Research Article

Structural optimization of baffle internals for fast particle pyrolysis in a downer reactor using the discrete element method

Bing Liu*

National Institute of Clean-and-Low-Carbon Energy, CHN Energy Investment, Beijing 102211, P.R. China

*Corresponding author. E-mail: 20032357@chnenergy.com.cn

Abstract

The structural optimization of baffle internals for fast pyrolysis of coal with particulate mixing and heat transfer in a downer reactor using the discrete element method (DEM) has been investigated in this research. The pyrolysis terminal temperature at the exit of the downer reactor is not only decided by the volume-feeding-rate ratio of the coal to the sand, but also is affected by the inner structural design of the baffle internals in the downer reactor. As presented in the previous publication of the author, the inhibition from the baffle internals in a downer reactor can improve the particulate-mixing degree and heat carrier, and increase the mean residence time of the coal and heat-carrier particles in the downer reactor. The structure of the baffle internals in the downer reactor mentioned in this research can be optimized by the independently developed 3D soft-sphere model of the DEM programme of a 40-mm baffle length, a 30° baffle-slope angle and at least four baffles designed in the downer reactor, which is beneficial for the process design of coal pyrolysis with a heat carrier in the downer reactor.
Keywords: structural optimization; baffle internals; downer reactor; DEM; coal pyrolysis

Introduction

The downer reactor is considered a high-efficiency chemical reactor in the twenty-first century, which has a very broad application prospect in energy conversion and chemical engineering [1–4]. The characteristics of a downer reactor can be summarized as follows: (i) it has a high flow rate of the solid phase [5–7]; (ii) the radial concentration of the solid phase is uniformly distributed and the phenomenon of the axial back mixing can be ignored [8, 9]; (iii) the mixture ratio of the solid and gas is not limited, which is especially suitable for high-load solid particles [5, 10]; (iv) low energy consumption in pneumatic conveying; (v) the mean residence time (MRT) of the solid particles is short and the residence time distribution is narrow [6, 7].

Based on these advantages, downer reactors can operate under some difficult process conditions, such as the rapid pyrolysis process of coal or biomass [11–14]. As mentioned in previous research [15–18], a pyrolysis downer reactor is generally coupled with a fluidized-bed reactor. Pulverized coal charged from a pot at the top of the downer reactor is mixed with the hot ash or silica sand (heat carrier) discharged from the fluidized-bed reactor, which heats the coal to release gaseous volatile substances.

Rapidly heating the coal particles can increase the yield of the light liquid products and fine chemicals. The coal-particle temperature at the exit of the downer reactor can be determined by the volume-feeding-rate ratio of the coal to the heat-carrier particle, but the rapid heating of coal particles is the most important factor during the coal-pyrolysis process, which is affected by the rapid mixing between the coal and the sand (a commonly used heat-carrier particle). Thus, some internal baffles can be designed and distributed in the downer reactor to enhance the mixing and heat transfer [19–22] between the pulverized coal, the sand and the circulating hot ash. The baffle internals can increase the MRT of particles in the downer reactor to ensure the terminal thermal balance temperature and also to improve the mixing of coal and hot ash.

In this research, the internal design of the baffle has been optimized using the developed 3D soft-sphere model of the discrete element method (DEM) to simulate the rapid pyrolysis of coal in the downer reactor. Increasing the baffle length can raise the coal-pyrolysis temperature at the exit of the downer reactor. The baffle length on a horizontal projection should be no less than the width of the particle-feeding entrance. Increasing the baffle angle...
can raise the coal-pyrolysis temperature at the exit of the
donner reactor both by fixing the horizontal-projection
length of the baffle and the actual baffle length. Increasing
the baffle number in the downer reactor not only can in-
crease the particle MRT in the downer reactor, but also can
enlarge the contact space for thermal conduction through
particle contact, which can raise the particle-pyrolysis
temperature at the exit of the downer reactor. The larger
the number of baffles in the downer reactor, the closer the
coa approaches thermal equilibrium.

