Tomography-Based Analysis of Radiative Transfer in Reacting Packed Beds Undergoing a Solid-Gas Thermochemical Transformation

A reacting packed-bed undergoing a high-temperature thermochemical solid-gas transformation is considered. The steam- and dry-gasification of carbonaceous materials to syngas is selected as the model reaction. The exact 3D digital geometrical representation of the packed-bed is obtained by computer tomography and used in direct pore-level simulations to characterize its morphological and radiative transport properties as a function of the reaction extent. Two-point correlation functions and mathematical morphology operations are applied to calculate porosities, specific surfaces, particle-size distributions, and representative elementary volumes. The collision-based Monte Carlo method is applied to determine the probability distribution of attenuation path length and direction of incidence at the solid-fluid boundary, which are linked to the extinction coefficient, scattering phase function, and scattering albedo. These effective properties can then be incorporated in continuum models of the reacting packed-bed.

[DOI: 10.1115/1.4000749]

Keywords: packed-bed, radiation, solar energy, gasification, chemical reactors

1 Introduction

Morphological and effective heat/mass transfer properties of complex porous media are needed for the engineering design, optimization, and scale-up of thermochemical reactors and processes in particular for packed beds. Their complex solid-gas structures can be incorporated in direct pore-level simulations for determining their morphological-dependent effective transport properties for continuum domain. This approach has been successfully applied for the geometrical characterization of packed beds and foams [1–5] and for the determination of the effective radiative heat transfer properties of opaque and semitransparent packed beds [3,6–8] and foams [5,9,10], of the effective conductivity of packed beds and foams [11–14], of convective heat transfer properties [13,15], and of the effective fluid flow properties [15,16] through foams. These pore-level computations allow for more in-depth investigations vis-à-vis classical empirical models for radiative [17,18], convective [19], convective [20], and fluid flow [19,21,22] properties.

In this study, computer tomography (CT) is employed to obtain the exact 3D digital geometrical representation of a packed-bed of carbonaceous materials undergoing high-temperature gasification. Thus, the numerically calculated effective properties are based on the exact morphology of the reacting packed-bed, which varies with time and process parameters (e.g., temperature, gasifying agent, partial pressure, and feedstock size) as the reaction progresses. These effective properties can then be applied for the accurate derivation of the reaction kinetics and for the design and optimization of packed-bed reactors.

2 Gasification Experiments

A packed-bed of tire shreds is selected as the model reactor. The gasification of this waste carbonaceous material into high-quality synthesis gas (syngas, mainly H₂ and CO, used for power generation in efficient combined-cycles and fuel cells or further processed to Fischer–Tropsch liquid fuels) is investigated in a packed-bed reactor using concentrated solar energy as the source of high-temperature process heat [23]. In this study, a laboratory packed-bed reactor, schematically shown in Fig. 1, is used to conduct the gasification reaction at controlled conditions and to produce sample materials at different reaction extents. These samples are then scanned by tomography. Their BET specific surface area is measured by N₂ adsorption (Micromeritics TriStar 3000) and their particle-size distribution is measured by laser scattering (HORIBA LA-950 analyzer). Outlet gas composition is monitored by mass spectrometry (MS, Pfeiffer Vacuum Omnistar GSD 301 O1) and gas chromatography (GC, Varian CP-4900 Micro GC).

Proximity analysis of the tire shreds indicates 63 wt % volatiles, 29 wt % fixed carbon, 7 wt % ash and 1 wt % moisture. Elemental analysis indicates 82 wt % C, 7 wt % H, 3 wt % O, 2 wt % S, and heavy metal impurities. Energy dispersive X-ray spectrometer analysis shows that the main components in the ash are Si, Zn, and Fe based oxides. Samples are first pyrolyzed to release volatiles. Approximately 3 g of pyrolyzed material is loaded in a 2.6 cm inside diameter quartz tube, rapidly heated by a radiative source, and gasified either by steam or CO₂ diluted by Ar. Once the reaction reaches a desired carbon conversion, the quartz tube is removed from the furnace and rapidly cooled. The partially reacted sample is extracted. The carbon conversion (or reaction extent) is defined by

