# NUMERICAL SIMULATION OF THE HOMOGENIZATION PROCESS OF A BINARY MIXTURE IN A BALL MILL

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Mechanical mixing of powder mixtures in various kinds of mills is a widespread method of obtaining a homogenized system [1]. It is known that the rate of chemical reaction of two substances directly depends on their common contact area, which, in the case of a powder mixture, directly depends on the homogeneity of the system [2].

It is obvious that the transition of the system from a heterogeneous state to a homogeneous one during mechanical mixing leads to an increase in the contact area of the two substances. However, it is still difficult or impossible to evaluate this parameter directly in various technological processes. To estimate the size of the reaction surface area, we constructed a numerical model (Fig.1.).

In our work, the results of numerical simulation of the mixing process of a binary mixture in LIGGGHTS® open source Discrete Element Method (Particle Simulation Software) are presented. The similarity of numerical calculations to the real experiment was estimated using the methodology proposed in [3] for comparing the degree of homogeneity of the real 3Ni + Al mixture to its model analog at fixed time points.

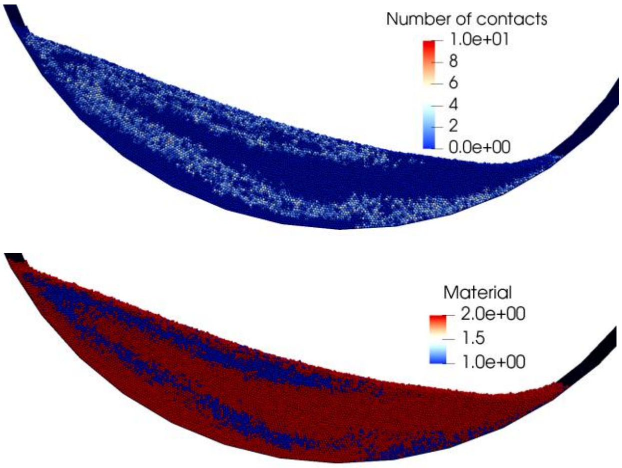


Fig.1. Indication and counting of the number of contacts between simulated nickel (red) and aluminum (blue) particles.

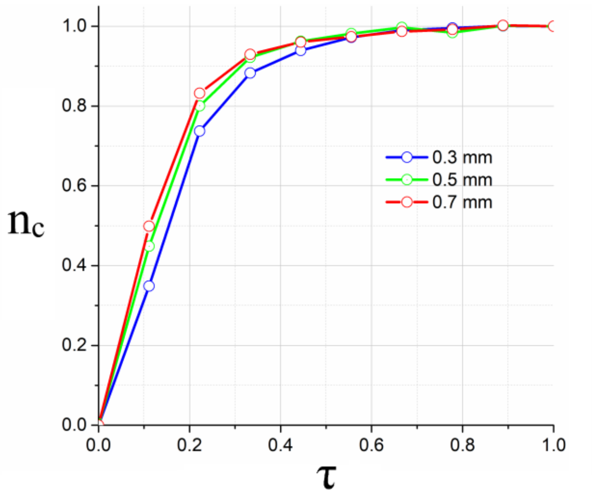


Fig.2. The dependence of the degree of homogenization (the number of heterogeneous contacts) on time at different particle diameter.

The calculation of the number of contacts between the particles was carried out using the LIGGGHTS® function, adapted for calculating contacts only between particles of different materials (heterogeneous contacts).

Numerical simulation results (Fig.2.) was presented in dimensionless parameters $n_c = N / N^*$ and $\tau = t / t^*$, where $N$ – the current number of heterogeneous contacts, $N^*$ – maximum number of heterogeneous contacts, $t$ – time, $t^*$ – time of reaching $N^*$ during mixing. It was found that the rate of homogenization of the binary mixture increases with increasing particle size. A good compliance of numerical calculations with experimental data is obtained.

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