1 Mathematical modelling

The DEM [23, 24] is a Lagrangian method for calculating
and recording the information of each particle in a granular
system, including the space position vector $\vec{x}_i$, phase pos-
tion vector $\vec{\phi}_i$, translational movement velocity vector $\vec{v}_i$,
rotating movement velocity vector $\vec{\omega}_i$, net force vector $\vec{F}_i$
, total moment vector $\vec{M}_i$, particle temperature $T_i$ and the
enthalpy value $H_i$.

The basic hypotheses of the DEM can be summarized
as follows: (i) the particles are assumed to be spherical; (ii)
when collision or compression happens, a certain overlap
area between two particles is allowed, the size of which
is small compared with the particle surface area. The al-
gorithm structure of the DEM is composed of the status
analysis, the kinematics analysis and the search algorithm
for particle collisions. Fig. 1 illustrates the main elements
of the developed algorithm of the DEM.

In this research, the motion of all particles in a downer
reactor is determined by the gravitational force $\vec{G}_i$, the col-
lision force $\vec{F}_c$ and the forces from the gas phase—that is,
the buoyancy force $\vec{F}_b$ and the drag force $\vec{F}_d$. The analysis
of the collision force between particles has been presented

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Fig. 1: Foundational principle of the developed DEM software package coupling with the particulate heat-transfer model
in previous research \cite{25, 26}. The calculation method of the buoyancy force and the drag force can be listed as shown in Equations (1)–(3).

\begin{equation}
\vec{G}_i = m_i g
\end{equation}

\begin{equation}
\vec{F}_{b,i} = -\rho g \frac{m_i}{V_i} \vec{v}_i = \nabla \left( \rho \vec{v}_i \right) - \frac{2}{3} \pi r_i^3 \rho g \vec{g}
\end{equation}

\begin{equation}
\begin{cases}
\vec{F}_{d,i} = \zeta \cdot A_{w,i} \cdot \frac{1}{2} \rho g \left| \vec{u}_g - \vec{v}_i \right| \left| \vec{u}_g - \vec{v}_i \right|
\end{cases}
\end{equation}

\begin{align}
\zeta = \begin{cases}
\frac{24}{k_e} & \text{Re}_i < 2 \\
\frac{18 \zeta_e}{k_e} & 2 < \text{Re}_i < 500 \\
0.445 & 500 < \text{Re}_i < 2 \times 10^5
\end{cases}
\end{align}

Therefore, the forces and momentum balance of particle \(i\) can be calculated as Equation (4):

\begin{equation}
\begin{cases}
\vec{F}_i = \vec{F}_{c,i} + \vec{F}_{b,i} + \vec{F}_{d,i} + \vec{G}_i \\
\vec{M}_i = \vec{M}_{t,i} + \vec{M}_{r,i}
\end{cases}
\end{equation}

The enthalpy of the solid particle is assumed to be a function of temperature. Thus, the particle temperature of the \(i\)th particle \(T_i\) is based on the enthalpy difference \(\Delta H_i\), which can be calculated using Equation (5):

\begin{equation}
T_i = T_{i,0} + \frac{\Delta H_i}{m_i c_{p,i}}
\end{equation}

The net force acting on the particle is governed by Newton’s Second Law of Motion (Equation (6a)), which determines the translational movement of the particle. The particle rotation is determined by Newton’s Law of Rotation (Equation (6b)):

\begin{equation}
\begin{cases}
\vec{F}_i = m_i \vec{a}_i = m_i \frac{d^2 \vec{x}}{dt^2} = m_i \omega \times \vec{x} \quad (a) \\
\vec{M}_i = I_{ij} \vec{\omega}_i = I_{ij} \frac{d \vec{\omega}_i}{dt} = I_{ij} \frac{d^2 \vec{\phi}_i}{dt^2} \quad (b)
\end{cases}
\end{equation}

