Simulation of crack formation in an anisotropic coke using discrete element method

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HIGHLIGHTS

▶ Cracks are initiated at a stress concentrating point.
▶ Cracks are developed following stress paths at the same time and independently.
▶ Strength has positive relation to the number of broken bondings between particles.
▶ Low stress concentrating pore structure can be more dangerous when it fails.

ABSTRACT

The Discrete Element Method (DEM) is a powerful computational method to simulate mechanical properties of cokes including its failure mechanisms. This study investigates the effects of an anisotropic pore structure on the stress concentration patterns and failure mechanisms of a brittle coke by describing it as a 2-dimensional DEM model assembly which consists of hundreds of element particles. The adjoining element particles are bound to each other using parallel-bonds which are assumed to be broken when the developing stress exceeds the target strength. The voids between element particles are considered to represent micro-defects, and several macro-pores are intentionally imbedded to investigate the effect of macroscopic pore-structures on the coke strength. The macro-pores have a shape of elongated ellipse and their long axes are arranged in three directions: normal, 45° angled and parallel to the loading direction. These pore layouts reflect the different stress concentration patterns during a tensile test.

Based on the simulated results, the coke strength has a positive relation with the load bearing matrix area, or, the number of broken bonds when the assembly has the same long axis as the pores. However, if their long axis directions are changed to decrease the stress concentration, the assembly can stand higher strength with the same load bearing matrix area. Decreasing the stress concentration makes the assembly much stronger against the failure and also avoids being shattered disastrously into small fragments at failure.

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1. Introduction

Strength is one of the most important properties for coke fed into a blast furnace (BF) because, as the only solid material in the lower high temperature zone, coke has to maintain its permeability for the uniform liquid phase drainage and upward gas flow in the BF. As an industrial practice, the coke strength has been measured using a drum index (DI). However, the DI does not quantify the coke strength itself but represents the tendency for breakage or abrasion of cokes. Therefore, many attempts have been made to relate the coke's physicochemical properties to the coke strength directly. There are many factors such as various pores, coke matrix textures and micro/macro-cracks which affect the coke strength,

but, among them, the macroscopic pore structure has been considered to be the most influential factor [1,2].

Generally, when the effects of pore parameters on the porous and brittle material's strength are discussed, two kinds of models [3,4] are proposed. The Minimum Contact Area (MCA) model considers the effect of porosity on the load-bearing coke matrix area. In other words, the increased porosity reduces the matrix area fraction, and, as a result, the material must withstand a smaller amount of stress. In contrast, the Stress Concentration Effects (SCE) model considers the effect of pore structure on the stress concentration or stress interference. In this case, pore's shape and directional change are significant factors.

Computational investigations have been carried out to find out the main factors of pore structure which affect coke breakage through various computational methods [5–8], however, the answer is still not clear. For example, Ueoka et al. simulated the effect of pore shapes on the direct tensile test using the homogenization

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method [5]. The homogenization model can simulate the stress concentration patterns of the simple pore layout easily, but due to its complex calculation algorithm to express breakage between elements, this simulation method is not appropriate to examine the validity of the SCE and MCA models.

On the other hand, DEM provides a simple and intuitive algorithm for the breakage simulation of cokes. It can easily make a complex structured coke model just by binding a large number of small element particles, and the breakage is simulated by eliminating bondings between element particles when a transferred stress exceeds the particular bonding strength. DEM does not require any calculation interruption or parameter modification when a failure occurs. Therefore, although it demands a long calculation time, DEM can be an excellent method/tool to compare and verify the breakage models directly.

The previous study [7] which used 3-dimensional (3-D) DEM investigated the effect of pore structure such as porosity, pores' size/number and arrangement on the coke strength by applying compression and indirect tensile test to cylinder-shaped coke specimen models. It confirmed the positive relation between matrix area and coke strength as the MCA model's suggestion. However, due to the spherical pore's shape, it was hard to verify the effect of stress concentration.

