Development of Analytical Method of Predicting Fissures Formation for Carbonization Process of Coke

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The development of a numerical method for fissure formation during the carbonization of coke is needed because the formed fissures determine the coke's particle size. In this study, we proposed and developed a novel numerical method that can represent initiation, extension, and branching of multiple cracks. Fundamental tests (i.e., bending of a beam, stress analysis of a center crack plate, and crack propagation in a plate under tensile loading) were performed using the proposed method. The test results showed that the numerical accuracy of stress analysis and the fracture analysis using the proposed method were high and were comparable to other standard numerical methods. Furthermore, we applied the proposed method for the coupled analysis of heat conduction and thermal stress and performed numerical simulations for the formation of fissures in coke during carbonization. The numerical simulation results showed that major fissures extended in a linear direction, perpendicular to the direction of an oven wall. And the numerical results reflected qualitative features of an actual coke-making process using a chamber oven. Therefore, the proposed method could be used to reproduce the formation of fissures in coke during the carbonization process.

KEY WORDS: metallurgical coke; fissure formation; finite element method; fracture analysis; carbonization process.

1. Introduction

The size of metallurgical coke must be large enough to sustain the flow of gas and liquid in a blast furnace.1–3 Cracks are one of the factors that affects the size of coke as they cause failure of the coke cake.4–7) Major fissures and secondary fissures are of concern as they manifest large cracks in the coke cake. The fissures are formed during the carbonization process, and their number and spacing determines the size of the coke.8–10) Therefore, it is important in the coke making process to have a prediction technique for fissure initiation and propagation.

The major fissures that develop in coke run in a perpendicular direction from the coke oven wall due to the differences in temperature distribution in the coke oven. The secondary fissures are believed to be extended in the perpendicular direction from the major fissure due to the transfer of radiation heat within the major fissure. Hence, knowledge and a good understanding of the temperature distribution and thermal stress caused by the temperature gradient in the coke oven is necessary for the prediction of the formation of fissures during the carbonization of coke. Numerical analysis through models such as the finite element method (FEM) have been widely used to simulate the mechanical response of the coke6,11–13) and for thermal stress analyses8,14–18) Sato et al.16) Goto et al.17) and Jenkins et al.18) performed the thermal stress analyses of coke models with major fissures using FEM and investigated the mechanism for the formation of fissures and factors that influence their spacing. However, although the shape of fissures that develop in coke during carbonization is generally complex, only linear major fissures were considered in the previous study. Besides, location of the fissure was prescribed in advance, and its shape was simplified. Three-dimensional thermal stress analysis without fissures has been performed,19) however, none has been conducted that includes fissures. Consequently, thermal analyses that considers fissures requires a three-dimensional method that can represent their complex shapes to improve the numerical accuracy.

In earlier studies, many numerical methods that could reproduce the crack formation were proposed which...
analyses of coke during carbonization using DEM and RBSM can model fissure formation easily, and fracture cracks by breaking springs between elements. The DEM displacement is constant within an element and describe crete element method (DEM) and rigid-bodies springs around the tip of a crack with high accuracy.

With an adaptive method can analyze stress distributions around the tip of a crack with high accuracy. In particular, the remeshing approach with an adaptive method can analyze stress distributions around the tip of a crack with high accuracy. The discrete element method (DEM) and rigid-bodies springs model (RBSM) are numerical methods which assume that displacement is constant within an element and describe cracks by breaking springs between elements. The DEM and RBSM can model fissure formation easily, and fracture analyses of coke during carbonization using DEM and RBSM has been reported. Various fracture analysis methods were proposed, however, they were considered unsuitable as their use for modelling may have brought about some challenges for predicting the formation of fissures during the carbonization of coke. This is because the remeshing method cannot represent the complex shape of a crack because the neighboring or branching cracks cannot be automatically remeshed. In X-FEM as with the remeshing method, representing the complex shape with a function is challenging due to its inability to represent the neighboring or branching cracks. The RBSM and DEM methods can represent the propagation of cracks with several branches, however, the numerical accuracy of stress analysis using these methods was low, and material properties such as the Young’s modulus and Poisson’s ratio cannot be directly used. The particle discretization scheme finite element method (PDS-FEM) was proposed by Oguni et al. to overcome the challenges of the RBSM and DEM. The PDS-FEM represents the displacement inside a tetrahedral element using a specific discontinuity function and represent the initiation and extension of cracks easily as it considers that they form inside the tetrahedral element. This allows it to perform the stress analysis with a high accuracy. The PDS-FEM was used to model crack formation that results from the shrinkage of material that is comparable to the carbonization of coke and reproduced the fissure extension from the surface to the interior.

