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14. ABSTRACT
Three major objectives of the basic research grant have been met. First, a physic based chemical kinetic model for high-temperature gas is developed and verified by comparing with data from the RAM-C-II probe and the Stardust sample return capsule. In the absence of an externally applied electromagnetic field, the Lorentz force and Joule heating in the globally neutral ionized gas is insignificant. Meanwhile the energy transfer from the translation and vibration degrees of freedom to electronic excitation is found to be negligible and the energy exchange is dominated by the chemical process for conductive-convective heat transfer. A simplified and more efficient energy conservation formulation has been verified against the published results of the fastest reentry objective – Stardust capsule. Second, a multi-spectral group approach for simulating nonequilibrium radiation heat transfer is accomplished. Accurate simulation for axisymmetric and three-dimensional configuration using the half-moment method and tracing technique for solving the nonequilibrium radiation intensity equations. The numerical result not only generates equally accurate prediction from the NASA ST centers, but also reveals for the first time the radiation frequency shift phenomenon. Third, in analyzing radiative heat transfer for thermal protection, a rigorous interface boundary condition for the ablating material has been derived via the Reynolds' transportation theorem. The basic formation explicitly includes the surface ablation and recession rate as well as the stress component for evaluation.

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Thermo-chemical phenomena Simulation for Ablation

AFOSR GRANT FA9550-08-1-0361

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Ablation is a multi-disciplinary phenomenon of thermo-chemical in nonequlibrium state. The dominant and the least understand problems for ablating simulation are the nonequilibrium chemical kinetics, energy cascading between the internal degrees of freedom of gaseous medium, radiative energy propagation, and the interaction of high-temperature gas and ablating material [1-4]. For an effective and productive basic research endeavor, a fewer selected and highly focused areas become mandatory. Therefore, three major objectives of the present research grant have been identified as stipulated in the original proposal.

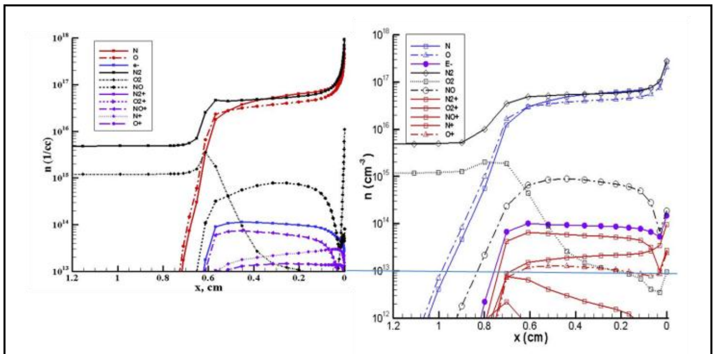

Figure 1. Comparison of nonequilbrium chemical composition along stagnation streamline with/without electronic energy conservation equation

First, it has found by the present effort that in the absence of an externally applied electromagnetic field, the Lorentz force and Joule heating of the globally neutral ionized gas are insignificant at the reentry speed up to 12 km/s [4-6]. Through a direct comparison of the kinetic models of Park [7] and Treanor et al [8], the relaxation rate among the translation and vibration internal degrees of excitations is also found to be rather insensitive to dissociation. All observations indicate energy exchange between internal degrees of freedom to electronic state is still dominated by the chemical kinetic process up to the environment of the Stardust capsule reentry [6-8]. This observation can also be made by the comparison nonequlibrium chemical composition along the stagnation streamline of the RAM-C-II probe in Figure 1. It has been shown the energy transfer between the electronic excitation and lower energy modes has a limited effect to conductive and convective heat transfer [4].

The most meaningful evaluation for the different kinetic models of the nonequilbrium hypersonic flow past the RAM-C-II is directly comparing the electron number density measurements adjacent to the vehicle surface [4]. These flight data were collected by two different devices, the major portion of data was collected by a four-frequency microwave reflector near the forebody of the vehicle. A single measurement at the last data collecting location was made by using an iridium electrostatic probe which has a different data scattering band than the rest of the measurements. The direct comparison with benchmark computations by Candler et al, Josyula et al and the flight data by Jones [4,5] is displayed in Figure 2. It is seen that all computational results using the rational kinetic gas models yield compatible agreement with the flight test data.

