

Thermophysical Properties for Dense Multicomponent High Temperature Media

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Abstract. The investigations of a matter with significant interparticle interaction (a non-ideal matter) are progressing rapidly due to the development of prospective technical projects, combustion and explosion problems modelling. The design of new technology devices and the necessary modeling of high energy density combustion and explosion phenomena assume the knowledge of the thermophysical properties of a high temperature dense matter. These properties include: thermodynamical, transport, optical and rheology characteristics of dense matter. Complete thermodynamic analysis of the thermodynamical model of real non-ideal high temperature matter is provided. The model approaches to the calculation of the total set of non-ideal matter transport coefficients, optical and rheology properties of a matter are discussed. It is discussed, in general, the situation at the Burnett level which can arise in combustion problems. The realization of the models for the determination of thermodynamic properties, the total set transport coefficients, optical and rheology properties of a multicomponent high temperature dense matter as the computer codes complex, calculations of the thermophysical properties of practically important substances and mixtures has permitted one to consider a number of high-temperature topical problems.

The investigations of a matter with significant interparticle interaction (a non-ideal matter) are progressing rapidly due to the development of prospective technical projects, combustion and explosion problems modelling. The examples of such media are discussed, which contain dense neutral gases, neutral and charged liquids (including electrolytes and their solutions), a low temperature plasma with strong particle coupling, high density substances under extreme pressure and temperature and so on. The design of new technology devices and the necessary modeling of high energy density combustion and explosion phenomena assume the knowledge of the thermophysical properties of a high temperature dense matter. These properties include: thermodynamical, transport, optical and rheology characteristics of dense matter. The main difficulty arising in the investigation of non-ideal high temperature media thermophysical properties is connected with the impossibility of a consistent theoretical description of the media present. Because of that, the model approaches based either on the charged (or neutral) fluid theory ideas or on gas plasma theory together with existing experimental information are of special importance. It is expedient to use the results on one and two-component Coulomb and neutral systems as theoretical asymptotics in the derivation of a model. The theory of the thermophysical properties of Coulomb systems with strong interparticle coupling is considered.

Thermodynamic functions and equation of state of the system are studied. There are two approaches commonly used for determination of the high temperature media thermophysical properties. The approaches are named as the physical and chemical models. The more customary chemical model is considered in the most cases. This model beforehand assumes the presence of the certain types of the particles which have a continuous energy spectrum and interact under definite laws. The influence of the inner structure of the particles (bounded states) on the thermodynamic functions of a matter is accounted by the individual partition functions of the particles. This circumstance along with the postulating of the lowest of interparticle interactions are the sources of the difficulties connected with the convention of the boundary which divides the particle energy spectrum into the discrete and continuous parts. In practice, the different definitions of the individual particle partition functions, which

correspond to their discrete spectrum, are introduced on the base of some physical assumptions. The thermodynamic analysis of a high temperature dense media may be conditionally subdivided into two parts. First, the full set of thermodynamic functions calculations are made under presumed temperature, pressure, and shares of the chemical elements, which consist the matter. Besides, the thermodynamic stability of a matter should be investigated. Second, the calculation of certain important auxiliary quantities, such as the system composition, different shares of subsystems (free electrons and ions, atoms, molecules etc.) are carried out within the framework of the chemical model of a matter. The existing approximate methods for the calculation of the thermophysical properties of high temperature dense media are founded on the utilization of the auxiliary quantities.

The physical kinetics of high temperature dense media is considered using the chemical model of the dense media. The kinetic description of a real medium may in most events be of only model nature which bases on the theory of more simple systems. The problem of the determination of the total set of transport coefficients for the chemically reacting high temperature dense media is considered. The set contains viscosity coefficients, thermoconductivity, multicomponent diffusion and thermodiffusion coefficients, electrical conductivity and thermoelectric power which determine fluxes of momentum, heat, mass and charge in the present medium. The model approach to the calculation of the total set of transport coefficients of the media is discussed based on the analysis of existing experimental data for various substances and accounting for the results of theory of kinetic equations for a weakly non-ideal media and the theory of linear response for Coulomb and neutral systems with strong interparticle coupling. The linear response theory (LRT) which is used in the report is valid for media with arbitrary interparticle coupling. The effective transport coefficients are introduced which connect chemical elements mass fluxes and convective heat flux with gradients of temperature, mass concentrations of chemical elements, electric field in a matter. Using the effective transport coefficients significantly simplifies the description of transport processes in the local thermodynamic equilibrium approximation if the number of components is greater than the number of chemical elements composing the matter. The examples of calculations of transport coefficients are presented and compared with experimental data. The scheme of calculating effective transport coefficients propounded in the report is sufficiently complicated, that the general restrictions on the nonlinear non-diagonal matrix of effective coefficients are studied for verification of numerical values of effective transport coefficients. The properties of the present matrix (and the matrix connected with it at major derivatives in the system of conservation equations for media with strong interparticle coupling) are also important in using a complete set of effective transport coefficients and thermodynamics characteristics in high-temperature combustion and explosion problems. It is discussed, in general, the situation at the Burnett level which can arise in combustion problems.

The determination of the spectral absorption coefficient for some high temperature substances is considered in detail. This coefficient is necessary for calculation of the radiation field in a matter by the equation of radiant energy transfer. It is noted that interparticle interactions especially affect the optical properties of high temperature dense matter. Report contains also the approach to the determination of the reflection and absorption coefficients of electromagnetic radiation and the power of radiation scattered by a Coulomb system with strong interparticle interactions. This approach is based on using exact frequency moments of a response function and time correlation functions of Coulomb system which are used for the calculation of mentioned optical characteristics. The frequency moments are essentially the thermodynamic characteristics of Coulomb systems, the comparative analysis of the frequency moments is performed. Thus, the detailed comparative analysis of thermodynamic, transport and optical characteristics of Coulomb systems are performed. LRT methods has permitted us to reveal the set of exact correlations between present characteristics.

The realization of the models for the determination of thermodynamic properties, the total set transport coefficients, optical and rheology properties of a multicomponent high temperature dense matter as the computer codes complex, calculations of the thermophysical properties of practically important substances and mixtures has permitted one to consider a number of high-temperature topical problems. The heat and mass transfer characteristics at hypersonic flow around a space probe in atmospheres of the planets are investigated. The interaction of the main physical processes within a shock layer matter between separated shock wave and the surface of the probe are consistently accounted for in the estimation of convective and radiant heat current at the probe. The processes mentioned are: the injection of thermal protection coating into a shock layer under action of the intensive heat fluxes, radiant and convective heat transfer through a shock layer to the probe surface and the multicomponent character of diffusive mixing matter components in the shock layer. The approach associated with the introduction of effective transport coefficients is utilized in the present problem. The heating regimes of the space probe heat protection were studied by computer experiments. Besides, the critical phenomena in the high temperature dense matter during rest and in motion are studied. The interaction of multicomponent diffusion and volume heat sources in the gas phase nuclear reactor fuel element (thermodiffusion instability) and the phenomenon of "hydrodynamic explosion" in the low temperature plasma with a strong dependency of viscosity and thermal conductivity coefficients on temperature are investigated.