From this reason, this study has investigated the effect of anisotropic pore-structures on the coke strength and the fracture mechanism by simulating the indirect tensile test to 2 dimensional (2-D) disk-shaped coke specimen models having elongated pores. This study adopts a 2-D model rather than a 3-D model because a 2-D model much clearly shows crack developing mechanism near pores. Also, a 2-D model requires much shorter calculation time to get a simulation result. As a result, it is possible to increase repeatability which is necessary for the computational investigation using DEM. The developed model is highly simplified in a sense. However, the ultimate aim of this study is to clarify the effect of stress distribution developed by the pore shape and their layouts on the fracture mechanism. The various layouts of pores will make the effect of stress concentrations on the coke fracture mechanism clear. As already reported [5], externally applied stresses concentrate strongly at the small areas where pore's shape changes significantly. Therefore, this study adopts elongated pores rather than spherical pores to intentionally generate strongly stress concentrating regions. By manipulating the direction of the elongated pores and their layouts, the effect of the stress interference patterns between pores on the fracture are investigate.

2. Simulation setup

2.1. Indirect tensile test

The "Indirect tensile test" (sometimes called the "Brazilian test") applies load to a lying cylindrical specimen by compressing it at the top and bottom. Then, indirect tensile forces develop which are perpendicular to the forced cross-section, and vertical fracture occurs following the forced cross-section in the sample. That is why the indirect tensile test is also called the "Cleavage test".

Following the suggestion of the International Society for Rock Mechanics [9], the 2-D indirect tensile strength of the specimen (σ_t) is calculated by the equation:

$$\sigma_t = 0.636P/D \text{ (MPa)} \tag{1}$$

where P is the load at failure (N) and D is the diameter of the test specimen (mm).

In the real case, coke particles receive stress at various directions. Usually, a coke particle receiving multiple stresses or confin-

ing forces stands much larger loading force compared with a particle receiving uniaxial stress. However, multiple stresses show complex stress interference, and it is very difficult to observe the effect of pore structures. Therefore this study uses only uniaxial stress to focus on the effect of pore structures on the stress distribution.

2.2. DEM modeling of anisotropic coke lumps

This study uses PFC2D, a commercial 2-D DEM code, to simulate the indirect tensile test of cokes. The numerical framework for DEM or PFC2D is already well explained in previous papers [10,11], hence, this paper do not describe it. In the PFC2D program, the element particle's type is a disk-shaped rigid body. Hence, generating complex shaped and breakable model requires assembling stage by *gluing* a large number of small element particles to the desired shape. Usually, 'wall's which are provided as lines at PFC2D are used to form a mold to generate desired model shape by filling the inside of mold with element particles. Walls are eliminated at the final model generating stage.

Fig. 1 shows the coke model of this study which is a 2-D porous disk having a diameter of 8 mm and two pore types of A and B. the details about two pore types will be explained in the last part of this section. The coke model consists of about 530 element particles which have 0.1–0.2 mm radius variation following the Gaussian distribution. The element particle's size is decided to be smaller than the fine particle's size (0.5 mm) shown at Aizawa et al.'s experimental results [12]. According to the Koyama and Jing's reports about the effect of element particles' dimension on the PFC2D simulation results [13], the chosen element particle's size is expected to cause within 10% acceptable variation to the results. Although the variation seems a little bit large than usual, this paper adopts this value to increase repeatability of simulations by decreasing computational cost drastically. The element particle's size distribution is also chosen to secure stable heterogeneity to the model according to the reference. The material properties such as density, stiffness and friction are unified for every element particle to simplify the coke model. The element particles are connected at each contact site using a parallel-bond which is an
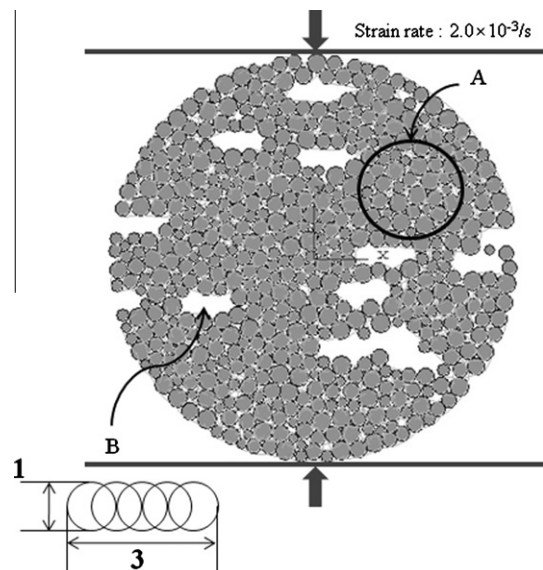

Fig. 1. Depiction of a 2-dimensional coke particle model including two types of pores: A type pores: small voids between closely packed element particles, B type pores: elongated large voids which are made by removing overlapping the five temporary pore–particles embedded in the matrix with the ratio of 1:3 as shown.