Heat transfer to the particle takes place because of particle collisions or interactions with walls through thermal conduction, the interaction with the gas phase via thermal convection and the radiative heat transfer.
The model of particulate thermal conduction uses the following assumptions: (i) when two particles collide, the direction of the temperature gradient is perpendicular to their contact surface; (ii) thermal conduction takes places in the area of overlap of two colliding particles; (iii) there is a gap with a thickness of $4 \times 10^{-10}$ m between the contact surfaces of two colliding particles [27, 28], through which the heat can be transferred; the thermal resistance of this gap is calculated as follows:

$$R_{\text{con}} = \frac{d}{k_{\text{p}}},$$

where $d$ is the diameter of particle $i$, in m; $k_{\text{p}}$ represents the gas-phase thermal-conduction coefficient, in W·m$^{-1}$·K$^{-1}$; $Nu$ stands for the Nusselt number [29, 30]; $Re$ and $Pr$ are the Reynolds number of particle $i$ and the Prandtl number, respectively; $c_{\text{p}}$ is the heat capacity of the gas, in kJ·kg$^{-1}$·K$^{-1}$; $\mu$ is the gas-phase dynamic viscosity, in Pa·s; $\rho$ stands for the density of the gas phase, in kg·m$^{-3}$; $|\vec{u}_g - \vec{u}_i|$ means the gas velocity relative to the particle, in m·s$^{-1}$.

The radiative heat transfer between the particle and the main zone of the downer reactor cannot be neglected because of the high temperature of the reactor surface. Kirchhoff's law of thermal radiation can be used to calculate the radiative flux as follows:

$$Q_{\text{rad}} = \sigma_{\text{gas}} \varepsilon_i A_i (T_i^4 - T_b^4)$$  \hspace{1cm} (12)

where $\sigma_{\text{gas}}$ is the Stefan-Boltzmann constant, $5.67 \times 10^{-8}$ W·m$^{-2}$·K$^{-4}$; $\varepsilon_i$ is the particle $i$ emissivity, $\cdot$; $A_i$ is the heat-transfer area between particle $i$ and the reactor bulk, in m$^2$; $T_i$ is the particle $i$ temperature, in K; $T_b$ is the bed temperature, in K.

The indicator for describing the mixing degree of the coal particle and the heat carrier can employ the variance or standard deviation of the concentrations of the key components (coal particles) in each position of the particle-motion space. A low value of standard deviation represents good mixing of the particles within the model domain. The calculation method can be summarized as follows:

Table 1: Parameter values of coal and silica sand in the model of mechanics and thermodynamics

| Particulate materials | Coal  | Sand |
|-----------------------|-------|------|
| Particle density $\rho$ /kg·m$^{-3}$ | 1250  | 2450 |
| Particle diameter $d$ /mm | 5     | 5    |
| Elastic modulus $E$ /Pa | $5.08 \times 10^9$ | $4.10 \times 10^{10}$ |
| Poisson ratio $\nu$ | 0.28  | 0.22 |
| Sliding friction coefficient $\mu$ | 0.51  | 0.66 |
| Rolling friction coefficient $\mu$ | $5 \times 10^{-4}$ | $5 \times 10^{-5}$ |
| Recovery coefficient $\epsilon$ | 0.85  | 0.90 |
| Specific thermal capacity $c$ /J·K$^{-1}$·kg$^{-1}$ | 1.13  | 0.92 |
| Thermal-conduction coefficient $k$ /W·m$^{-1}$·K$^{-1}$ | 0.26  | 0.52 |
| Blackness $\zeta$ | 0.85  | 0.70 |

Fig. 4: Particulate mixing and temperature of coal and sand in a downer reactor simulated by the DEM software package.
(i) The volume fraction (as concentration) $x_{\text{coal},i}$ of coal particles (as key components) in spatial sample $i$ at any position of the mixing zone of the downer reactor can be calculated as

$$x_{\text{coal},i} = \frac{V_{\text{coal}}}{V_{\text{coal}} + V_{\text{sand}}}$$  \hspace{1cm} (13)

(ii) It is worth noting that the particle number $n_p$ in each spatial sample at any position of the mixing zone of the downer reactor may be different, because the volume of the spatial sample is fixed. Therefore, the variance or standard variation of the volume fraction of coal particles $x_{\text{coal},i}$ of the whole reactor space can be calculated as

$$\bar{x}_{\text{coal}} = \frac{\sum_{i=1}^{N} w_i \cdot x_{\text{coal},i}}{\sum_{i=1}^{N} w_i}$$  \hspace{1cm} (14)

$$\sigma = \sqrt{\frac{\sum_{i=1}^{N} w_i \cdot (x_{\text{coal},i} - \bar{x}_{\text{coal}})^2}{\sum_{i=1}^{N} w_i}}$$  \hspace{1cm} (15)