---

Contributed by the Heat Transfer Division of ASME for publication in the JOURNAL OF HEAT TRANSFER. Manuscript received May 15, 2009; final manuscript received October 22, 2009; published online March 25, 2010. Assoc. Editor: Walter W. Yuen.
Samples at $X$ type of feedstock. Carbon conversions are shown in Fig. 2 as a type of gasifying agent, partial pressure of gasifying agent, and CO$_2$ 1273 CO$_2$ 0.8 Granular, Powder 1273 H$_2$O 0.8 Powder, 5

$T$ Reference 1273 H$_2$O 0.8 Granular, $d_a=1$

Powder 1273 H$_2$O 0.8 Powder, $d_a=0.5$

$T$ 1173 H$_2$O 0.8 Granular, $d_a=1$

Reduced $p_{H_2}O$ 1273 H$_2$O 0.4 Granular, $d_a=1$

CO$_2$ 1273 CO$_2$ 0.8 Granular, $d_a=1$

The distance of a random point in the sample to the phase boundary is found by following a generic ray in small steps (searching for the root). Afterward, the bisection method is used to find the
exact value. The normal unit vector at the interface is determined by computing the gradient of the gray values at the specific position.

4 Morphological Characterization

4.1 Experimental. Porosity is determined by weight measurements, assuming the approximate intrinsic density to increase linearly with decreasing carbon content, and is given by

\[ \rho = \rho_{\text{ash}} + \rho_c (1 - X_C) \]

with \( \rho_c = 1700 \, \text{kg m}^{-3} \) and \( \rho_{\text{ash}} = 2500 \, \text{kg m}^{-3} \). \( \rho_{\text{ash}} \) of the initial tire shreds (before pyrolysis) is measured by He pycnometry (AccuPyc 1330) to be 1200 kg m\(^{-3}\). \( X_C \) is shown in Fig. 5 as a function of the carbon conversion for the five experimental runs listed in Table 1. The porosity peaks at \( X_C = 0.55 \) as a result of growing pores and break-up of fragile particles [25]. The measured values correspond to a loosely packed-bed of randomly oriented and located non-spherical particles having uniform size and sphericity (fraction of surface area of volume-equivalent sphere to surface area of particle) smaller than 0.25 [26], indicating highly porous particles. The measured porosity is fitted to a second order polynomial function (RMS = 0.04).

\[ \varepsilon_{\text{ex}}(X_C) = -0.243X_C^2 + 0.269X_C + 0.856 \]  

The porosity of the unreacted packed-bed of tire shreds is determined to be \( \varepsilon_{\text{ex}} = 0.60 \pm 0.05 \), which corresponds to a packed-bed of non-spherical particles of uniform size and with sphericity of 0.55 [26].

The BET specific surface area and the corresponding fraction resulting from nanopores (\( d_p < 2 \, \text{nm} \)) is shown Fig. 6 as a function of the carbon conversion for the five experimental runs listed in Table 1. Before pyrolysis, BET surface area is 0.6 m\(^2\) g\(^{-1}\) for the granular and 1.6 m\(^2\) g\(^{-1}\) for the powder feedstock, and no nanopores are detected. During pyrolysis, it increases to 70 m\(^2\) g\(^{-1}\) of which a small fraction (\( \approx 5\% \)) is associated to nanopores. During gasification, the BET specific surface area increases up to \( \sim 700 \, \text{m}^2 \text{g}^{-1} \) for \( X_C = 0.7 \) and decreases for the residual ash (\( X_C = 1 \)), which is consistent with the variation in porosity in Fig. 5. The fraction of nanopores increases and peaks at 60% for \( X_C = 0.3 \). No nanopores are detected in the ash. The different values obtained for H\(_2\)O and CO\(_2\) gasifying agents are presumable the result of different mechanisms as CO\(_2\) mainly reacts at the external surface while H\(_2\)O diffuses to the particle core [27]. In general, the variation in the reaction temperature, partial pressure, gasifying agent, and particle-size (as described in Table 1) do not significantly affect the morphology of the sample at the same
carbon conversion.

