A Visualization Method of Quantifying Carbon Combustion Energy in the Sintering Packed Bed

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Carbon combustion provides energy to reach essential temperatures in the sintering packed bed. A visual and quantitative evaluation on the energy input distribution inside the bed is urgently demanded to learn energy-saving potential of sintering process and subsequently to suppress greenhouse gas emission. Herein, after a two-dimensional simplified model of sintering packed bed is established and validated against the temperature measurements on the sintering pot experiment, this work highlights a mesh-based visualization method of quantifying carbon combustion energy in the packed bed. To be more specific, local transient temperature distributions in all meshed grids are first extracted from numerical simulation results. Then each grid is colorized according to the specific criteria on five pre-defined energy input (EI) states. As a result, the effects of carbon segregation and cross-sectional shape on the energy efficiency of sintering packed bed are quantitatively compared and optimized. These two case studies not only demonstrate the principle, process, and application of the proposed visualization method, but also stimulate its future potential in various areas.

KEY WORDS: visualization method; carbon combustion energy; sintering packed bed; carbon segregation; cross-sectional shape.

1. Introduction

The packed bed reactor have wide applications in the different chemical processes, such as the absorption,¹⁾ the distillation,²⁾ the stripping,³⁾ the separation,⁴⁾ the solid fuel combustion,⁵⁾ and the iron ore sintering process.^{6,7)} The carbon combustion in the packed bed supports desired temperatures for the chemical reactions in the sintering process,⁸⁾ which significantly affects yield and quality of products.^{9,10)} Therefore, lots of efforts on temperature profile optimization have been made by controlling carbon grain size distribution,^{11,12)} blowing natural gas,^{13,14)} and so on.

On the other hand, the duration above a specific temperature also makes an important influence on the reaction kinetics in the packed bed,^{15,16)} which has been widely investigated by experimental^{17–23)} and numerical^{24–29)} studies over the past decades. Machida *et al.*³⁰⁾ established a relationship between products' strength and the duration

above melting temperature, and the total heat available in the critical melt formation stage⁹⁾ was further determined.³¹⁾ Meanwhile, either one-dimensional^{32,33)} or two-dimensional model¹⁰⁾ was solved to predict the temperature profiles against the time, and a residence time of approximately 10 mins at 1 473–1 673 K was expected to be reasonable for liquid phase generation in the packed bed.³⁴⁾

Although lots of work has successfully established the relations between the temperature profile and the sintering time, few works focus on proposing a visualization method to quantitatively evaluate carbon combustion energy in the packed bed. Therefore, this work first predicts and validates the transient temperature versus the time in a carbon combustion packed bed through a two-dimensional simplified model. Then five energy input (EI) states are defined based on the specific criteria, and the cross section of the carbon combustion packed bed is colorized and evaluated based on the meshed grids. Furthermore, two case studies, namely the effects of the carbon segregation and the cross-sectional shape on the energy efficiency in the packed bed,

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are demonstrated to understand the definition, process and application of the proposed visualization method, as well as to stimulate its future prospects in other fields.

2. Experimental and Numerical Methods

The laboratory-scale sintering pot experiment is used to simulate the carbon combustion in a packed bed, and its schematic diagram is shown in the Fig. 1. The pot has an inner diameter of 40 cm and a height of 63 cm. Three thermocouples are respectively installed at H=15, 33, and 48 cm measured from the bottom, to record the transient temperatures in the whole process. After approximately 60 kg raw materials including 3.2 wt% carbon are charged into the pot, the combustion starts when the carbon is ignited by the liquefied gas from the top at a negative pressure of 15 kPa.

Meanwhile, a 1:1 scale two-dimensional simplified Euler-Euler model for the numerical simulation is established in terms of mass, momentum, energy and specie conservation equations of gas and solid phases respectively in Eqs. (1)–(6).