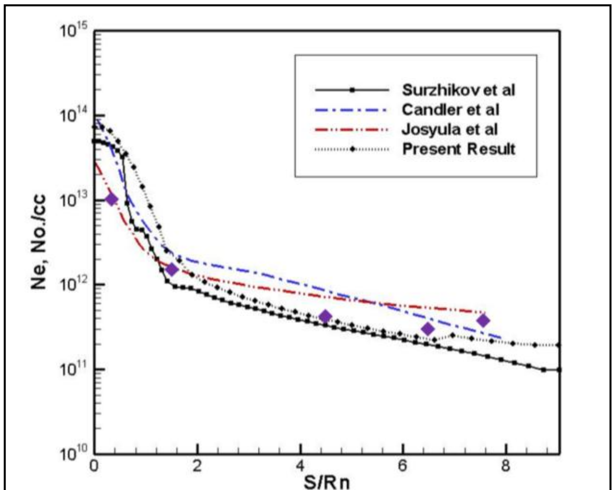

Figure 2. Comparison of electron number density profilesat RAM-C-II surface (Alt=71.0 km)

The simplified chemical kinetics model for conductive-convective heat transfer model has shown an equally accurate prediction in comparison with the established procedures of the NASA S&T centers for thermal protection [5,9-12] but at a 27% computational resource saving. The additional evaluation for the different nonequilibrium kinetic models of hypersonic flow past the RAM-C-II probe and Stardust Sample Return Capsule has convincingly illustrated by directly comparing the chemical composition in the shock layer and convective heat transfer rates with simulated results in open literature [4-6].

In the hypersonic reentry environment, radiation heat transfer contributes a substantial amount of energy transfer in addition to the conductive and diffusive processes. In fact, at the maximum heat loading condition for the Stardust reentry, the radiation heat transfer rate is 120 w/cm^2 versus the convective-conductive heat transfer rate of 1,100 w/cm^2 [1,2]. Therefore it is critically important to understand the basic mechanism and to develop an accurate and efficient predictive method. The high-temperature gas mixture in shock layers and wakes of entering space vehicles contain optically active components as CO_2, H_2O, N_2, O_2, NO, N_2^+, C_2, CO, etc. The radiative heat transfer computation requires not only predicting the spectral radiation fluxes on the vehicle surface but also inside the radiating volume bounded by the bow shock.

The energy exchanging mechanism of radiative heat transfer is fundamentally different from the convective or conductive process. For thermal radiation, it’s a phenomenon associated with any quantum transition of molecule and electronic transition in atom which has a spectrum from the far infra-red (25~1000μm) to near ultra-violet (0.4~0.7μm). Therefore, the electronic excitation is not ignorable in radiative calculation as that in convective-conductive heat transfer simulation [13,14].

According to astrophysics, all electronic transitions can be divided by into bound-bound, bound-free, and free-free groups via the continuity criterion or the discreteness of the energy spectrum of the initial and final quantum of atom or molecule [7,13]. In high-temperature air, the most important optical activity molecules are well known and they are; the transitions for O_2 (Schumann-Runge; $B^3\Sigma_g^- \rightarrow X^3\Sigma_g^-$), N_2 (2nd positive; $C^3\Pi_u \rightarrow B^3\Pi_g$, and 1st Positive; $B^3\Pi_g \rightarrow A^3\Sigma_u^+$, NO (β-band; $B^2\Pi \rightarrow X^2\Pi$, γ-band; $A^2\Sigma^+ \rightarrow X^2\Pi$), N_2^+ (1st negative; $B^3\Sigma_u^- \rightarrow X^2\Sigma_g^+$), and O_2^+ (1st negative; $b^4\Sigma_g^- \rightarrow a^4\Pi_u$). When the hypersonic reentry phenomenon involves carbonaceous ablating surface, at least six additional optically active species such as the C2, $C2^-$, $C2^+$, CN, CO, CO^+ add to a substantial amount of complexity to the electronic bands to be included into radiative heat transfer analysis [9-12]. According to the work by Laux et al [16,17], for blunt body with a reentry speed around 10 km/s and the strong absorption by C and CO has been detected in the vacuum ultraviolet (80 -200 nm) and ultraviolet spectra. The emission of cyanide (CN) has also been noted, as well as, a low intensity absorption by CO_2 within the boundary layer. In all, the nonequilibrium radiation is responsible for 26% of the total radiation flux in the spectra of 80-600 nm. Some of these transition processes are not fully understood but become critical mechanisms for the radiative heat transfer process [1-7,16,17].