However, it is challenging to directly apply the general algorithm used in the finite element (FE) analyses in the PDS-FEM when other factors such as the viscosity and finite deformation of a material, and radiation heat transfer from the crack plane are considered. This is because the PDS-FEM is a unique method and may have limitations to its extensive application that have not yet been realized.

In the present study, we proposed a novel three-dimensional analytical method based on the FEM to simulate the fissure formation of coke during carbonization. Fundamental tests were performed using the general FEM and our proposed method for comparative purposes and for its validation. Moreover, three-dimensional thermal stress analyses coupled with heat conduction and the formation of fissures in coke during carbonization was conducted. The proposed method for carbonization of coke was validated through a comparative analysis of the experimental results with the previous numerical analysis results of the two-dimensional numerical analysis.

2. A Numerical Method to Represent Initiation, Extension, and Branched Cracks

A tetrahedral element can be divided into four hexahedral elements with four types of vertices (i.e., a vertices of the tetrahedron, the mid-point of the sides, and the gravity center of the triangle plane and the gravity center of the element). The presented method uses the hexahedral elements generated as above for stress analysis. For example, if a crack is assumed to initiate from the hexahedral elements inside a tetrahedron, its initiation can be represented by separating the connection of the hexahedral elements. Thereby, a node located on the fracture plane can be divided by generating another node at the same coordinate and this allows the hexahedral elements to be separated. The propagation and branching of cracks can be described by defining more than two planes inside the tetrahedral element as fracture planes, hence, the connections of the hexahedrons in a tetrahedron will separate one after another as shown in Fig. 1. In the proposed method, the shape of a crack in a tetrahedron was preliminarily prescribed. When a tetrahedron is divided into four hexahedral elements, six quadrangular planes exist inside the tetrahedron and the number of the patterns of fracture plane generated in the tetrahedron is 63, however, when considering the symmetry,

![Fig. 1. Schematic of crack formation in a two-dimensional triangle element and a three-dimensional hexahedral element. (Online version in color.)](image-url)
the number of fracture plane patterns is 10 as shown in Fig. 2. Therefore, the shape of a complex crack can be expressed by separating hexahedral elements in each tetrahedron. For simplification, the application of the above method to the two-dimensional quadrangular elements gives a description of the formation of complex cracks with branches that are shown in Fig. 3. In the case of three-dimensional elements, cracks that initiate from the element group that share a side of neighboring tetrahedrons, the shape of the fracture plane will be polygonal because separating shared nodes at the neighboring quadrangular plane is required. Figure 4 shows a group of five tetrahedral elements sharing one vertical side and has a pentagonal fracture plane composed of five quadrilaterals because horizontal cracks are generated in the five tetrahedral elements of the group simultaneously. We presumed that the breakage of linkage of elements occurs when tensile stress between hexahedral elements exceeds a certain threshold, and fracture planes are generated simultaneously. Furthermore, the proposed method can be applied to an existing stress analysis program using FEM for the fracture analysis because it was implemented in the pre- and post-processes as shown in Fig. 5.

The proposed method is a type of remeshing technique, hence, the shape of cracks is not completely arbitrary because their pattern is prescribed in advance. However, undesired termination in remeshing when describing the complex shape of a crack does not occur, and many cracks can be represented without any preprocessing or treatment. Thus, our analysis for the propagation of complex crack can be continuous without failure unlike when using the general remeshing methods and the X-FEM. Moreover, the interpolation of physical quantities in space, which is conducted in general remeshing methods, is not needed because the shape of the hexahedral element does not change before and after dividing the mesh. In the proposed method, the physical quantities remain the same before and after remeshing. The location of the crack planes generated using the proposed method are comparable to the ones generated using the PDS-FEM, suggesting that the proposed method can directly express crack simulated using the PDS-FEM. The proposed method uses more nodes in comparison to the PDS-FEM, hence, it has higher computational costs. However, in our method numerical simulations consider the viscosity of materials, large deformation, and radiation heat transfer of the fissures and these can be performed easily in comparison to the PDS-FEM. This is because it can use existing FEM programs, and fracture planes can be treated as boundary planes.

