Determination of Size of Representative Volume Element for Coke Using Homogenization Method Based on Digital Image of Actual Microstructure

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When the homogenization method based on the digital image of actual microstructure is used to analyze the strength of coke, the representative volume element (RVE) is a crucial input to predict reliable results. The shape of RVE was identified as square, due to the two-dimensional numerical analysis with the research object being a section image of a coke sample being studied. The variation of multi-scale mechanical properties of coke according to a large number of unit cells with various scales was investigated to determine the proper RVE size. The resolution of calculation equaling original resolution was considered as Case 1. The other low resolution of calculation was considered as Case 2. The results showed that, in the macro-scale (homogenization) analysis, the proper size of RVE on coke’s sample should be chosen larger than 874.8 μm, due to the mean calculated homogenized Young’s modulus was almost constant in the case of unit cell larger than 874.8 μm. In the micro-scale (localization) analysis, in Case 1, unit cell of a large scale was prone to stress concentration which happened at the relative thin parts of structure around large pores. In Case 2, it was considered that high resolution was necessary, because low resolution changed the structural characteristic. Finally, the optimum size of RVE on coke’s sample was determined as 2 624.4 μm, which could represent the structural relativity of the research object.

KEY WORDS: coke strength; homogenization method; RVE; microstructure; stress concentration.

1. Introduction

High strength coke proves effective in improving blast-furnace performance, because coke serves as a heat source, as a reducing agent, and as the skeleton for supporting burden and providing the permeability of liquid and gas in blast furnace.1 Due to the large requirement of iron and steel in developing countries for economic development, it is a challenge to increase the availability of non- or slightly-caking coal to ensure the supply stability of raw material for coke making without deteriorating coke strength.

Coke is a porous material consisting of matrix and pore. The distribution of pores is irregular and complex.2 The sufficient information about microstructure also includes microcracks, grain boundaries, phase separation when more than one chemical entity is present, ordered and amorphous material, as well as the presence of inert materials.3 These structural parameters influence coke strength.

In conventional approaches, drum and tumbler test are used as indices of coke strength. Recently the coke strength has been studied by computational simulation,4–7 which can in-depth understand the relationship between the microstructure and mechanical property of coke. Asakuma et al.5 demonstrated that the distribution of both cracks and pores in coke was an important factor for the microscopic fracture.

Ueoka et al.6 concluded that the coke with regular arrangement of equal sized inerts was expected for the improvement of coke strength. Furthermore, it was important to prevent inerts from being close to each other in irregularly arrangement in order to produce the coke with high strength. The above two examples were using homogenization method. Their studies were just based on the simulated random microstructure, which considered particles of regular geometric shape and size in a matrix phase.

When the homogenization method was used to analyze the strength of coke, the simulation process must be based on the actual microstructure of coke. Then the finer microstructure details can be represented accurately, and the analysis can result in better insight into the critical structure parameters that influence the strength of coke. In this case, the calculated effective properties of coke depend on the selected unit cell. The notion of representative volume element (RVE) is of paramount importance. The unit cell which can statistically represent the composite, i.e., to effectively include a sampling of all microstructural heterogeneities that occur in the composite is regarded as RVE.8 RVE is a crucial input to predict reliable results. However, there is almost no report about the RVE for coke. In this study, the shape of RVE for coke was identified as square due to discussing the two-dimensional numerical analysis. The
purpose of this study was to determine the size of RVE for coke. The variation of multi-scale mechanical properties of coke according to a large number of unit cells with various scales was investigated.

2. Digital Image Analysis

The coke for study was produced by 50% caking coals and 50% non- or slightly-caking coals with particle size less than 1 mm. The research object for numerical analysis was a two-dimensional digital image (resolution of 2.43 μm/pixel) had a size of 11,284 μm × 11,284 μm on a section of the above type of coke. Software WinROOF Ver. 6.1 was used to binarize and analyze the digital image. Porosity was calculated from area ratio of coke matrix and pore. Mean pore area was calculated by averaging individual pore area in binary image. Pore roundness was given by the following equation as:

\[
\text{Roundness} = \frac{4\pi S}{L^2}, \quad (1)
\]

where \( S \) is area and \( L \) is perimeter of each pore. Pore-wall thickness was calculated by drawing the line horizontally to the microscopic image and counting the average number of pixels of coke matrix.