where $w_i$ is the weight of sample $i$, which can be calculated by $w_i = n_i/n$; $n_i$ is the particle number in the spatial sample $i$; $n$ is the total particle number in the mixing zone of the downer reactor; $N$ is the number of spatial samples in the mixing zone of the downer reactor. The maximum and the minimum of the standard variance can be calculated by:

$$\left\{ \begin{array}{l}
\sigma_0 = \sqrt{x_{\text{coal}} \cdot (1 - x_{\text{coal}})} \\
\sigma_r = \frac{\sigma - \bar{x}_{\text{coal}}}{\bar{x}_{\text{coal}}}
\end{array} \right.$$  \hspace{1cm} (16)

An index of mixing of the coal and the sand for real-time analysis $M_{\text{real-time}}$ can be defined as:

$$M_{\text{real-time}} = \frac{\sigma - \sigma_r}{\sigma_0 - \sigma_r}$$  \hspace{1cm} (17)

The reactor internals can affect not only the coal-particle temperature at the exit of the downer reactor, but also the rate of change of the temperature of the particles within the reactor by the process of solid–solid heat transfer. The rate of particle-temperature change is influenced by the heat transfer as determined by the temperature difference between the particle and its surrounding, the heat-transfer coefficient and the physical chemical properties of the particulate material itself. The rate of change of the $i$th particle temperature can be defined as follows:

$$\alpha_i = \frac{\partial \theta_i(\vec{x}, t)}{\partial t} = \lim_{\Delta t \to 0} \frac{\theta_i(\vec{x}, t + \Delta t) - \theta_i(\vec{x}, t - \Delta t)}{2 \Delta t}$$  \hspace{1cm} (18)

Fig. 5: Effect of the baffle length on the particulate-mixing degree of coal and sand simulated by the developed DEM software package
2 Simulation conditions

In order to research the influence of the baffle internals on the particle mixing and heat transfer in the downer reactor, the developed algorithms of a 3D DEM software package were used to establish the numerical-simulation system. The correctness of the software package and the rationality of the particle parameters have been validated in past research [25, 26]. The shape and size of the downer reactor with baffle internals are illustrated in Fig. 2, showing the front and side views.

As described in Fig. 2, the downer reactor mainly consists of two hoppers, each containing a different kind of granular material and a long vertical tube, which is the main zone for particulate mixing and heat transfer. In particular, there are two vertical baffles at the exits of the two hoppers—that is, the entrance of the mixing zone of the downer reactor—to avoid disturbing the evaluation of the effect of baffle internals on the particulate mixing and heat transfer in the downer reactor. The results of particulate mixing and heat transfer will consider the structure and shape of the entrance of the mixing zone of the downer reactor if no vertical baffle is installed and the effect of the internal baffles on particulate mixing and heat transfer in the mixing zone of the downer reactor will be unclear. A series of baffle internals are installed in the main zone of the traditional type of downer reactor to form the new type of baffle downer reactor, as shown in Fig. 2. The angle of the baffle with respect to the downer-reactor wall of the six baffles is 45°, the length of the six baffles is 70.70 mm and the interval between the baffles along the vertical direction is 250 mm. In this study, the flow type and mixing behaviour of particulate materials affected by the baffle internals in the downer reactor can be investigated clearly. In addition, the design of the baffle internals has been optimized to strengthen the mixing and heat-transfer behaviour of the particles using the developed algorithm of the 3D DEM software package.

The initial conditions and basic assumptions for simulating the particulate mixing and heat transfer in the downer reactor are as follows: (i) to simplify the simulation, the gas phase in the downer reactor is considered...
to be still dry air; the gas-phase density and viscosity are functions of temperature, as illustrated in Fig. 3; (ii) uniform temperature on the inner surface of the downer reactor is assumed during the calculation; (iii) at a temperature of 0°C, the specific enthalpy of the material components in downer reactor is 0 kJ·kg⁻¹; (iv) the physical properties of the coal and the sand have been listed in Table 1 [31–33].