3. Verification

3.1. Bending of a Beam

A hexahedral element is generated by dividing a tetrahe-
dron and this distorts the shape of the element leading to a decrease in numerical accuracy. Hence, the accuracy of the stress analysis was verified using numerical simulations of tetrahedral elements that were generally used in the FE analyses or hexahedral elements that were generated by dividing tetrahedrons. During verification, stress analyses based on a beam bending test was conducted as shown in Fig. 6. The Young’s modulus and Poisson’s ratio were used as material properties and were set at 10 GPa and 0.3, respectively. In this case, the formation of cracks was not represented because the purpose of this numerical simulation was only to evaluate stress distribution. Three linear tetrahedral meshes different in the number of nodes were used and also generated quadratic tetrahedral and hexahedral meshes. The location of vertex nodes of the quadratic tetrahedral and hexahedral meshes were the same as those of the linear tetrahedral. Mid-points or gravity centers were added onto the quadratic tetrahedral and hexahedral meshes. The number of nodes and elements divided by each mesh is listed in Table 1. The numerical accuracy of the stress analyses was investigated by calculating the degrees of freedom (DOF) of the linear tetrahedral meshes and the displacement at point P on the y-axis direction ($u_y$) as shown in Fig. 7. The value of the DOF was a multiple of dimensions (i.e., three) and the nodes of linear tetrahedral elements. The theoretical solution was calculated based on the classical beam theory. The numerical results of the linear tetrahedral elements and quadratic tetrahedral elements were comparable to the theoretical solution as the DOF increased, and the hexahedral elements also converged. The results show that the hexahedral elements decreased error with an increase in the DOF and it was comparable to the elements used in the general FE analysis. A comparison of the numerical results determined using tetrahedral elements to with the results determined using hexahedral elements shows that the error of displacement for the hexahedral elements was less than that of the linear tetrahedral elements, however, it was larger than that of the quadratic tetrahedral elements ones. This is because the function of the order of shape function with hexahedral elements was higher than that with linear tetrahedral elements and lower than that with quadratic tetrahedral elements. Note that fracture analysis was performed with ease using hexahedral elements in comparison to the linear and quadratic tetrahedral elements. The results suggest that the numerical accuracy of the stress analysis using hexahedral elements is higher than that when using

| 1st-order tetrahedron | Number of nodes | 134 | 646 | 3 663 | 2nd-order tetrahedron | Number of nodes | 773 | 4 170 | 25 864 | 1st-order hexahedron | Number of nodes | 2 043 | 11 953 | 78 183 | Number of elements | 1 544 | 9 804 | 67 560 |
the linear tetrahedral elements, however, it is lower than that when using quadratic tetrahedral elements. The deformation of the beam and von Mises stress distribution is presented in Fig. 8. The stress distribution using the hexahedral elements was comparable to the stress distribution using the quadratic tetrahedral elements. The above results show that the numerical solution of the stress analysis for the hexahedral elements used in this study was comparable to that of the general tetrahedral elements. Therefore, the results suggest that the numerical accuracy of stress analysis using hexahedral meshes generated by the proposed method was high and comparable to that of the conventional FE analyses.

3.2. Stress Analysis of a Center Crack on a Plate

Based on the stress distribution around a crack tip, the numerical accuracy of stress analyses with using structured cubic elements and unstructured hexahedral elements generated using our proposed method was compared. In general, the numerical accuracy of the numerical simulation with cubic elements is high. For verification problem, a uniaxial tensile test for a plane with a straight crack shown in Fig. 9 was simulated. The boundary conditions indicated in Fig. 9(a) were applied for cubic elements, and a quarter of the plate was analyzed using symmetry boundary condition due to its properties of symmetry. The crack had a free boundary and node displacement was unconstrained. When the stress analysis was performed using the proposed method, the analytical object indicated in Fig. 9(b) was used and the domain of the plate without cracks was divided into hexahedral elements. A crack was added on the domain by separating hexahedral elements located on and this resulted in it becoming nonlinear. The Young’s modulus and Poisson’s ratio were set at 10 GPa and 0.3, respectively. In this case, the development of cracks was not represented because the purpose of this numerical simulation was only to evaluate stress distribution.