The experimentally measured particle-size distribution is shown in Fig. 7 for the reference case at \( X_C = 0.3, 0.7, 1 \). As expected, the main peak shifts to the left as particles shrink, and the small peaks—associated with smaller particles resulting from particle break-up—increase during the reaction. Note that these distributions are qualitative as particles are not spherical.

### 4.2 Numerical

The two-point correlation function

\[
s_2(r) = \frac{\int \int \int \phi(r) \phi(r+s) d\Omega dV}{4\pi}\ (5)
\]

is applied to calculate the porosity and specific surface area of the sample since \( s_2(0) = \varepsilon \) and \( dV/dr\bigg|_{\text{voxel}} = \frac{\varepsilon_0}{4} \) [1]. The particle-size distribution is calculated by an opening; a morphology operation consisting of an erosion followed by a dilation with the same structuring element [28]. A sphere is used as the structuring element. The determined opening porosity is related to the size distribution by

\[
f(d) = \frac{d}{d^3} \left( 1 - \frac{\varepsilon_{\text{sub}}}{\varepsilon_0} \right) (6)
\]

The calculated porosity of the unreacted packed-bed of 0.61 compares well to the experimentally determined one of 0.60 ± 0.05. Figure 8 shows the experimentally measured and numerically calculated porosity as a function of the carbon conversion during gasification for the reference case. The failure in predicting the porosity and its increase with increasing \( X_C \) is related to the resolution of the tomographic scans, which is limited by the tomographic setup, the subsequent image processing (especially filtering) and the relative increase in optically thick material, which distorts the tomographic image. The impact of the insufficient scanning resolution and subsequent image processing is roughly calculated to be \((1 - \varepsilon)\varepsilon_{\text{sub}} \approx 0.1\), where \( \varepsilon_{\text{sub}} \approx 0.2\) for \( X_C = 0.3\) is the porosity of the particle only detectable by the high-resolution tomography. Nanopores are not detectable but obviously present as indicated by the BET measurements. Calculated specific surface shows an increase up to \( X_C = 0.7 \) but the experimentally observed decrease for the ash is not elucidated.

The numerically calculated particle-size distributions, shown in Fig. 9 for the reference case at \( X_C = 0, 0.3, 0.7, 1 \), are based on the largest sphere that fits inside the particle. Therefore, for non-spherical, complex, porous and fractal-like particles, these distributions deviate from those experimentally measured. The calculations are limited by the voxel size of the CT scans (\( d_{\text{min}} = 4\cdot\text{voxel size} \)). Since the particle-size distribution is calculated based on the solid phase, the limited resolution of the CT scans leads to an over prediction of the particle-size due to virtual particle agglomeration. The measurements show (see Fig. 7) that the amount of particles in the 10 \( \mu\text{m} \) range is small compared with that in the 100 \( \mu\text{m} \) range. Therefore the influence of this distortion is assumed negligible on the particle-size distribution in the...
range of 60–100 \( \mu m \). Indeed, an increase in small particles due to shrinkage and breakup of the initial ones during the reaction is observed.

The representative elementary volume (REV)—the smallest volume that can be considered as continuum—is determined by calculating the porosity of a subsequently growing subsample until its variation is within a tolerance band of \( \pm 0.05 \) [3]. The edge length of the REV, \( L_{\text{REV}} \), was found to be equal to 5 mm, independent of the process parameters.

