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NUMERICAL SIMULATION OF CHEMICAL REACTIONS IN POWDER MIXTURES TAKING INTO ACCOUNT MELTING

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This paper presents a numerical model of chemically reacting powders mixture under explosive loading conditions. Such mixtures make it possible to obtain homogeneous solid reaction products of high density and homogeneity.

The processes of elastic-plastic deformation of particles and diffusion processes are simulated based on the meshless method of smooth particles [1, 2]. To simulate the motion of the medium it is suggested to use a weak variational formulation of the equations of motion [3], which allows one to reduce requirements for order of spatial derivatives of the solution and ensures fulfillment of conservation laws.

Diffusion and heat conduction processes are also modelled by the meshless smooth particle method [4] with the use of Morris [5] and Schweiger [6] approximations. Under the conditions considered, the initiation of reaction takes place at the particle contact boundaries, resulting in temperature rise and melting of one of the mixture components, after which the flow of the molten component and diffusion in the melt starts to play an important role. A special feature of the approach is that SPH allows transition from the model of an elastic-plastic medium to a fluid medium without explicitly identifying the boundaries.

Numerical simulations show that two scenarios of reaction propagation are possible in such a reaction - when reaction initiation in the whole volume is carried out by a passing shockwave, and when shockwave initiation occurs in a limited volume of reacting materials [7], which causes their heating, and the heat released in this case is a factor of reaction propagation in the surrounding volume of the powders mixture. Assuming that reactions in powder mixtures occur at the solid-liquid interface, in the second case, the heat exchange conditions between the particles and the initial temperature may influence the final result of the reaction by influencing the wetting of the more refractory components of the mixture by the more fusible ones. The approach and numerical model proposed in this work allow us to investigate on a micro level the melting process of the fusible component of the mixture and its interaction with refractory components with account to heat transfer and diffusion of components in chemically reaction media.

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