A WIDE-RANGE NUMERICAL MODEL OF EXOTHERMIC REACTIONS UNDER SHOCK-WAVE LOADING

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Shock-wave compaction of reacting mixtures is a promising method for producing homogeneous and high-density products [1]. However, the mechanism of chemical reaction development under these conditions is not yet fully understood due to the rapid process occurring at high pressures and temperatures. In processes like this, the chemical reaction is typically described using a phenomenological model of irreversible chemical transformations based on zero-order kinetics [2]. The objective of this study was to develop a comprehensive wide-range model of exothermic reactions for an Al/CuO mixture under shock-wave loading.

Two potential chemical reaction mechanisms were evaluated: a zero-order and first-order reactions.

The zero-order reaction model has the following form:

$$\frac{d\eta}{dt} = \begin{cases} 0, & \eta = 1 \text{ OR } \left(P < P_{crit} \text{ AND } T < T_{crit} \right) \\ f(P), & \text{otherwise;} \end{cases} \tag{1}$$

$$f(P) = \begin{cases} K_0, & \text{if } \left(P < P_{crit} \right) \\ K_P K_0, & \text{otherwise;} \end{cases} \tag{2}$$

where η is the reaction depth, $P, T, K_0, K_P, P_{crit}, T_{crit}$ are pressure, temperature and reaction parameters. The proposed model assumes a constant reaction rate, while taking into account the experimentally observed effect of reaction acceleration at high pressure.

The first-order reaction model has the following form [3]:

$$\frac{d\eta}{dt} = \begin{cases} 0, & \text{if } \left(P < P_{crit} \text{ AND } T < T_{crit} \right) \\ K_0 (1-\eta)\left(1 + K_1 \left(P - P_{crit} \right)\right), & \text{if } \left(P < P_{crit} \text{ OR } T < T_{crit} \right); \end{cases} \tag{3}$$

The Al/CuO mixture experimental data [4] can be accurately described by the proposed first-order reaction model with the following parameters: $P_{crit} = 1.6$ GPa, $T_{crit} = 493$K, $K_0 = 260$GJ/(kg*s), $K_1 = 6$/GPa. It was also shown that the zero-order reaction model can be used for a first-order approximation.

The first-order reaction model is preferred from a theoretical standpoint as it corresponds better to the assumed process mechanism. This involves the reaction of the plastic or liquid phase of one component with the solid surface of particles of the second component. Based on this reaction mechanism, the reaction rate decreases as the depth of conversion increases because the surface area of the second component solids, where the chemical transformation occurs, decreases.

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