Structural characteristic of the coke sample’s section was summarized as follows: the porosity was 51.9%, mean pore area was 1,041.6 μm², mean pore roundness was 0.617 and mean pore-wall thickness was 47.7 μm. The image of the section is shown in Fig. 1. Figure 1(a) is the original image and Fig. 1(b) is the binary image. Coke matrix (green color) can be clearly separated from the pore (black color) in the binary image.

3. Experimental Measurement of Young’s Modulus of Coke

In this section, the experimental measurement of Young’s modulus of coke was introduced. The value of Young’s modulus was derived from Hook’s law, which relied on the linear part of the relationship between tensile stress and strain of coke breakage behavior in the diametral-compression test. The schematic diagram of the diametral-compression test is shown in Fig. 2.

In this test, coke specimens were made into the discs with the diameter \( d \) of 15 mm and thickness \( l \) from 5 to 7 mm. The eleven discs were measured. The test was carried out using a universal-testing machine. The tensile stress \( \sigma_t \) of coke was measured during the test. The detail was described by Patrick et al.9) The strain \( \varepsilon_t \) was measured by attaching strain gauges to the test specimens across the diameter perpendicular to the line of the applied load \( P \) during the compression test. The frequency of data record of strain development was consistent with universal-testing machine setting condition. The standard deviation of the measured Young’s modulus of the eleven discs was 1.4 GPa. Mean value of Young’s modulus equaling 5.4 GPa was defined as Young’s modulus of this type of coke. In the latter part of this paper, this value would be compared with the predicted one based on the homogenization method.

4. Numerical Analysis

4.1. Homogenization Method

Microscopic simulation should provide a maximum information depth in form of spatial-temporally resolved microstructures. Homogenization method is then used to reduce this data and to extract the effective properties in order to obtain information relevant for simulations on a larger length scale. Homogenization method makes the only assumption about the microstructure, namely its periodicity.10) This assumption is widely used, and numerical results fit well with experimental data.11) Homogenization method has reached a high level of sophistication and efficiency, especially in the case of linear properties such as thermal conductivity or elasticity.9)

The schematic diagram of a structure which has a periodic microstructure is shown in Fig. 3.12) It can explain the homogenization method. In this figure, a macroscopic structure \( \Omega \) is supposed to be made of a material that has periodical microstructure (unit cell \( Y \)). The material is approximated as a homogeneous one with regarding the unit cell as a point in the overall structure. The unit cell can represent
the global heterogeneity. The macroscopic properties can be
defined as the average of the microscopic properties in the
unit cell. Define the macroscopic scale $x$ and the microscop-
ic scale $y$, and define the scale ratio $\varepsilon$ that is usually a very
small positive number so that $y = x/\varepsilon$. Formulations of
homogenization method\(^5,13\) are introduced as following.

$\chi^m$ is a characteristic displacement that is a periodic
function with respect to the micro scale. The microscopic
equation to be solved for the unit cell $Y$ under the periodic
boundary conditions is as follows:

$$\int_Y (E_{ijkh} - E_{ijmn} \frac{\partial \chi^m_{ab}}{\partial y_j}) \frac{\partial v^i_a}{\partial y_j} dY = 0 \quad \text{for} \quad \forall v^i_a, \quad \cdots. \quad (2)$$

$E_{ijkh}^{\mu}$ is the homogenized elasticity tensor that is defined by:

$$E_{ijkh}^{\mu} = \frac{1}{|\Gamma|} \int_Y (E_{ijkh} - E_{ijmn} \frac{\partial \chi^m_{ab}}{\partial y_j}) \frac{\partial v^i_a}{\partial y_j} dY, \quad \cdots. \quad (3)$$

