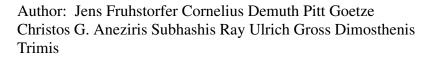
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## ACCEPTED MANUSCRIPT

# How the coarse fraction influences the microstructure and the effective thermal conductivity of alumina castables—an experimental and numerical study

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#### Abstract

This study investigates the particle size distribution's effect on the microstructure and effective thermal conductivity (ETC) of alumina castables. The ETC was measured by the transient plane source method and predicted numerically based on a two-scale model describing the structure on a fine and coarse scale. The prediction considered particle and pore size distributions, porosity (around 20%) and grain morphology. The microstructure was investigated by scanning electron microscopy. For a constant fines content, increasing the coarse grain fraction while decreasing the medium fraction enhanced sintering of the matrix. Small pores ( $\leq 250 \text{ nm}$ ) increased the sintering activity. The densest castable contained the most small pores. The particles' and pores' contributions to the sintering activity led to intensified microcracking and a decreased ETC. The numerical model did not consider constituents  $\leq 500 \text{ nm}$  like the small pores and microcracks and the calculated ETC values consequently deviated from the measured values.

Keywords: particle size distribution, pore size distribution, sintering, microcracking, refractory

#### 1. Introduction

A main requirement on most refractories is thermal shock resistance [1]. Otherwise, thermal stresses—caused by sudden heat loads and steep temperature gradients may result in the failure of the material. The distribution of such temperature gradients can be determined and controlled by the heat flow rate, specimen geometry, and (effective) thermal conductivity (ETC) [2]. Therefore, a numerical prediction of the ETC is important to evaluate the performance of refractories with respect to thermal shock resistance.

Several structural characteristics of refractories influence the ETC. Refractories contain porosity and cracks, which generally decrease the thermal conductivity [3, 4]. In addition, the ETC is affected by grain boundaries [5], shape of grains and pores [6] and their size distributions [7]. Defects like vacancies, impurities and isotopes [8], crystal imperfections like stacking faults and dislocations [9], and microcracks [10] influence the thermal conductivity, too. Although these studies partially contradict each other, it was found that an increasing defect density generally decreases the ETC.

Since the ETC is influenced by numerous refractory characteristics, its numerical prediction requires a simplified but adequate representation of the material structure. In a previous study [11], a modified random sequential adsorption (RSA) algorithm was introduced for the associated geometry generation. The classical RSA algorithm [12, 13] is unsuitable for packings with a high solid volume fraction [13–16] like dense refractories. Furthermore, the original algorithm employs exclusively spheres, i.e. nonspherical particles cannot be included. In contrast, the generation and insertion of non-spherical particles is possible in the modified approach. Additionally, particles or pores belonging to the same constituent, e.g. a single particle size fraction, are allowed to overlap. Therefore, higher volume fractions are attainable [11].

After generating the simplified material structure, the heat conduction equation is solved [17]. For the numerical solution the finite volume method [18, 19] was applied in the previous study [11]. Subsequently, the ETC was determined according to the averaged Fourier's law of heat conduction as a function of the average steady-state heat flux. Nevertheless, the prior study [11] did not consider thermal resistances which impair the conductive heat transfer. Particularly, the thermal boundary resistance between different phases like alumina and air decreases the heat transfer by conduction [5]. Microcracks also reduce the conductive heat transfer, but their consideration in the numerical prediction is not straightforward.

Microcracks are caused by a thermal expansion or shrinkage mismatch. They develop due to thermal expansion

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