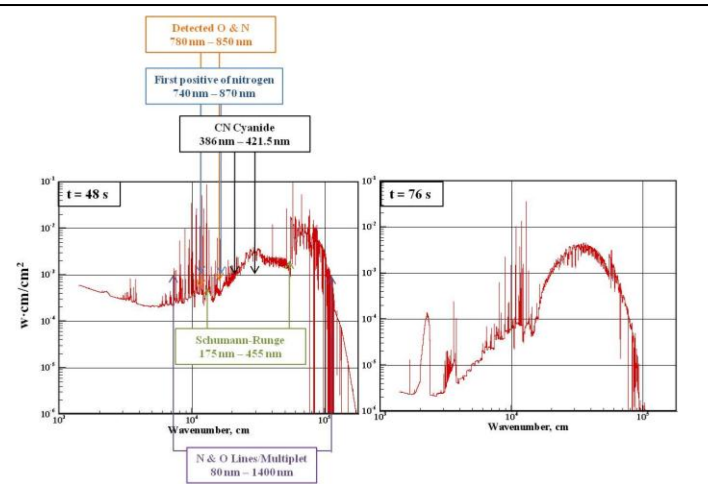

Figure 3. Radiative frequency shift of Stardust sample return capsule from the early to the later stages of reentry

An incisive investigation is being conducted for the radiative heat transfer, which is fundamentally different from the conductive-convective process [13,14]. The intensity of emission and absorption of radiation is controlled by the electronic excited state and the binding energy of the species. However in this process, the emission and absorption is limited in intensity and confined to the infrared spectrum [13]. The high-temperature gas mixture during the earth reentry usually is electronic excited, both the discrete and continuous radiative processes in energy spectrum occurred. Under this circumstance, the radiation energy transfer to Stardust capsule reentry has the wide spectra from infrared to vacuum ultraviolet [13,14]. The computation for radiation heat transfer is based on multi-group model in a given spectrum. Within the divided bandwidth of each spectral group, the averaged absorption coefficients are used including the wide-band and narrow-band models of a spectrum, or by the Line-by-line integration over the full spectrum [14,16,17]. The equation of radiation intensity is solved in the divided band with frequency-independent spectral coefficients of emission and absorption. The overall absorptivity and emissivity of the full spectral range is determined by summing over all the averaged values of these individual bands. As expected, the physical fidelity can be improved but at the expense of computational efficiency with an increasing number of spectral groups considered. In Figure 3, the computational result reveals for the first time that during the Stardust reentry that the frequency shifts of the maximal radiative intensity during the reentry from the visible to near infrared region. This behavior can be explained by the Wien' law [13] and has been confirmed by a removal observation location from the stagnation point of the reentering capsule [15].

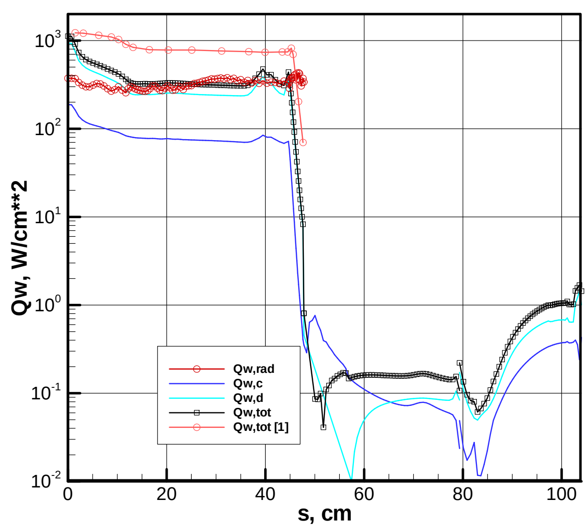

Figure 4. Contributions from conductive, diffusive, and radiative heat transfer and comparison of the total rate with results of Olynick et al [1]

The assessment of numerical resolution for a complex physical phenomenon is extremely challenged. In the present computational simulation, numerical accuracy is controlled by established a uniformly enforced convergent criterion for all dependent variables to the relative error of 10^{-5} and by a series of study on grid topology. The comparison of the peaking heat transfer rate with results in literature becomes ultimate assessment of the research achievement. Figure 4 shows the distribution of all heat fluxes on the surface in the plane of symmetry of the Stardust spacecraft, including conductive, diffusion, and radiative components. The combined conductive and diffusive heat transfer rates yield a value of 1.19×10^3 w/cm^2 at the stagnation point of the capsule. The present total heat transfer rate without active ablation, is in a very good agreement with the results by Olynick et al [1] of 1.2×10^3 w/cm^2 and agrees equally well with the laminar flow result of Park [2] at 1.189×10^3/cm^2. The radiative heat transfer rate over the forebody also reveals a comparable value of 248 w/cm^2 with the results by Olynick et al and by Park. The good agreements by comparison ensure that the thermodynamic states and composition of all pertaining chemical species have duplicated the chemical-physical phenomena for radiative heat exchange evaluation.