The macroscopic equation is derived from the weak forms
for the homogenized macroscopic body as:

$$\int_\Omega E_{ijkh}^{\mu} \frac{\partial u^i_a}{\partial x_j} \frac{\partial v^j_a}{\partial x_i} d\Omega = \int_{\Gamma^r} t^i_a v^j_a d\Gamma \quad \text{for} \quad \forall v^i_a, \quad \cdots. \quad (4)$$

The microscopic stress can be calculated by the following
equation:

$$\sigma_{ij} = (E_{ijkh} - E_{ijmn} \frac{\partial \chi^m_{ab}}{\partial y_j}) \frac{\partial u^i_a}{\partial x_j}, \quad \cdots. \quad (5)$$

The finite element discretization was used to solve the
partial differential equations. The detail was described by
Asakuma \textit{et al.}\(^5\) Isoparametric finite element method was
applied for the calculation.

### 4.2. Numerical Conditions

Boundary condition for the macro-scale analysis was
shown in \textbf{Fig. 4}. Tensile strength of industrial coke is
approximately 5 MPa.\(^{14}\) The load of 1 MPa in the test piece
was determined. Macroscopic and microscopic behaviors
were analyzed using the finite element homogenization
method. An element located in the middle of the bottom was
set as the micro-scale analysis region, in which the macro-

scopic strain ($\frac{\partial u^i_a}{\partial x_j}$) was constant in the unit cell $Y$, as
shown in \textbf{Fig. 4}. So the scale ratio $\varepsilon$ equaled 0.02. Mathematical theory of homogenization method demands $\varepsilon$ tending
to 0. But it is said that, the calculation result using
homogenization method with the value of $\varepsilon$ less than 0.1 is
approximate the result calculated with the value of $\varepsilon$ tending
to 0.\(^{15}\) Thus the scale ratio was a reasonable setting.

\textbf{Table 1} shows mechanical parameters of unit cell.
Young’s modulus of coke matrix was determined according to
the measurement of elastic modulus of coke texture using
nano-indentation method.\(^{16}\) Young’s modulus of pore was
determined 10$^{-4}$ times of Young’s modulus of coke matrix.
Poisson’s ratio of both coke matrix and pore was taken as
0.3.\(^{17}\)

In the homogenization method, the structure of the material is assumed periodic. Under this periodicity assumption, the
coke structure was idealized as a periodic assembly of many unit cells.\(^{18,19}\) \textbf{Figure 5} shows the image of periodic
tiled microstructure unit cells.

### 4.3. The Choice of Unit Cells

In this section, the choice of unit cells was discussed.
Bobzin \textit{et al.}\(^{10}\) proceeded calculations by asymptotic
homogenization with the defined RVE size by discussing the component ratio distribution. It implies that component ratio is an important parameter. Besides that, the morphology of the microstructure usually depends on the volume fractions of the constituent material phases,\(^{(18)}\) which also emphasized the importance of component ratio. In addition, the RVE should represent the global structural characteristic. Therefore, unit cells chosen for analysis had almost same porosity that equaled the porosity of the research object. The shape of unit cells was all square. Side length of square represented the dimension of the unit cell.

Table 2 shows the simulation information about unit cells. The more pixels of unit cell, the more CPU time required for computational calculation. When the square was 1 200 × 1 200 pixels, because of the limit of the work station’s storage capacity, the program of homogenization method could not be executed. In this condition, when the original dimension of square was 4 617.0 \(\mu\)m, resolution of calculation was changed to 4.86 \(\mu\)m/pixel, corresponding to 950 × 950 pixels. When the original dimension of square was 9 234.0 \(\mu\)m, resolution of calculation was changed to 9.72 \(\mu\)m/pixel, corresponding to 950 × 950 pixels. The largest original dimension of square with the resolution of calculation being 2.43 \(\mu\)m/pixel, which equaled the original digital image resolution, was 2 624.4 \(\mu\)m, corresponding to 1 080 × 1 080 pixels. The chosen unit cells of the definite scale were as much as possible to avoid overlapping each other. In Table 2, the resolution of calculation equaling 2.43 \(\mu\)m/pixel was considered as Case 1. The low resolution of calculation in Case 1 was almost did not influence the whole tendency in Case 1. The value at the scale of 1 749.6 \(\mu\)m and 1 458.0 \(\mu\)m, the large figure was not shown, but the black part was used to show the position of pore in coke.