5 Radiative Heat Transfer Characterization

The packed-bed of the carbonaceous material is assumed to be opaque for visible and near-infrared radiation, which is the spectral range encountered in the solar-driven reactor [23]. The fluid phase is assumed to be radiatively non-participating. Hence, the variation in the radiative intensity in continuum models is described by a single equation of radiative transfer (RTE) [29,30].

\[
\frac{dI_n(s,s')}{ds} + \beta_n I_n(s,s') = \kappa_n I_{n,b}(s,s') + \frac{\sigma_n \lambda}{4\pi} \int_{4\pi} I_n(s,s') \Phi_n(s,s') d\Omega_n
\]

(7)

Since the smallest pores or particles detected by CT and consequently employed in the analysis are larger than the voxel sizes of the low-resolution scans, geometric optics can be assumed for radiation wavelengths smaller than 1 \( \mu m \) [17]. Collision-based Monte Carlo (MC) method is applied to compute the cumulative distribution functions of the radiation mean free path \( G_e(s) \) and of the cosine of incidence at the solid wall \( F_{\mu_{in}}(\mu_{in}) \) defined as

\[
G_e(s) = \int_0^s \frac{1}{N} \sum_{j=1}^{N_s} \delta(s' - s_j) ds'
\]

\[
F_{\mu_{in}}(\mu_{in}) = \int_0^{N_s} \delta(\mu_{in} - \mu_{in,j})
\]

(8)

(9)

\( G_e(s) \) and \( F_{\mu_{in}}(\mu_{in}) \) are related to \( \beta_n \) and \( \Phi_n \) [2,5,8] by

\[
\Phi(\mu) = 2 \int_{\mu_{in}=0}^{1} \int_{\varphi_{in}=0}^{\pi} \int_{\mu_{in}=0}^{1} \delta(\mu_{in} - \sqrt{(1 - \mu_{in}^2)(1 - \mu_{in}^2)} \cos \varphi - \mu_{in}\mu_{in}) p^2(\mu_{in},\mu_{in},\varphi_{in}) F_{\mu_{in}} \mu_{in} d\mu_{in} d\varphi_{in} d\mu_{in}
\]

\[
\int_{\mu_{in}=0}^{1} \int_{\varphi_{in}=0}^{\pi} \int_{\mu_{in}=0}^{1} p^2(\mu_{in},\mu_{in},\varphi_{in}) F_{\mu_{in}} \mu_{in} d\mu_{in} d\varphi_{in} d\mu_{in}
\]

(10)

(11)

The absorption characteristics of the samples and the contribution of dependent scattering vary with the reaction extent since ash is less absorbing than coal \( (\rho_{d,\text{ash}}=0.273, \rho_{d,A,C}=0.1, \rho_{d,sp,ash} =0.092, \text{ and } \rho_{d,sp,ash}=0.75 \) [31,32]). Gas, packed-sphere, liquid, and modified liquid models are used to estimate the corresponding deviations of the scattering and absorption coefficients from the corresponding values obtained by assuming independent scattering [33]. For a packed-bed with \( d_{in}=0.4 \) and 1 mm \( (d_{m} \) of particlesize distribution shown in Fig. 7 at \( X_c=1 \) and 0, respectively), the maximum deviation of the scattering efficiency (appearing at the largest radiation wavelength in our spectral range of interest 1 \( \mu m \)) is 5% and 23% for \( \varepsilon_{\text{ext}}=0.88 \) and 0.86, respectively, (measured and depicted in Fig. 5 at \( X_c=1 \) and 0, respectively). Consequently, dependent scattering effects are neglected in the radiative transfer analysis.

The cumulative distribution function of the cosine of incidence at the solid wall and the scattering phase function are computed for two limiting cases: a specular and a diffuse solid-gas interface. For tire shreds, a combination of these two cases is anticipated to be valid. The specular directional-hemispherical reflectivity is calculated using Fresnel’s equations for the complex refractive index of the carbon-ash mixture \( m=(1-X_c)m_C+X_cm_{\text{ash}} \), where \( m_C \) and of the initial ones during the reaction is observed.