Gas phase mass conservation:

$$\frac{\partial}{\partial t}(\varepsilon \cdot \rho_g) + \frac{\partial}{\partial y}(\varepsilon \cdot \rho_g \cdot u_g) = \sum_{k=1}^n \dot{m}_k \quad \dots\dots\dots (1)$$

Gas phase momentum conservation:

$$\frac{\partial}{\partial t}(\varepsilon \cdot \rho_g \cdot u_g) + \frac{\partial}{\partial y}(\varepsilon \cdot \rho_g \cdot u_g \cdot u_g) = -\varepsilon \cdot \frac{\partial P}{\partial y} - F_v \quad \dots\dots\dots (2)$$

Gas phase energy conservation:

$$\frac{\partial}{\partial t}(\varepsilon \cdot \rho_g \cdot h_g) + \frac{\partial}{\partial y}(\varepsilon \cdot \rho_g \cdot u_g \cdot h_g) = h_{conv} \cdot A_s \cdot (T_g - T_s) + \sum_{k=1}^n \dot{q}_{g,k} \quad \dots\dots\dots (3)$$

Gas phase specie i conservation ($i=O_2, CO, CO_2, N_2$ and H_2O):

$$\frac{\partial}{\partial t}(\varepsilon \cdot \rho_g \cdot Y_i) + \frac{\partial}{\partial y}(\varepsilon \cdot \rho_g \cdot u_g \cdot Y_i) = \sum_{k=1}^n \sum_i \dot{m}_{i,k} \quad \dots\dots\dots (4)$$

Solid phase mass conservation:

Fig. 1. The schematic diagram of the laboratory-scale sintering pot experiment and the corresponding dimensions and boundary conditions for the numerical simulation. (Online version in color.)

$$\frac{\partial \rho_s}{\partial t} = -\sum_{k=1}^n \dot{m}_k \quad \dots\dots\dots (5)$$

Solid phase energy conservation:

$$\frac{\partial}{\partial t}(\rho_s \cdot h_s) = \frac{\partial}{\partial y} \left(\frac{k_{s,eff}}{C_{ps}} \cdot \frac{\partial h_s}{\partial y} \right) + h_{conv} \cdot A_s \cdot (T_g - T_s) + \sum_{k=1}^n \dot{q}_{s,k} \quad \dots\dots\dots (6)$$

Besides, the carbon combustion reaction in the present model has two intermediate steps:³⁵⁾ the carbon is first oxidized to CO by O_2 , and then it is further oxidized to CO_2 . The corresponding reaction rates are determined by Eqs. (7)³⁶⁾ and (8),³⁷⁾ respectively.

$$R_{carbon} = \frac{2A_c W_c C_{O_2}}{\frac{1}{\xi k_c} + \frac{1}{k_{film}} + \frac{1}{k_{coating}}} \quad \dots\dots\dots (7)$$

$$R_{co} = 3.25 \cdot 10^7 C_{co} C_{O_2}^{1/2} C_{H_2O}^{1/2} \exp \left(-\frac{15089}{T_g} \right) \quad \dots\dots\dots (8)$$

where, k_c is the rate constant, k_{film} is the film mass transfer coefficient, $k_{coating}$ is the mass transfer coefficient through the coating solids and the developing ash layer. Besides, the particle radius r_0 is initialized as 0.002 m, while the carbon radius $r_{i,carbon}$ decreases as the combustion proceeds, which is described by Eq. (9).

$$r_{i,carbon} = r_0 \left(1 - \frac{(Y_{0,carbon} - Y_{i,carbon})}{Y_{0,carbon}} \right)^{\frac{1}{3}} \quad \dots\dots\dots (9)$$

where, $Y_{0,carbon}$ is initial carbon mass fraction, $Y_{i,carbon}$ is the transient carbon mass fraction.

For boundary conditions, the top surface is the gas velocity inlet while the bottom is the gas pressure outlet, both side-wall are stationary and adiabatic. The bed voidage is supposed to have a linear relationship with the temperature by fitting the data from Wang *et al.*' work.³⁸⁾ The pre-test results of the established model reveals that the transient carbon particle radius and bed voidage make limited effect on the carbon combustion rate, while the prediction of the

Table 1. The parameters for the numerical simulation.

Parameters	Values
Gas temperature at the inlet (ignition stage) (K)	1 273
Gas pressure at the outlet (ignition stage) (kPa)	−15
Ignition duration period(s)	120
Gas temperature at the inlet (combustion stage) (K)	300
Gas pressure at the outlet (combustion stage) (kPa)	−10
Initial solid temperature (K)	300
Solid density (kg/m ³)	2 719
Solid specific heat J/(kg·K)	871
Voidage in the packed bed (−)	0.35
Particle radius (m)	0.002
Time step (s)	1
Calculation time (s)	3 000

bed voidage distribution by directly solving conservation equations is challenging. Alternatively, the bed voidage is considered to be constant (0.35) in the following analysis. The other specific parameters^{39–41)} for numerical simulation are listed in the **Table 1**.

