MODEL OF ZONE CHEMICAL REACTION
OF A LIQUID SINTER OF CONDENSED PHASE
ON THE SURFACE OF COKING THERMAL PROTECTIVE MATERIALS

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A new mathematical model of the hot spot reaction and evolution of the liquid agglomerate of metal oxides on the surface of charring thermal protective materials of multilayer walls is proposed. Within the framework of a local one-dimensional model, a parametric computer simulation has been carried out of the unsteady heating and mass ablation in the chemical hot spot reaction of the gas-liquid agglomerate of the condensed aluminum oxide phase with a rubberlike thermal protective material under the characteristic conditions of stagnation zones in a high-temperature two-phase medium.

In the interaction of high-temperature two-phase flows with ablating thermal protective materials (TP), the inertially precipitated liquid particles of the condensed phase (k-phase) metal oxides produce a thermal, chemical, and mechanical effect, leading to increased ablation and in some cases to anomalous operating conditions of the energy units. In this case, the mechanisms of drop, hot spot, and film chemical reactions of the liquid particles with degraded TP are of great importance [1]. In [1, 2], the mechanism of the drop chemical reaction has been studied on the basis of a continuous diffusional-kinetic model for the thermochemical destruction of carbon–graphite and carbon–composite TP in a high-temperature two-phase flow containing active oxygen-containing components (H₂O, CO₂, etc.).

This paper deals with the mathematical modeling of the chemical hot spot reaction and evolution of the liquid metal-oxide agglomerate on the surface of charring TP of multilayer walls.

According to the physical model [1], the chemical hot spot reaction results in the formation of large agglomerates ("ingots") of the liquid particles on the surface of charring TP of multilayer walls under the low mass flow rate of inertially precipitated polydisperse liquid particles. At the locations of agglomerate precipitation, local cavities (hot spots) appear, which is typical for the stagnation zones of a high-temperature two-phase flow, where the conduction-radiation heat transfer is the determining factor. The occurrence of the hot spots is associated with an endothermic reduction reaction proceeding between solid carbon and the charred layer of liquid metal oxides under continuous contact between the phases. In the liquid agglomerate, which is gradually increasing in size, the barbotage of the gaseous products formed in the chemical reduction reactions and due to thermal destruction of the organic binder occurs. In this connection, the liquid agglomerate can be treated as a gas-liquid system [4].

The bubble regime of barbotage of the gaseous products through the liquid metal-oxide agglomerate on the surface of the charred layer with a fine-pored structure typical of elevated pressures is considered. In the barbotage, the gas bubble sizes change due to their compression or expansion depending on the pressure and temperature distribution over the thickness of the liquid layer. As a result of convection, the gas bubbles cool the liquid agglomerate. The physical diagram of the chemical hot spot reaction is shown in Fig. 1.
Fig. 1. Physical diagram of the chemical hot spot reaction of the gas-liquid agglomerate on the surface of charring TP of multilayer walls.

Taking into account the complicated physical nature of the hydrodynamic, physicochemical, and heat and mass transfer processes during TP degradation, we introduce the following major assumptions:

1) The two basic assumptions of the mechanics of multiphase mixtures hold true [4]. The liquid agglomerate is treated in the approximation of a two-phase, two-velocity, single-temperature, \((N_g + N_{za} + 1)\) component gas-liquid medium;

2) The problem of the dynamics of chemical hot spot reaction of the gas-liquid agglomerate of the metal oxide particles on the surface of charring TP of multilayer walls is solved in a plane two-dimensional formulation for the stagnation zone of a high-temperature two-phase medium, in which friction, convective heat transfer and diffusion can be neglected;

3) Liquid agglomerate is a complex body of revolution confined between the free surface and the surface of the chemical reaction hot spot that has a time-dependent radius in the equatorial plane. The problem is symmetric about the axis \(x = 0\);

4) We consider the evolution regime of the liquid agglomerate on the surface of charring TP during the precipitation of polydispersed liquid particles distributed previously into a finite number of size fractions. The mass addition of the particles per second exceeds their loss due to the chemical reduction reaction. The mechanical ablation of the agglomerate is lacking;

5) The thermochemical ablation of charring TP proceeds by an overall heterogeneous reduction reaction at the contact between the carbon of the charred layer and the melt, which is described by the following stoichiometric equation:

\[
\nu_C(c.) + \nu_{MeO} MeO(l.) \rightarrow \sum_i \nu_i A_i + \sum_s \nu_s A_s(c.), \quad i = 1, N_{za}, \quad s = 1, N_s,
\]

where \(MeO, A_i, A_s\) are the conventional chemical symbols for metal oxides, and the gaseous and condensed reaction products respectively; \(\nu_C, \nu_{MeO}, \nu_i, \nu_s\) are the stoichiometric coefficients; \(N_{za}, N_s\) is the number of gaseous and condensed components of the reaction;

6) The gas phase in the liquid agglomerate represents an ensemble of bubbles containing a mixture of the gaseous products from the thermal destruction of the organic binder and the chemical reduction reaction;

7) The surface ablation of charring TP in the areas without the agglomerate is lacking;

8) The conditions of an ideal thermal contact between the liquid agglomerate and charring TP, and also between the layers of the plane multilayer wall are met;

9) The heat and mass transfer processes in the charring TP are described in terms of the general laws of conservation for a two-phase, \((N_g + 1)\)-component, single-temperature, isotropic, nondeforming, porous reacting medium [5, 6].

The mathematical modeling of the hydrodynamic, physicochemical, and heat and mass exchange processes of the chemical hot spot reaction of the gas-liquid metal-oxide agglomerate on the surface of charring TP of multilayer walls is carried out in the range \((x, y) \in \Omega, \quad t > 0\), subject to symmetry conditions.