The representative elementary volume (REV)—the smallest volume that can be considered as continuum—is determined by calculating the porosity of a subsequently growing subsample until its variation is within a tolerance band of \( \pm 0.05 \) [3]. The edge length of the REV, \( L_{\text{REV}} \), was found to be equal to 5 mm, independent of the process parameters.

The packed-bed of the carbonaceous material is assumed to be opaque for visible and near-infrared radiation, which is the spectral range encountered in the solar-driven reactor [23]. The fluid phase is assumed to be radiatively non-participating. Hence, the variation in the radiative intensity in continuum models is described by a single equation of radiative transfer (RTE) [29,30].

\[
\frac{dI_n(s,s')}{ds} + \beta_n I_n(s,s') = \kappa_n I_{n,b}(s,s') + \frac{\sigma_n \lambda}{4\pi} \int_{4\pi} I_n(s,s') \Phi_n(s,s') d\Omega_n
\]

(7)

Since the smallest pores or particles detected by CT and consequently employed in the analysis are larger than the voxel sizes of the low-resolution scans, geometric optics can be assumed for radiation wavelengths smaller than 1 \( \mu m \) [17]. Collision-based Monte Carlo (MC) method is applied to compute the cumulative distribution functions of the radiation mean free path \( G_e(s) \) and of the cosine of incidence at the solid wall \( F_{\mu_{in}}(\mu_{in}) \) defined as

\[
G_e(s) = \int_0^s \frac{1}{N} \sum_{j=1}^{N_s} \delta(s' - s_j) ds'
\]

\[
F_{\mu_{in}}(\mu_{in}) = \int_0^{N_s} \delta(\mu_{in} - \mu_{in,j})
\]

(8)

(9)

\( G_e(s) \) and \( F_{\mu_{in}}(\mu_{in}) \) are related to \( \beta_n \) and \( \Phi_n \) [2,5,8] by

\[
\Phi(\mu) = 2 \int_{\mu_{in}=0}^{1} \int_{\varphi_{in}=0}^{\pi} \int_{\mu_{in}=0}^{1} \delta(\mu_{in} - \sqrt{(1 - \mu_{in}^2)(1 - \mu_{in}^2)} \cos \varphi - \mu_{in}\mu_{in}) p^2(\mu_{in},\mu_{in},\varphi_{in}) F_{\mu_{in}} \mu_{in} d\mu_{in} d\varphi_{in} d\mu_{in}
\]

\[
\int_{\mu_{in}=0}^{1} \int_{\varphi_{in}=0}^{\pi} \int_{\mu_{in}=0}^{1} p^2(\mu_{in},\mu_{in},\varphi_{in}) F_{\mu_{in}} \mu_{in} d\mu_{in} d\varphi_{in} d\mu_{in}
\]

(10)

(11)

The absorption characteristics of the samples and the contribution of dependent scattering vary with the reaction extent since ash is less absorbing than coal \( (\rho_{d,\text{ash}}=0.273, \rho_{d,A,C}=0.1, \rho_{d,sp,ash} =0.092, \text{ and } \rho_{d,sp,ash}=0.75 \) [31,32]). Gas, packed-sphere, liquid, and modified liquid models are used to estimate the corresponding deviations of the scattering and absorption coefficients from the corresponding values obtained by assuming independent scattering [33]. For a packed-bed with \( d_{in}=0.4 \) and 1 mm \( (d_{m} \) of particle-size distribution shown in Fig. 7 at \( X_c=1 \) and 0, respectively), the maximum deviation of the scattering efficiency (appearing at the largest radiation wavelength in our spectral range of interest 1 \( \mu m \)) is 5% and 23% for \( \varepsilon_{\text{ext}}=0.88 \) and 0.86, respectively, (measured and depicted in Fig. 5 at \( X_c=1 \) and 0, respectively). Consequently, dependent scattering effects are neglected in the radiative transfer analysis.