The simulated transient temperatures at $H=15, 33$, and 48 cm against the process time are compared with the experimental measurements in the **Fig. 2(a)**. The differences in the maximum temperatures and the periods to reach the corresponding maximum temperatures between the measured and simulated results are less than 75 K and 24 s, respectively. In addition, the measured sintering time and the times when the flame front (FF) reaching specific heights or the times when the temperature starts to rise, are compared with the simulated results in the **Fig. 2(b)**. The difference in the sintering time between the experiment and simulation is less than 3 minutes, while the simulated times when the FF reaches individual heights is shorter than the measured counterparts. The discrepancies in the temperature profile and the corresponding FF distributions between the experimental and numerical results attribute to the following two reasons. First, the established model is simplified by neglecting other complex physical and chemical processes, such as the melting and solidification process, the migration process of water, the shrinkage process of bed height after combustion, and so on. Second, the sealing problems strengthen the heat loss in the lower part of sintering pot. Nevertheless, the consistent trends in temperature distributions with acceptable differences agree that this simplified model is capable of providing quantitative data to introduce the visualization method. Meanwhile, the snaps of the solid temperature profiles at 120 s, 1100 s, and 2155 s are demonstrated in the **Fig. 2(c)**. The solid temperature increases to 1273 K when the ignition finishes at 120 s, and the thickness of the high temperature zone between 923 and 1621 K is approximately 3 cm in the vertical direction. At 1100

s, the maximum solid temperature is increased by 458 K and the thickness of the aforementioned high temperature zone enlarges to 18 cm. When the carbon combustion in the packed bed closes to the end, the maximum solid temperature and the thickness of the high temperature zone reach as great as 1621 K and 19 cm, respectively. In short, the transient temperature profile versus the process time in the **Fig. 2(d)** provides quantitative information to evaluate the energy storage effect.^{42–44)}

Fig. 3. The transient temperature profiles of the solid in the carbon combustion packed bed at different time nodes (inset: the transient temperature profile of the white dotted square against the time marked with the upper and lower limits of the critical temperatures and the valid duration). (Online version in color.)

Fig. 2. (a) The comparison between the measured and simulated transient temperatures at $H=15$ cm, 33 cm, and 48 cm measured from the bottom, (b) the comparisons of measured and simulated sintering time and the time when the flame front (FF) reaching different heights, (c) the snaps of the simulated solid temperature profiles at 120 s, 1100 s and 2155 s, and (d) the transient temperature distribution versus the increasing time in the packed bed. (Online version in color.)

3. Results and Discussion

3.1. Visualization Method of Quantifying Carbon Combustion Energy

First of all, the cross-section of the sintering packed bed is divided into grids with the proper mesh size. Second, taking the white dotted square in the **Fig. 3** as an example, the transient temperature is subjected to change at different time nodes as depicted in the inset. Third, based on the favorable conditions for liquid phase production,^{45,46)} the upper and lower limits of the critical temperature range are 1 573 and 1 373 K, respectively, while the valid duration

is between 180 and 300 s. As a result, five visualization EI states, namely EI(0), EI(+), EI(++), EI(-), and EI(--), are defined and explained in the **Table 2**.

The EI(0) state (marked in green) means the local temperature is between 1 373 and 1 573 K for 180–300 s. In contrast, when the local temperature is higher than 1 573 K or lower than 1 373 K, it is in the EI(++ state (marked in red) or in the EI(--) state (marked in grey blue). Besides, although the local temperature is between 1 373 and 1 573 K, it is in the EI(+) state (marked in yellow) when its valid duration is longer than 300 s, while it is in the EI(-) state (marked in dark blue) when shorter than 180 s. Overall, in

Table 2. Symbols, criterions and marked colors of the five energy input (EI) states. (Online version in color.)