The third contribution of the present research grant is the derivation of interface boundary conditions for the ablating surface by the rigorous Reynolds transportation theorem. In the past, the majority of research efforts have been concentrated on the interface boundary conditions either from physical observations or by some insights [1-3,9-12]. These rigorous interface conditions are summarized as follows;

For species conservation equations;

$$[\rho_+ c_{i+}(\vec{u}_+ + \vec{u}_{+i} - u_{b+}) - \rho_- c_{i-}(\vec{u}_- + \vec{u}_{-i} - u_{b-})]\cdot n_+ A = \lim_{v\to 0}[\iiint \dot{w}_i dV - \frac{d}{dt}\iiint \rho c_i dV] \to 0.$$

For momentum conservation equation;

$$[\rho_+ \vec{u}_+(\vec{u}_+ - \vec{u}_{b+}) - \rho_- \vec{u}_-(\vec{u}_- - \vec{u}_{b-}) - (\tilde{\sigma}_+ - \tilde{\sigma}_-)]\cdot n_+ A = \lim_{v\to 0}[\iiint \rho \sum_{i=1}^{n} c_i \vec{f}_i dV - \frac{d}{dt}\iiint \rho \vec{u} dV] \to 0.$$

For internal energy conservation equation;

$$[\rho_+ e_+(\vec{u}_+ - \vec{u}_{b+}) - \rho_- e_-(\vec{u}_- - \vec{u}_{b-}) + \vec{q}_+ - \vec{q}_- - \vec{u}_+ \cdot \tilde{\sigma}_+ + \vec{u}_- \cdot \tilde{\sigma}_-]\cdot n_+ A$$

$$= \lim_{v\to 0}[\iiint \dot{q} dV + \iiint \rho \sum_{i=1}^{n} c_i \vec{f}_i \cdot (\vec{u} + \vec{u}_i) dV - \frac{d}{dt}\iiint \rho e dV] \to 0.$$

In the above equations, the subscript symbols + and – denote the variables evaluated above or beneath the ablating interface, thus separate the required descriptions for the non-equilibrium gas from the ablator. The velocity of the recessing surface is indicated as u_b which is permitted to vary from point to point on the control surface. In this formulation, the ejection velocity of pyrolysis gas and the release vapor rate of the sublimated material on the ablating surface are required. Therefore the detailed of gaseous motion through the porous ablating material is relegated to the research results of ablative material. The heat transfer term q accommodates the heat flux by conduction, convection, as well as, radiation transfer according to the energy conservation equation, equations [4-6,16,17]. Finally, the normal stress component is designated as $\tilde{\sigma}$ and it's the only tensoral stress component that can contribute to the work done by the gas media; the non-equilibrium gas, sublimating vapor, and pyrolysis gas of the ablating material.

The formulation is derived from the structure of the governing equations and has the direct link to the eigenvector of the partial differential equations system. This result intends to show these interface boundary conditions are much more complex for an ablating surface in the existing literatures. Addition efforts are still required as how these conditions can be implemented and ensured to maintain the computational stability.

The first attempt by simulating the fastest man-make object - Stardust sample return capsule in three-dimensional earth reentry has also been achieved by the present research grant. In Figure 5, the three-dimensional result at eight-degree of angle of attack exhibits a significant 3-D relief effect which has not been resolved by all known previous investigations [17]. The pressure contour and the surface shear stress vector trace are present together; the post-shock expansion at the angle of attack condition is spreading into a very large lower pressure sector from the stagnation region indicating by the surface shear flow direction and the pressure contour. At an angle of attack, a rapid expansion immediately downstream to the bow shock of the three-dimensional flow is not constrained only in the downstream planar surface like that of the axisymmetric flows [1,2,4]. However, it's important to observe that the effect of ablating surface indicates a reduced heat load to the capsule can be as high as 35 percent at the peak heating condition [1]. In short, the total heat transfer rate for capsule by the present effort is in a very good agreement with the results by Olynick et al [1] and Park [2] including the radiative heat transfer rate.