The cumulative distribution function of the cosine of incidence at the solid wall and the scattering phase function are computed for two limiting cases: a specular and a diffuse solid-gas interface. For tire shreds, a combination of these two cases is anticipated to be valid. The specular directional-hemispherical reflectivity is calculated using Fresnel’s equations for the complex refractive index of the carbon-ash mixture \( m=(1-X_c)m_C+X_cm_{\text{ash}} \), where \( m_C \) and of the initial ones during the reaction is observed.
The scattering albedo, $s$ for spheres and for diffuse reflecting identical overlapping opaque functions for diffuse reflecting identical overlapping transparent functions for diffuse reflecting identical overlapping transparent functions for diffuse reflecting identical overlapping opaque functions, for diffuse reflecting identical overlapping opaque functions. For the specular solid-gas interface, this result is consistent with the small differences obtained between the phase functions for diffuse reflecting identical overlapping transparent spheres and for diffuse reflecting identical overlapping opaque spheres, although largely differing in morphology. The extinction coefficient is inversely proportional to the characteristic path length, and consequently, the extinction coefficient are independent on the refractive index and therefore $X_C$. Further studies are directed to the determination of the effective properties for conduction heat transfer (thermal conductivity), convection heat transfer (interfacial heat transfer coefficient), and for fluid flow (permeability and Dupuit–Forchheimer coefficient).

### Nomenclature

- $A_0$: specific surface, m$^{-1}$
- $b$: bit number of image
- $c$: constant, indicating gamma correction regime change
- $d$: particle diameter, m
- $F$: probability density function
- $f$: size distribution function, m$^{-1}$
- $f_γ$: two-step gamma correction function
- $G_x$: cumulative distribution function of extinction length
- $I$: radiative intensity, W m$^{-3}$ sr$^{-1}$
- $m$: complex refractive index
- $N_r$: number of rays
- $N_e$: number of extincted rays
- $n$: number of moles
- $n_i$: molar flow rate
- $p$: (partial) pressure, bar
- $r$: distance between two points in the sample, m
- $r$: position vector for spatial coordinates in the sample
- $s$: path length, m
- $s_x$: two-point correlation function
- $\hat{s}$: unit vector of path direction
- $T$: temperature, K
- $t$: time, s
- $V$: total sample volume, m$^3$
- $X_C$: carbon conversion
- $x$: molar fraction
- $x$: spatial location vector, m

### Greek

- $\alpha$: density value of tomographic scans
- $\alpha_0$: threshold density value for phase segmentation
- $\beta$: extinction coefficient, m$^{-1}$
- $\delta$: Dirac delta function
- $\varepsilon$: porosity
- $\gamma$: gamma constant
- $\kappa$: absorption coefficient, m$^{-1}$
- $\lambda$: radiation wavelength, m
- $\mu$: directional cosine
- $\rho$: intrinsic density, kg m$^{-3}$
- $\rho_r$: hemispherical reflectance
- $\sigma$: scattering coefficient, m$^{-1}$
- $\varphi_x$: difference between azimuthal angle of incidence and reflection, rad
- $\Phi$: scattering phase function

### Table 2

<table>
<thead>
<tr>
<th>$X_C$</th>
<th>$A$</th>
<th>$b$</th>
<th>$c$</th>
<th>RMS</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.986</td>
<td>5.031 × 10$^{-7}$</td>
<td>13.55</td>
<td>0.017</td>
</tr>
<tr>
<td>0.3</td>
<td>0.899</td>
<td>1.415 × 10$^{-2}$</td>
<td>4.057</td>
<td>0.001</td>
</tr>
<tr>
<td>0.7</td>
<td>0.750</td>
<td>3.622 × 10$^{-2}$</td>
<td>4.017</td>
<td>0.009</td>
</tr>
<tr>
<td>1</td>
<td>0.614</td>
<td>6.377 × 10$^{-3}$</td>
<td>6.697</td>
<td>0.124</td>
</tr>
</tbody>
</table>

$\varepsilon = 2.2\times 1.12/\varepsilon$ is the complex refractive index of carbon and $m_{ash} = 1.5 - 0.02 \varepsilon$ is the complex refractive index of ash [17,34]. Note that the cumulative distribution function of radiation mean free path, and consequently, the extinction coefficient are independent of the interface reflection type in the geometrical optics range.

