation for all three cases (Figure 3).

The relative imbalance of the total mass and energy was monitored throughout the calculation. The definition of the relative imbalance can be found in the work of Juřena and Hájek (2011). The values at 250 s and the maximum reported values are listed in Table 2.

Table 2: Comparison of the maximum mass and energy relative imbalances recorded throughout the simulated period 250 s. RO – randomly oriented particles, SC – extinction coefficient is given by Shin and Choi (2000), PP – particles perpendicular to the radiative flux direction.

		RO	SC	PP
mass	maximum	0.0036 %	0.00024 %	0.00024 %
	final	0.0013 %	0.00023 %	0.00024 %
energy	maximum	0.040 %	0.39 %	0.57 %
	final	0.030 %	0.26 %	0.39 %

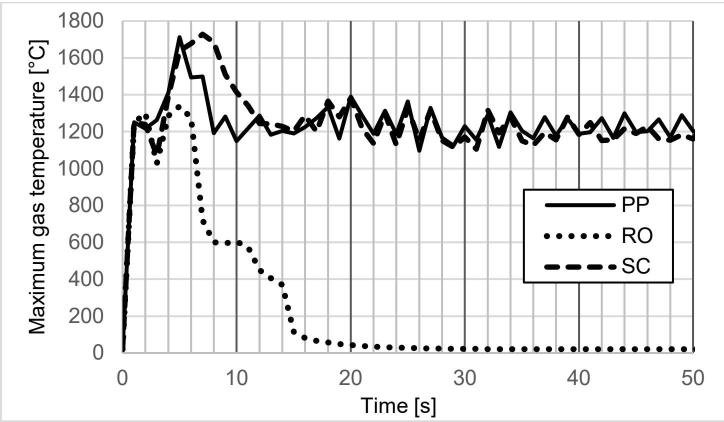

Figure 3: Temperature profiles during the first minute of simulated combustion, obtained using three models for β_s. Temperatures in the range of 727°C – 1,027°C were measured during the experiments (Zhou et al., 2005).

Nine points representing the thermocouples in the experimental reactor were placed at the reactor axis inside the bed. These were labelled from the bed bottom to the top as T2-T9. The period between the same given gas temperature is recorded at the furthest thermocouple (T6). The periods were almost identical for both the SC (218 s) and PP case (224 s) and the temperatures reported by experimenters (≈ 230 s). The average temperature recorder during the 250 s was 1,197°C (PP) and 1,173°C (SC), being significantly higher compared to the maximum temperatures observed during experiments (727°C–1,027°C). As both the PP and SC models differ from the experiment almost identically, the cause of the higher temperature might be expected to relate to using too high an estimation of the straw LHV.
Predicted molar fractions of CO_2 and CO at the bed top were 12.04 % and 4.7 % for the PP and 11.7 % and 5.11 % for the SC case. Predicted contents were lower compared to the experiment (approximately 16 % of CO_2 and 13 % of CO).

5. Conclusions

Simulation of three minutes of the combustion process demonstrated the difference in assuming a particular arrangement of fuel particles even when all the particle properties and the bed porosity are identical. For the case of the experimental reactor and straw bed, the main results are the following:

- No significant difference was observed between the original expression for the extinction coefficient proposed by Shin and Choi (2000) and the expression derived from the randomly placed particles oriented perpendicularly to the radiation direction was observed.
- Using the model with randomly orientated straw particles led to the flame extinction within 2 s after the artificial heat source representing the auxiliary gas burner was turned off. The value of the extinction coefficient for this particle arrangement

The observed difference points to the fact, that the bed structure cannot be automatically considered as an insignificant parameter compared to other parameters, although in practice and namely in the case of heterogeneous fuels, e.g., municipal solid waste, the structure cannot be always predicted in such a detailed level to obtain the accurate distribution of particle orientations.

Nomenclature

d_p – fuel particle diameter, m
I – radiative intensity, W/(m^2·sr)
n – number of particles per unit volume, 1/m^3
P – probability, -
$\vec{s}$ – directional vector, -
S_{RTE} – energy source term in RTE, W/(m^3·sr)
T – temperature, °C
w – weighting factor, -
α – absorption coefficient, 1/m
ΔS_{rad} – enthalpy source term, W/m^3
Δx – path distance, m
ε – emissivity, -
η – external porosity, -
θ – angle, rad
ξ – number of particles per unit area and unit solid angle, 1/(m^2·sr)
σ – scattering coefficient, 1/m
σ_R – Stefan-Boltzmann constant, W/(m^2·K^4)
Φ_s – scattering function, -
Ω – solid angle, sr

Subscripts

g – gas
s – solid
p – particle

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