Displacement changed drastically on the position with the crack in each case as shown in Fig. 10(a). Our method can also represent the discontinuity of displacement as with the method using cubic elements. The distribution of the $\sigma_y$, which is the component of the stress that opens the crack...
is shown in Fig. 10(b). The stress concentrated at the crack tip and similar stress distributions were shown in both cases. Figure 11 shows the spatial distribution of $\sigma_{yy}$ at $y = 0$. The stress increased closer to the location of the tip of the crack at $x = 0.4$, and our method reproduced the solution with cubic elements. Therefore, the application of the proposed method to the stress analysis for material with a crack gave numerical solutions with a high accuracy comparable to the general method with hexahedral elements.

3.3. Crack Propagation in a Plate under Tensile Loading

The numerical results of the proposed method were compared to those by Khoei et al.\textsuperscript{20} to investigate the propagation behavior of a crack. Khoei et al. used the adaptive FEM that can analyze propagation of simple cracks with high accuracy. Referring to the analysis by Kohei et al., a fracture analysis for the analytical object shown in Fig. 12 was performed. The applied boundary conditions were shown in Fig. 12, and the Young’s modulus and Poisson’s ratio were set at 20 MPa and 0.3, respectively. An iterative calculation was performed during the simulation of the propagation of cracks. A criterion of crack initiation was not set, however, five planes with the highest tensile stress were defined as fracture planes and treated as free boundary conditions at each iteration. This is because the load was assumed as large enough to develop cracks in this calculation. Since the propagation direction of cracks depends on the shape of mesh in the proposed method, 10 types of analytical objects were employed. These analytical objects were generated using the tetrahedral mesh generation software, Tetgen,\textsuperscript{35} and the arrangements of nodes in the objects were different in each mesh. Crack propagation from a notch tip that were simulated by Khoei et al., were reproduced and the cracks
Crack propagation, shape and stress distribution were evaluated at each step as shown in Fig. 13. Each crack propagated from each notch tip to the center of the plate. The stress was concentrated on tip of the crack, and cracks propagated because of stress. The results suggest that the proposed can also be used to analyze the propagation of cracks. Furthermore, crack propagation was calculated using 10 different meshes as shown in Fig. 14 with the earlier study. The shape of cracks formed is focused because of different algorithms. The shapes of the cracks that were simulated using our method were different in each mesh. However, the averaged crack wake obtained by the present analysis reproduced that by the earlier study. This would be because our method can simulate stress around a with high accuracy. The results, that the proposed method can be used to analyze the propagation of with high accuracy.


4.1. Numerical Method

The results presented in section 3 suggested that the proposed method could represent crack initiation and extension, and the branching of cracks. We applied the proposed method to a coupled analysis of heat conduction and thermal stress using the FEM and performed numerical simulations for coke during carbonization. The analytical object was a rectangular cake of coke with a width of 300 mm, a depth of 300 mm, and a height of 200 mm. The domain was divided into 70 718 tetrahedrons, and then these elements were divided into hexahedral elements. In the analysis of heat conduction, the non-linear heat conduction equation was discretized using the experimental results of Miura et al.,36) which is an effective thermal diffusivity as shown in Fig. 15(a). The boundary conditions were set for the upper side of the analytical object and were assumed to be a wall boundary heated from 400°C to 1 000°C at a heating rate of 10°C/min. Adiabatic boundary condition were set for the other faces. The stress equilibrium equation for thermal stress analysis was discretized. The infinite strain was assumed as a relationship between displacement and strain. The coke was assumed to be a linear elastic material, and referring to experimental results of Fukada et al.,37) the temperature-dependent elastic modulus and contraction coefficient shown in Figs. 15(b) and 15(c) were used, respectively. The Poisson’s ratio was set to 0.3 constant. The displacement on a bottom face was constrained as a boundary condition, and free boundary conditions were set for the other faces. The proposed method was used to represent the formation of cracks, and a criterion of crack initiation was set to 20 MPa. Fracture planes were treated as adiabatic boundaries during heat conduction analysis and as free boundaries during thermal stress analysis. The time increment was set at 4 min in each analysis.