	Insufficient energy input		Reasonable energy input	Excess energy input	
symbol	EI(--)	EI(-)	EI(0)	EI(+)	EI(++)
criterion	$T < 1\,373\text{ K}$	$1\,373\text{ K} < T < 1\,573\text{ K},$ $t < 180\text{ s}$	$1\,373\text{ K} \leq T \leq 1\,573\text{ K},$ $180\text{ s} \leq t \leq 300\text{ s}$	$1\,373\text{ K} < T < 1\,573\text{ K},$ $t > 300\text{ s}$	$T > 1\,573\text{ K}$
marked color

Fig. 4. Energy optimization through the carbon segregation in the 6 layer-structure packed beds: (a) the carbon concentration distributions (wt%), (b) the predicted EI state distributions, (c) the transient temperature at H=42 cm and (d) the maximum central temperature distributions. (Online version in color.)

contrast to the local regions in the EI(0) state, those in the EI(-) and EI(--) states require more energy input whereas that in the EI(+) and EI(++) states waste a considerable amount of energy. Therefore, the proposed method provides a quantitative and visual guidance to balance the energy input distribution in the sintering packed bed, thus expecting to achieve higher energy efficiency.

3.2. Case Study I: Carbon Segregation in a Rectangular Cross-section of Packed Bed

This case study demonstrates how to use the aforementioned visualization method to compare and evaluate the effect of the carbon segregation on the energy efficiency in a rectangular cross-section of packed bed. The 6 packed beds in the Fig. 4(a) have 1, 2, 3, 4, 5 and 6-layer structures, respectively with different carbon concentrations. Then their cross-sections are discretized into 3×3 cm square grids. Based on the transient temperature profile against the time extracted from the numerical results, each grid is judged and colorized as one of the previously defined EI states in the Fig. 4(b). Meanwhile, the transient temperature profiles at $H=42$ cm, and maximum central temperature profiles are further compared in the Figs. 4(c)–4(d), respectively. To be more specific, in the base case, 3.2 wt% carbon is uniformly distributed in the packed bed. The results show that less than 15% of the cross section is in the EI(0) state. In contrast,

more than 33% of the region in the upper part of the packed bed requires more energy input while approximately 50% in the lower part wastes excess energy. These quantitative results indicate that carbon should be unevenly distributed to balance the energy distribution in the vertical direction of the packed bed. Therefore, another 5 cases are studied with 2- to 6-layer structure packed beds. Three points are worthy of note. First, although the average carbon concentrations in the base or 1, 2 and 3-layer cases are the same, the latter two cases make better use of the heat storage effect, and approximately 90% of the region is in the EI(++) state, which provides great potential to reduce carbon consumption. Second, the 3 to 6-layer cases not only uniform the energy distribution, but also reduce the total carbon consumption by at most 43.8% under present numerical conditions. Because the maximum transient temperature in the packed bed is decreased significantly while it is still above the critical temperature.

3.3. Case Study II: Cross-sectional Shape Optimization of Packed Bed with Uniform Carbon Distribution

This second case demonstrates how to use the aforementioned visualization method to compare and evaluate the effect of the cross-sectional shape on the energy efficiency of the packed bed with uniform carbon distribution. The upper base length of the isosceles trapezoidal-shaped cross section

Fig. 5. Energy optimization through increasing upper base length of the trapezoidal cross sections of the packed beds: (a) the geometric dimensions, (b)(c) the predicted EI state distributions, and (d) the vertical sintering speed in the center and edge. (Online version in color.)

Fig. 6. (a) The geometric dimensions of the trapezoidal cross sections with 50 cm and 30 cm upper base, and the correspondingly predicted EI state distributions, (b) further comparison in terms of individual EI state, and (c) the vertical sintering speed in the center and edge. (Online version in color.)

of the packed bed in the Fig. 5(a) is increased from 50 cm to 60 cm and then to 70 cm, while the lower base length is accordingly decreased from 30 cm to 20 cm and then to 10 cm, respectively, while the cross-sectional area is constant. The EI state distributions are predicted and compared in the Figs. 5(b)–5(c). In addition to the V-shaped distributions, 24.2%, 30.0%, and 33.7% of the region are in the EI(0) state while 37.4%, 65.6% and 60.1% are in the EI(–) or EI(–) state. The vertical sintering speeds in the center and edge are also compared in the Fig. 5(d). First of all, the vertical sintering speeds in the trapezoid-shaped cross-section of packed bed is higher than the counterpart in the base case (17.5 mm·min^{–1}). The results indicate that the trapezoid-shaped cross-section with the long upper base length, in comparison to the rectangular one, can increase the sinter yield. Second, when the upper base length is increased from 40 cm to as long as 70 cm, the vertical sintering speeds in the central and edge regions is respectively increased by at most 50.2% and 45.2%, and an increasing unevenness of the vertical sintering speed between center and edge is noticed.