The extinction coefficient $\beta$ and scattering phase function $\Phi$ are shown in Figs. 10 and 11, respectively, for the reference case at $X_C=0, 0.3, 0.7, 1$. $\beta$ increases with $X_C$ as particles shrink and shorten the attenuation path length. An empirical correlation of the extinction coefficient inversely proportional to the characteristic diameter supports this trend [18]. The extinction coefficient is fitted to an exponential function (RMS/β_{X_C=0}=0.09):

$$ \beta_{mc}(X_C) = 4024 + 32.14 \exp(5.93X_C) \quad (12) $$

In contrast, the scattering phase function for specularly reflecting particles exhibits a large forward scattering peak. This peak is enhanced with increasing $X_C$ due to the decrease in the real part of the refractive index of the carbon-ash particle. The coefficients of the exponential fit, described by Eq. (14), are listed in Table 2.

$$ \Phi_{ip} = a + b \exp(c\mu_s) \quad (14) $$

The scattering albedo ($\sigma_i/\beta$) can be approximately calculated as

$$ \sigma_i/\beta = (1 - X_C) \rho_{ip} + X_C \rho_{ash} \quad (15) $$

For the specular solid-gas interface, $\sigma_i/\beta = 0.273$ and 0.092 at $X_C=0$ and 1, respectively. For the diffuse solid-gas interface $\sigma_i/\beta = 0.1$ and 0.75, respectively, [31,32].

### Conclusions

CT-based computational techniques were used to characterize the morphology (porosity, specific surface, particle-size distribution, and the REV for continuum domain) and the effective radiative heat transfer properties (extinction coefficient, scattering phase function, albedo) of a packed-bed undergoing a thermochemical reaction. The study was performed for the gasification of carbonaceous waste materials (tire shreds) to produce high-quality syngas. The variation in the morphology of the packed-bed was investigated at discrete carbon conversion steps ($X_C=0, 0.3, 0.7, 1$) and for different process parameters (feedstock size, furnace temperature, gasifying agent, and ambient pressure of gasifying agent). The CT scans were digitally improved to allow for more accurate phase segmentation. Numerical calculated and experimentally measured porosity (by weight), BET surface (by $N_2$-adsorption), and particle-size distribution (by laser scattering) were compared. Discrepancies were due to limitations in the CT scan resolutions and to image distortions around optically thick heavy metal impurities. The morphological results can be used for the determination of structural parameters [25] needed in kinetic models. The extinction coefficient increased as particles shrunk and shortened the attenuation path length. For diffuse reflecting particles, the scattering phase function was found to be independent of the reaction extent. For specularly reflecting particles, the scattering phase function exhibited a strong forward peak and dependency on the refractive index and therefore $X_C$. Further studies are directed to the determination of the effective properties for conduction heat transfer (thermal conductivity), convection heat transfer (interfacial heat transfer coefficient), and for fluid flow (permeability and Dupuit–Forchheimer coefficient).
\[ \psi = \text{pore-space indicator function} \]
\[ \Omega = \text{solid angle, sr} \]

**Subscripts**
- b = blackbody
- C = carbon
- d = diffuse
- ex = experimental
- ga = gasifying agent
- in = incidence
- m = mean
- min = minimal
- op = opening
- r = reflection
- s = scattering
- sp = specular
- sub = submicron
- 0 = initial

**References**