4.2. Results and Discussion

Fissure initiation and propagation during carbonization are discussed with a focus on the deformation of coke shown in Fig. 16, the temperature change shown in Fig. 17, and von Mises stress distribution shown in Fig. 18. Numerous fissures formed on the upper face of the coke cake in the initial stages of the analysis at \( t = 120 \) min as shown in Figs. 16 and 19. The coke cake near the heated wall was heated up to over 800°C (Fig. 17), and then high thermal stress occurred (Fig. 18). This was due to the large temperature gradient around the upper face heated, and the high thermal stress that developed. After \( t = 200 \) min, Fig. 16 shows a part of fissure was extended straight in a perpendicular direction to the oven wall. This was possibly because the coke cake shrank as the carbonization progressed, and thermal stress occurred away from the oven wall (Fig. 18). These cracks that extended straight were comparable to actual fissure formation that occurs in the actual coke oven. As carbonization progressed at times, \( t = 400 \) and 600
min, the number of propagating cracks decreased as shown in Figs. 16 and 19. Some major fissures propagated to the bottom of the coke cake resulting in the coke cake dividing into as carbonization progressed. The decrease in the number of propagating cracks was possibly due to a decrease in thermal stress around the fissure tip as shown in Fig. 18. The decrease in thermal stress was attributed to a decrease in temperature gradient with distance from the heated wall as shown in Fig. 17. The variation of predicted fissure length on cross-sectional planes at \( t = 800 \) min are shown in Fig. 19 and that the number of cracks decreased with increasing distance from the heated wall. The results are comparable to Jenkins et al., who theoretically and experimentally showed that the spacing of the major fissure in the coke oven was narrow around the heated wall but widen as the distance from the wall increased. Our numerical result qualitatively reflected their feature. Unfortunately, our model was not compared with actual fissuring of a coke cake because precise material properties during carbonization in coke were not sufficiency and experimental evaluation of fissure formation was not comparable. Secondary fissures were not formed in our analysis. This is possibly because the fracture plane was assumed to be the adiabatic boundary in the heat
conduction analysis and irradiation was not considered. In previous studies using the two-dimensional analyses, most of the results were evaluated using the distance of fissure extension and the spacing between fissures.\(^{8-10}\) The results show that the proposed method can be used to evaluate the length of fissure extension and the cross-sectional area of coke divided on the heated wall. The fissure in the coke cake is extended by the dropping impact, and the size and shape of coke particles can be determined by the size and shape of the coke cake divided by some fissures. Therefore, our proposed method would accurately and directly evaluate the size of coke particle which had been challenging thus far. The pieces of the divided coke cake after carbonization were of different sizes due to the random nature of the size and shape of elements generated in advance that were used in the model. Hence, the novel method also would enable the determination of the size distribution of coke particles based on the spacing and distribution of the fissures. Recently, the relationship between the fissure formation on cross-sectional area and size distribution of coke particles were studied experimentally.\(^{38}\) If the relationship between the shape of shattered coke particles and three-dimensional fissure formation of coke measurement from X-ray CT analysis is evaluated, our numerical method would be a useful tool to predict the size and distribution of coke particles.

5. Conclusion

In this study, we proposed a novel three-dimensional numerical method for predicting the formation fissuring during carbonization process of coke. The numerical accuracy of stress analysis of the proposed method was high because the method is based on the finite element method. Initiation, extension, and branching of cracks was analyzed based on the priori definition of the crack shape in a tetrahedral element. The numerical accuracy of the fracture analysis of the model was high. Furthermore, a numerical analysis for the carbonization of coke in a coke oven was performed and reproduced the qualitative features of the actual phenomenon. We deduced that amount of crack decreased with increasing distance from heated wall. Therefore, the proposed method can reproduce the complicated shapes of fissure formed in actual coke. As shown, as the method is based on the three-dimensional analysis, it could be used to evaluate the particle size of coke and predict its particle size distribution. Overall, the proposed method has the potential to be a useful tool for numerical simulations of the carbonization process of coke.

### Nomenclature

\[ t: \text{Time [s]} \]
\[ u: \text{Displacement [m]} \]
\[ \sigma: \text{Stress [Pa]} \]

### Greek symbol

\[ \varepsilon \]

### REFERENCES