On the other hand, what if the trapezoidal cross section has a shorter upper base length? So the Fig. 6(a) introduces a new trapezoidal cross section with a 30 cm upper and a 50 cm lower base lengths, while the previous case with a 50 cm upper and a 30 cm lower base lengths is taken for comparison. The EI state distributions are predicted and compared in terms of individual states in the Fig. 6(b). The trapezoidal cross-section having shorter upper base length decreases the proportion of region in the EI(–) or EI(–) state from 37.4% to 29.3%, while that in the EI(+) or EI(++) state increases from 38.5% to 47.6%. However, the proportion in the EI(0) state is not significantly changed. When the upper base length is shorter than the lower base, the central temperature is higher than that near the edge. As a result, the EI state distribution changes from a V-shaped profile to a reversed V-shaped one. Besides, the vertical sintering speeds in the central and edge regions are further compared

in the Fig. 6(c). It is worth noting that the vertical sintering speed in the central region for the 30 cm upper base length case is less than half of the result for the 50 cm upper base length case. Besides, the uneven vertical sintering speed distribution between the center and edge regions in the former case greatly limits the yield. Overall, when the upper base length of the trapezoid-shaped cross-section of packed bed is decreased, the shortage of energy in the upper part can be relieved while the excess energy caused by the high central temperature in the lower part becomes the most prominent feature.

4. Conclusions

This work highlights a visualization method aiming to quantitatively evaluate the carbon combustion energy efficiency in the sintering packed bed. Its cross section is first discretized into 3 × 3 cm square grids, and the transient temperature profile with respect to the time in each grid is extracted from the numerical results, after the established model is validated against the experimental measurements. The five EI states are defined according to the criteria consisting of the critical temperature range and its duration. At last, two case studies, namely the effects of carbon segregation and cross-sectional shape on the energy efficiency of packed bed, are demonstrated to fully understand the definition, process, application of the visualization method, and to stimulate the application potential in other fields.

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Nomenclature

- A_C : volumetric surface area of carbon particle (m^2/m^3)
 A_S : specific surface area of convective heat transfer (m^2/m^3)
 C_{CO} : CO mole concentration (mol/m^3)
 C_{H_2O} : H_2O mole concentration (mol/m^3)
 C_{O_2} : O_2 mole concentration (mol/m^3)
 C_p : solid specific heat ($\text{J}/(\text{kg}\cdot\text{K})$)
 c_n : carbon concentration in the n th layer (wt%)
 F_V : gas flow resistance ($\text{Pa}\cdot\text{m}$)
 h_{conv} : convection heat transfer coefficient $\text{W}/(\text{m}^2\cdot\text{K})$
 h_s : solid enthalpy (kJ/mol)
 k_c : reaction rate constant (m/s)
 $k_{coating}$: mass transfer coefficient of ash layer (m/s)
 k_{film} : film mass transfer coefficient (m/s)
 $k_{s,eff}$: solid effective coefficient ($\text{W}/(\text{m}\cdot\text{K})$)
 $\dot{m}_k$: mass production rate ($\text{kg}/(\text{m}^3\cdot\text{s})$)
 P : pressure (Pa)
 $q_{g,k}$: volumetric heat source of gas ($\text{J}/(\text{m}^3\cdot\text{s})$)
 $q_{s,k}$: volumetric heat source of solid ($\text{J}/(\text{m}^3\cdot\text{s})$)
 R_{carbon} : reaction rate of carbon ($\text{kg}/\text{s}/\text{m}^3$)
 R_{CO} : reaction rate of CO ($\text{kg}/\text{s}/\text{m}^3$)
 r_0 : initial particle radius (m)
 r_{carbon} : transient carbon radius (m)
 T : temperature (K)
 W_C : carbon molecular weight (kg/mol)
 Y : mass fraction (-)
 y : coordinate value in y-axis (m)

Greek alphabets

- ε : packed bed porosity (-)
 u : velocity (m/s)
 μ : viscosity ($\text{Pa}\cdot\text{s}$)
 ξ : a factor of particle area (-)
 ρ : density (kg/m^3)

Subscripts

- g : gas
 s : solid
 0 : initial state
 i : transient state

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