3 Results and discussion

The granular-mixing and heat-transfer behaviour of the coal and the sand affected by internals in a downer reactor have been simulated by the developed DEM software package, which is shown in Fig. 4. The baffle internals can affect the mixing degree of the fuel particles and heat carriers in the downer reactor, and the change in the final coal-pyrolysis temperature and the particle-heating rate indirectly. Therefore, optimization of the design of baffle internals is important for the coal-pyrolysis process in a downer reactor.

3.1 Baffle length

The effect of the baffle length on the mixing degree of the coal and the sand particles has been simulated by the developed DEM software package, as shown in Fig. 5. \( l_{\text{baffle, proj}} \) stands for the projection of baffle length \( l_{\text{baffle}} \) onto the horizontal plane. \( \alpha_{\text{baffle}} \) is the angle between the vertical direction and the baffle-length direction, i.e. \( l_{\text{baffle, proj}} = l_{\text{baffle}} \sin \alpha_{\text{baffle}} \). The dimensionless parameter \( l_{\text{baffle, proj}} / d_{\text{gap}} \), the horizontal-projection length of the baffle divided by the gap width of the particle-feeding entrance (2.0 cm) shown in Fig. 5, should be optimized to maximize the coal-pyrolysis conditions in the downer reactor.

It can be concluded from Fig. 5 that \( l_{\text{baffle, proj}} \) should be no less than the width of the particle-feeding entrance \( d_{\text{gap}} \), which can mix the coal and the sand sufficiently. However, too large a baffle length cannot improve the mixing degree of the coal and the sand further, but will increase the particle-residence time unnecessarily. When the volume-feeding-rate ratio of coal to sand is fixed at 1:4, the wall temperature is equal to 684.57°C under the adiabatic condition. The effect of the baffle length in the downer reactor on the distribution of coal-particle temperatures along the height of the downer reactor simulated by the developed DEM software package is illustrated in Fig. 6.

As shown in Fig. 6, the coal-temperature distribution in the downer reactor is remarkably affected by the baffle-length design. The improvement in the coal-temperature distribution is affected by the enhancement of the heat transfer between the coal and the sand due to the effect of the mixing degree of the coal and the sand, especially
due to the horizontal length of the baffle ranging from 0 to 1.0 \(d_{gap}\). In addition, the MRT of coal particles in the downer reactor will increase from 0.497 to 0.859 sec when the dimensionless parameter \(l_{baffle, proj}/d_{gap}\) increases from 0 to 2.5. Therefore, the coal-particle-temperature distribution along the height of the downer reactor and the coal-pyrolysis temperature at the exit of the downer reactor are remarkably affected by the horizontal length of the baffle ranging from 0 to 1.0 \(d_{gap}\), as shown in Fig. 6c. Most importantly, the coal-heating rate can reach a maximum value when \(l_{baffle, proj}\) is equal to \(d_{gap}\). Therefore, the horizontal projection of the baffle length should be no less than the width of the particle-feeding entrance, which is a benefit for the fast pyrolysis of the coal in the downer reactor.

### 3.2 Baffle angle

The effect of the slope angle of the baffle internals on the particulate mixing of the coal and the sand in the downer reactor can be simulated by the developed DEM software package, as shown in Fig. 7.

It can be concluded from Fig. 7 that the mixing degree increases with the slope angle of the baffle internals in the downer reactor. When the volume-flow-rate ratio of coal to sand is fixed at 1:4, the wall temperature of the downer reactor can be calculated as 684.57°C. The effect of the slope angle of the baffle internals on the coal-particle terminal temperature and the average particle-heating rate are illustrated in Fig. 8.

It can be concluded from Fig. 8 that the coal-particle temperature increases with the particle distance from the entrance of the downer reactor. In addition, the coal-particle terminal temperature increases with the slope angle of the baffle internals in the downer reactor. The larger slope angle of the baffle internals makes the coal-particle terminal temperature closer to the wall temperature of the downer reactor. However, the slope angle of the baffle internals will increase the residence time of coal particles in the downer reactor. Therefore, the coal-particle-temperature heating in the downer reactor does not increase monotonically with the obstacle of the baffle internals. As is vividly shown in Fig. 8, the coal-particle heating rate increases...
with the obstacle of the internals from 0° to 30° and decreases after 30°. Therefore, a 30° slope angle of the baffle internals is beneficial for the rapid pyrolysis of coal under the condition of a fixed volume-flow-rate ratio of coal to sand.

