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# Numerical modeling of compaction and flow of coke/pitch mixtures using discrete element method

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## HIGHLIGHTS

- Discrete element method is capable of modeling composite materials.
- Burger's model can predict the rheological behavior of pitch at different temperatures.
- Temperature has a positive effect on compaction of coke and pitch mixtures.

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## ABSTRACT

A variety of composite materials are composed of a viscoelastic matrix and elastic fillers. These materials range from polymer matrix composites to asphalt concretes. Discrete element method (DEM) has the capability of explicitly modeling the mechanical and physical properties of both matrix and aggregates. In the present work, DEM is applied to simulate the compaction and deformation of mixtures of coal tar pitch and calcined coke at 135, 140, 145 and 150 °C. Rheological properties of pitch and those of the binder matrix (mixture of pitch and fine coke particles) were experimentally measured by means of a dynamic shear rheometer. Obtained data was then used to estimate the four parameters of Burger's viscoelastic model for pitch and binder matrix. The dynamic shear rheometer test was simulated by a three dimensional DEM model to verify the proposed viscoelastic model. Results showed that there is a very good agreement between the measured values and model predictions for complex, storage and loss moduli of pitch and binder matrix in a wide range of frequencies at all studied temperatures. The verified models were then used to study the compaction and densification of coke/pitch mixtures. Results showed that temperature has a positive effect on densification of coke/pitch mixtures and lower value of porosity is expected for the material pressed or vibrated at higher temperatures.

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## 1. Introduction

Aluminum oxide is reduced to metallic aluminum by means of the Hall-Héroult process. Carbon anodes, which participate in the main chemical reaction of the cell and are consumed during the process, are important elements of the reduction cells. Prebaked carbon anodes are made by mixing calcined coke aggregates with coal-tar or petroleum pitch. The mixture is called anode paste and at its forming temperature, 150 °C, exhibits a granulo-viscoelastic behavior [1]. Mixing and forming steps are of critical importance for the quality of anode and the efficiency of reduction cells. High permeability of the obtained mixture, as an example, results in an increased air and $CO_2$ reactivity [2]. Paste recipe as well as mixing and forming temperatures influence the density and homogeneity of the final product. Azari et al. [3] in 2013 showed the importance of coke particle granulometry on the compaction behavior and densification of anode paste. Anode paste is a complex material and because of existence of several material and process parameters, its deformation mechanics is not fully understood. Numerical simulation can potentially be an effective approach to understand the flow and deformation mechanisms in the anode paste compaction process.

Application of computers in mechanical modeling goes back to 1950s [4]. Since 1956 finite element analysis has been used in dif-

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ferent engineering applications for mechanical and thermo-mechanical modeling of materials and structures. However, when the size of discontinuities is large with respect to the scale of the problem domain, the continuity assumption which is usual in finite element method is no longer valid [5]. The extended finite element method has been developed to effectively address this problem. However, to deal with problems where large deformations and localizations exist, these continuum-based models fail to be practical [6].

Having been developed more than four decades ago, the discrete element method (DEM) is a powerful method to study the movements and interactions in a granular system. With ever increasing computational capacity, advanced simulation techniques like DEM are attracting more interest in computational materials science [7,8]. From particle flow [9] and sintering simulation [10] to mechanical modeling of glacial ice [11], concrete [12] and asphalt mixtures [13], DEM has been a powerful method for dealing with microstructural problems in materials modeling.

Apart from the basic elastic contact model which has been used to study particle packing [14] and flow problems [15], other contact models such as a simple viscoelastic model (based on Maxwell model) and Burger's model have also been developed to model the rheological behavior of viscoelastic materials. Burger's model, mostly in the Particle Flow Code (PFC3D) platform, has been used to predict the rheological properties of hot mix asphalts. As reported by Khattak et al. [16] and Dondi et al. [17], Burger's model embedded in DEM code can successfully predict the dynamic modulus of asphalt mixes.

In the previous article [18], the authors showed the power of DEM modeling in predicting the viscoelastic behavior of coal-tar pitch at 150 °C. The present work attempts to address some critical issues regarding effects of temperature on compaction and homogeneity of anode paste. DEM models of pitch at 135, 140, 145 and 150 °C as well as that of binder matrix (pitch + fine coke particles) at 150 °C are created. Then, static and dynamic responses of pitch and binder matrix mixtures with coke aggregates are studied.