Table 2. The simulation information about unit cells (Porosity = 51.9% ± 0.1%).

| Case number | Original dimension of square [\(\mu\)m] | Number of realizations | Resolution of calculation [\(\mu\)m/pixel] | Calculation dimensions [pixels] | Mean pore roundness [-] | Standard deviation of mean pore roundness |
|-------------|----------------------------------------|------------------------|--------------------------------------------|-------------------------------|------------------------|-----------------------------------------|
| Case 1      | 145.8                                  | 209                    | 2.43                                       | 60 × 60                       | 0.597                  | 0.0568                                  |
|             | 291.6                                  | 123                    | 2.43                                       | 120 × 120                     | 0.607                  | 0.0325                                  |
|             | 583.2                                  | 89                     | 2.43                                       | 240 × 240                     | 0.612                  | 0.0212                                  |
|             | 874.8                                  | 46                     | 2.43                                       | 360 × 360                     | 0.613                  | 0.0143                                  |
|             | 1 166.4                                | 43                     | 2.43                                       | 480 × 480                     | 0.617                  | 0.0103                                  |
|             | 1 458.0                                | 27                     | 2.43                                       | 600 × 600                     | 0.616                  | 0.0111                                  |
|             | 1 749.6                                | 22                     | 2.43                                       | 720 × 720                     | 0.618                  | 0.0085                                  |
|             | 2 624.4                                | 9                      | 2.43                                       | 1080 × 1080                   | 0.615                  | 0.0074                                  |
| Case 2      | 4 617.0                                | 5                      | 4.86                                       | 950 × 950                     | 0.662                  | 0.0091                                  |
|             | 9 234.0                                | 2                      | 9.72                                       | 950 × 950                     | 0.672                  | 0.0019                                  |

5. Results and Discussion

5.1. Macro-scale Analysis: Calculated Homogenized Young’s Modulus of Coke according to a Large Number of Unit Cells with Various Scales

The calculated homogenized Young’s modulus in \(x\) and \(y\) direction, that was horizontal and perpendicular to the digital image of the coke’s section, is shown in Fig. 6. The error bars represent the standard deviation values. Figure 6 revealed that the tendencies in both \(x\) and \(y\) directions were similar. Young’s modulus decreased as the scale of unit cells increased until it reached 4 617.0 \(\mu\)m, which had a little increase, but the degree of change was very small in the case of the unit cell larger than 874.8 \(\mu\)m. In other words, the mean calculated homogenized Young’s modulus was almost constant in the case of the unit cell larger than 874.8 \(\mu\)m. Based on such relationship, the proper size of RVE on coke’s sample should be chosen larger than 874.8 \(\mu\)m. This result indicated that the low resolution of calculation in Case 2 almost did not influence the whole tendency in Case 1.

5.2. Micro-scale Analysis: Stress and Microstructure for Unit Cells

Maximum von Mises stress for unit cell with various scales is shown in Fig. 7. The error bars represent the standard deviation values. In Case 1, Fig. 7 showed that, maximum von Mises stress increased from the scale of 145.8 to 2 624.4 \(\mu\)m. The value at the scale of 1 749.6 \(\mu\)m and 2 624.4 \(\mu\)m was almost equal. This relationship could be interpreted by stress distribution in unit cells at different scales as shown in Figs. 8 and 9. The calculated stress in pore was not shown, but the black part was used to show the position of pore in coke.