### 3.3 Baffle number

The number of baffles is one of the most important design parameters for the baffle-type downer reactor. The horizontal-projection length of the baffle is 2.5\(d_{\text{gap}}\) and the baffle-slope angle is 45°. The baffle interval is \(5l_{\text{baffle, proj}}\). The upper edge of the first top baffle is fixed at the position of \(4l_{\text{baffle, proj}}\) (20.0 cm) from the entrance of the sand hopper. The effect of the baffle number on the particulate mixing of coal and sand in the downer reactor can be simulated by the developed DEM software package coupling the particulate model of heat transfer, as shown in Fig. 9.

It can be concluded from Fig. 9 that the mixing degree increases with the internal-baffle number in the downer reactor. When the volume-flow-rate ratio of coal to sand is fixed at 1:4, the wall temperature of the...
downer reactor can be calculated as $684.57°C$. The effect of the internal-baffle number on the coal-particle terminal temperature and average particle-heating rate is illustrated in Fig. 10.

It can be concluded from Fig. 10 that the coal-particle temperature increases with the particle distance from the entrance of the downer reactor. In addition, the coal-particle terminal temperature increases with the internal-baffle number in the downer reactor. A large number of internal baffles makes the coal-particle terminal temperature closer to the wall temperature of the downer reactor. However, more internal baffles will increase the residence time of coal particles in the downer reactor, so the coal-particle-heating rate in the downer reactor will not increase monotonically with the increase in the internal-baffle number. As vividly shown in Fig. 10, the coal-particle-heating rate will not be raised when the number of internal baffles is larger than four. Therefore, no fewer than four internal baffles should be installed in the downer reactor for the rapid pyrolysis of coal under the condition of a fixed volume-flow-rate ratio of coal to sand.

It can be concluded from Sections 3.1–3.3 that the design of the internal baffles can affect the coal-particle-heating rate in the downer reactor for the pyrolysis process. The optimized baffle internal design is that the baffle length is 40 mm, the baffle-slope angle is 30° and the baffle number is no fewer than four. Under this condition, a higher coal-particle-heating rate can be obtained in the downer reactor for the pyrolysis process.

4 Conclusions
The structural optimization of baffle internals in a downer reactor has been discussed in this research. For one thing, the coal-pyrolysis temperature at the exit of the downer reactor can be determined by the volume-feeding-rate ratio of the coal to the sand. For another, it will be also affected by the structural design of the internals in the downer reactor. It can be concluded from the simulation results that the effect of the baffle internals not only can improve the mixing degree, but also can enlarge the MRT of particles in the downer reactor, which can make the fuel particles
achieve the predicted pyrolysis temperature in the downer reactor as soon as possible. The conclusions can be summarized as follows:

(i) Increasing the baffle length can raise the coal-pyrolysis temperature at the exit of the downer reactor, which is remarkable when the horizontal length of the baffle ranges from 0 to 1.0d_{gap}, and is weakened when the horizontal length of the baffle increases further. It is obvious that the baffle-length design is a benefit for the rapid pyrolysis of coal in the downer reactor, whose horizontal projection should be no less than the width of the particle-feeding entrance.

(ii) Increasing the baffle angle can raise the coal-pyrolysis temperature at the exit of the downer reactor both by fixing the horizontal-projection length of the baffle and by fixing the actual length of the baffle. When the baffle angle is −30°, a higher coal-particle-heating rate can be achieved.

(iii) Increasing the baffle number in the downer reactor not only can increase the particle MRT in the downer reactor, but also can enlarge the contact space for thermal conduction through particle contact. Therefore, increasing the baffle internals installed in the interior of the downer reactor can raise the particle-pyrolysis temperature at the exit of the downer reactor. The larger the number of baffles in the downer reactor, the closer the coal approaches the thermal equilibrium. Therefore, it can be concluded that the baffle length is 40 mm, the baffle-slope angle is 30° and the baffle number is no fewer than four, which is a benefit for the coal-pyrolysis process in the downer reactor.

Conflicts of Interest
None declared.

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