## 2. Numerical modeling

A typical DEM model is composed of a combination of spherical elements and walls. Geometrical features are modeled by the shape of the particle assembly and sometimes by clustering spherical particles to make irregular-shape particles. In contrast to the finite element method where elements carry the material properties, in DEM the contact model assigned to the interactions of elements simulates the material behavior. The calculation cycle of DEM simulations is composed of two main parts. First is the DEM platform algorithm which detects the contacts between the elements and also calculates the elements acceleration based on explicit (or implicit) solving of Newton's second law. The second part of the code takes into consideration the mechanical and physical features of the material. This part is composed of the contact model applied to the interactions and the geometrical features of the model such as particles position, shape and size.

An anode paste contains two types of materials: coke aggregate and pitch. Coke aggregate is considered as rigid and unbreakable under the process conditions. Interactions of coke-coke contacts are thus handled with the classic contact stiffness model. This model is simply like an elastic spring in normal and shear directions. In some cases, i.e. this study, where particles are not spherical, particles shape and size distribution should also be considered.

Pitch, however, is a viscoelastic material and an appropriate numerical model must be used to be able to simulate its time-dependent behavior. Burger's model is a widely used and well-documented model for simulating viscoelasticity. Advantages of Burger's model such as its relative simplicity and capability of predicting material behavior in both creep and relaxation have made it a very common model for viscoelastic materials [19]. Burger's model, as shown in Fig. 1(a), is a four-element model composed of two basic Maxwell and Kelvin models. The force-displacement equation of the Burger's model can be written as:

$$f + \left[\frac{C_k}{K_k} + C_m\left(\frac{1}{K_k} + \frac{1}{K_m}\right)\right]\dot{f} + \frac{C_k C_m}{K_k K_m}\ddot{f} = \pm C_m \dot{u} \pm \frac{C_k C_m}{K_k}\ddot{u} \tag{1}$$

Eq. (1) is the governing law defining the interaction of two bodies with Burger's model as their contact model. The present authors have already implemented this viscoelastic model in the open access DEM code, YADE [20].

In an anode formulation (a mixture of matrix and coke aggregates), where both elastic and viscoelastic materials are present, there are three types of contacts to be handled; coke-coke, coke-matrix, and matrix-matrix. These three contacts and their mathematic equivalent have been presented in Fig. 1. Although Fig. 1 is showing the normal direction, the tangent movement of two bodies in contact is also expressed with the same elements and parameters.

Viscoelasticity is often represented by the two response parameters, complex shear modulus, $G^*$, and phase angle, $\delta$ [17]. Dynamic Shear Rheometer (DSR), Shown in Fig. 2, is the laboratory equipment widely used to characterize the rheological properties of different types of binders and mastics, capable of determining these two parameters [14]. In this test, a sinusoidal stress is applied to a disc of material sandwiched between two plates at the desired temperature and the strain is measured. Both stress or strain-control schemes are possible. The induced strain is also in the sinusoidal form but with a time lag, which comes from the material's time dependent behavior. This time lag is called the phase angle ($\delta$). Frequency sweep is used to obtain the response by measuring the complex shear modulus and phase angle at different frequencies.

The spherical elements for the DEM models of pitch and binder matrix have chosen to have radius of r = 0.08 mm. The balance between the computation time and model resolution is the main factor in determining the size of elements. Time-step of the model was also determined by verifying the stability in the model at different time-steps. In DEM models here, $\Delta t = 2 \times 10^{-7}$ s was used.

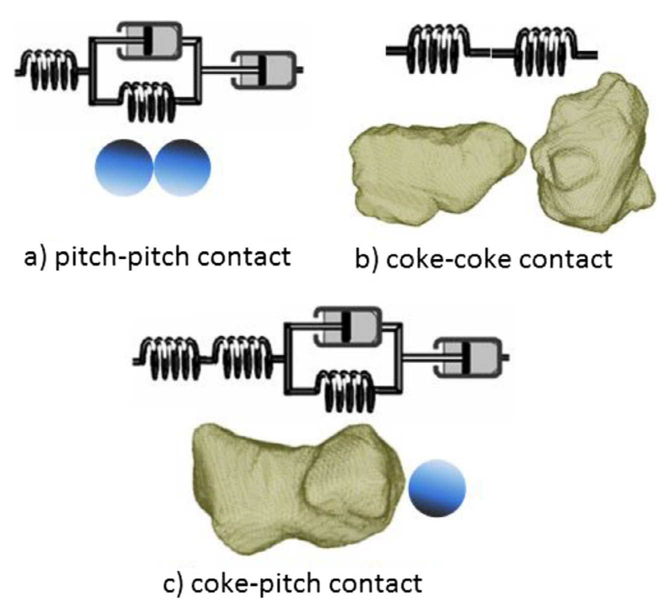


**Fig. 1.** Three contact types in the DEM model of coke/pitch mixtures.

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