Figure 8 shows stress distributions in unit cells at the scale of 291.6 \(\mu\)m, 874.8 \(\mu\)m and 1 749.6 \(\mu\)m. The large figures included some structures in small figures. From Fig. 8, it was found that unit cell of a large scale was prone to stress concentration which happened at the relative thin parts of structure around large pores. This phenomenon was considered to be the reason for the increasing of maximum von Mises stress. Figure 9 shows stress distributions in unit cells...
at the scale of 1 749.6 and 2 624.4 μm. In this figure, the stress concentration location and extent in the unit cell at the scale of 1 749.6 μm was almost consistent with the scale of 2 624.4 μm, owing to small change of structural relativity between these two scales, that is, the degree of thin structure was almost same at this two scales. So the maximum von Mises stress at the scale of 1 749.6 μm and 2 624.4 μm was almost equal. Besides that, Fig. 9 also revealed that inert had a lot of thin structures, but the pore in inert was relative small compared with the unit cell, so stress concentration almost did not happen in the inert.

From Figs. 8 and 9, it was suggested that the larger the unit cell was, the better it reflected the stress distribution characteristic of overall structure. In Fig. 9, the structures where the stress concentration happened in the unit cells at the scale of 2 624.4 μm were very thin, thus even in the whole section image (Fig. 1) they were also the thin parts, which meant that the unit cells at the scale of 2 624.4 μm could be able to represent the structural relativity of the whole section image. Absolutely, the scale which was larger than 2 624.4 μm could satisfy the requirement. Therefore, the maximum von Mises stress of unit cells with the scale larger than 2 624.4 μm was predicted to be consistent with the value at the scale of 2 624.4 μm.

In Case 2, Fig. 7 shows that the maximum von Mises stress at the scale of 4 617.0 μm satisfied the above predicted tendency based on the analysis of case 1, that the maximum von Mises stress of unit cells with the scale larger than 2 624.4 μm would be consistent with the value at the scale of 2 624.4 μm. However, the value at the scale of 9 234.0 μm had a great deviation from the tendency. The structural characteristic of unit cells with different resolutions at the last two large scales shown in Table 3 could explain such result.

Table 3. The structural characteristic of unit cells with different resolutions.

| Unit cell scale [μm] | Resolution [μm/pixel] | Mean porosity [%] | Mean pore roundness [-] | Mean pore area [μm²] | Mean pore-wall thickness [μm] |
|----------------------|-----------------------|-------------------|------------------------|---------------------|-----------------------------|
| 4 617.0              | 2.43                  | 51.9              | 0.617                  | 1 097               | 50.3                        |
| 9 234.0              | 9.72                  | 52.0              | 0.672                  | 2 969               | 64.6                        |
| Ratio relative to original | 0.000 | 0.087 | 1.928 | 0.380 |

In Table 3, when the resolution of calculation was 4.86 μm/pixel, the values of mean pore roundness, mean pore area and mean pore-wall thickness became larger. The mean pore area changed most obviously, and the change of mean pore roundness was smallest. The same variation appeared as the resolution became lower. But comparing the changes of mean pore area and mean pore-wall thickness with the results of the resolution decreased to 9.72 μm/pixel, these changes were distinct small, especially the change of mean pore area. Because of the small expansion of pore, the small amount of stress concentration structure became relative thinner, but a few of thin parts of structure also vanished. The resolution decreased to be 4.86 μm/pixel did not affect the value of maximum von Mises stress obviously. At the last scale of 9 234.0 μm with the resolution of calculation...
being 9.72 μm/pixel, the maximum von Mises stress was greatly decreased. It was considered that, mean pore-wall thickness became thicker and the mean area of pore expanded three times compared with the original digital image, which made many thin parts of structure vanished.

Nevertheless, in Case 2, the low resolution changed the structural characteristic. Therefore, the calculated results did not reflect the real structure. In order to get the reliable simulated results, the high resolution with large unit cell scale was necessary. The scale of 1 749.6 μm could be chosen as the RVE size. However, microstructure of coke was very complex. The larger size could better represent the global microstructural heterogeneities that occurred in coke. As the above reason, the optimum size of RVE on coke’s sample was determined as 2 624.4 μm, which corresponded to the standard deviation of mean pore roundness less than 0.01 in the case of original resolution.

5.3. Comparison the Predicted Effective Young's Modulus of Coke Based on the Simulation with the Experimental One

Due to the optimum size of RVE on coke’s sample being 2 624.4 μm, the mean calculated Young’s modulus for unit cells at this scale shown in Fig. 6 was regarded as the effective Young’s modulus of coke based on the simulation. Comparing this Young’s modulus with the value being 5.4 GPa obtained from the experiment measurement, which was described in section 3, it was obvious that the simulation provided result lower than the experimental one. It was not possible to determine the exact reasons for such difference. However, some explanations could be proposed. Firstly, the Young’s modulus of the pore phase was underdetermined. For example, the value of Young’s modulus of the pore element is determined as 0.024 GPa rather than 0.0024 GPa. On the other hand, perhaps experimental method overestimated the Young’s modulus of coke. Because the coal for coke making included 50% non- or slightly-caking coals. There were some defects in coke, such as cracks. So the fracture routes might be not across the perpendicular diameter of the discs in the diametral-compression test. The strain gauge did not measure the strain in the perpendicular diameter of the discs. The drawback of experimental method can be avoided by nondestructive testing, such as the pulse echo method based on sound velocity can be used to measure the Young’s modulus of material. Moreover, the predicted effective Young’s modulus was based on the two-dimensional digital image. If the simulation is based on the three-dimensional image, the predicted effective Young’s modulus might be increased, because the matrix with an orientation unparallel to the vertical direction between the two-dimensional images can be taken into account to enhance the Young’s modulus in those two-dimensional images.

6. Conclusions

The representative volume element (RVE) is a crucial input to predict reliable results, when the homogenization method based on the digital image of actual microstructure is used to analyze the strength of coke. In this paper, we focused on the determination of the proper RVE size for coke in the two-dimensional problem. The optimum size was determined by investigating the variation of multi-scale mechanical properties of coke according to a large number of unit cells with various scales. The resolution of calculation equaling 2.43 μm/pixel was considered as Case 1. The low resolution of calculation was considered as Case 2. Conclusions of this study are summarized as follows.

(1) In the macro-scale analysis, the proper size of RVE on coke’s sample should be chosen larger than 874.8 μm, due to the mean calculated homogenized Young’s modulus was almost constant in the case of unit cell larger than 874.8 μm.

(2) In the micro-scale analysis, in Case 1, unit cell of a large scale was prone to stress concentration which happened at the relative thin parts of structure around large pores. Owing to small change of structural relativity between the scale of 1 749.6 and 2 624.4 μm, stress concentration location and extent in the unit cell at these two scales was almost consistent. The unit cells at the scale of 2 624.4 μm could be able to represent the structural relativity of the research object, because the structures where the stress concentration happened in the unit cells at this scale were very thin, thus even in the whole section image they were also the thin parts. In Case 2, it was considered that high resolution was necessary, because low resolution changed the structural characteristic. The scale of 1 749.6 μm could be chosen as the RVE size. However, the larger size could better represent the global microstructural heterogeneities that occurred in coke. Finally, the optimum size of RVE on coke’s sample was determined as 2 624.4 μm, which corresponded to the standard deviation of mean pore roundness less than 0.01 in the case of original resolution.

(3) The predicted effective Young’s modulus of coke sample by homogenization method was lower than the experimental one. It was considered that Young’s modulus of the pore phase was underestimated, and experimental method might overestimate the Young’s modulus of coke. Moreover the simulation was not based on the three-dimensional images.

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Nomenclature

| Symbol | Unit |
|--------|------|
| L      | μm   |
| S      | μm²  |
| t      |      |
| u      |      |
| v      |      |
| x      | mm   |
| y      | mm   |
| Y      | μm   |
| ε      |      |
| Γ      | mm   |
| σ      |      |
| χ      |      |
| Ω      | mm   |

Superscript

| Symbol | Description |
|--------|-------------|
| 0      | macro-scale |
| 1      | micro-scale |

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