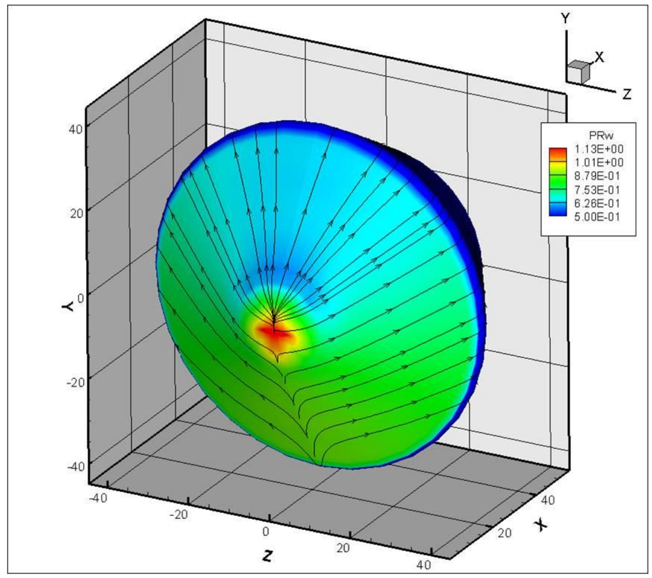

Figure 5. Pressure contour and surface shear stress trace on frontal surface of Stardust capsule at peak heating condition

In addition, the radiative heat transfer drops sharply at the juncture of the forebody and afterbody of the capsule like that of the convective heat transfer process. At the same instance, the diffusive heating in the wake region begins to rise through energy cascading from vibrational excitation and chemical species recombination as the nonequilibrium flow leaving the computational domain. The present efforts through in-depth research and incisive interpretation of research findings contribute to the basic understanding of nonequilibrium hypersonic flow.

Acknowledgment/Disclaimer

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Personnel Support during Duration of Grant

Shang, J.S.	Research Professor, Wright State University, Dayton OH
Huang, P.G.	Professor & Chair, Wright State University, Dayton OH
Surzhikov, Sergey	Visiting Professor, Russian Academy of Science, Moscow Russia
Fabio, Roveda	Visiting Scholar, Bologna University, Italy
Barnes, Caleb	Graduate student, Wright State University, Dayton OH
Evans, James	Student, Wright State University, Dayton OH

Publications

A total of 33 public releases documents have been produced during the performance period of the present research grant, including nine (9) archival journal publications and two (2) invited keynote speeches.

1. Shang, J.S., Huang, P.G., Yan, H., and Surzhikov, S.T., Electrodynamics of Direct Current Discharge, AIAA 2008-1101, Reno NV, January 2008.

2. Surzhikov, S.T. and Shang, J.S., Kinetic Models Analysis for Super-Orbital Aerophysics, AIAA 2008-1278, Reno NV, January 2008.

3. Shang, J.S., Surface Direct Current Discharge for Hypersonic Flow Control, AIAA 2008-1352, Reno NV, January 2008.

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Honors & Awards Received

USAF Basic Research Award, 1986
Fellow of AIAA, 1993
Outstanding and Exception Civilian Service Awards, 2001
AIAA Plasmadynamics and Laser Award, 2004
Keynote Speaker, 16th CFD Conference of Taiwan, 2009
Keynote Speaker, 17th International Conference on MHD Energy Conversion, 2009

AFRL Point of Contact

Dr. Donald B. Paul, AFRL/RB WPAFB, OH 937-255-7329, met weekly.
Dr. Richard Rivir, AFRL/RZ WPAFB, OH 937-255-2246, interacted monthly and actively participated in Window in Science Seminars.
Dr. Roger Kimmel, AFRL/RBAA WPAFB, OH 937-255-8295, interacted weekly.
Dr. Datta V. Gaitonde, AFRL/RBAC WPAFB, OH 937-904-4031, interacted weekly until he left for Ohio State University in September 2010.
Mr. Michael Zeigler, AFRL/RBAI WPAFB, OH 937-656-6307, interacted and met weekly.
Dr. Biswa Ganguly, AFRL/RZ WPAFB, OH 937-255-6782

Transitions

The objective of the present grant is to develop a numerically efficient and physically accurate modeling and simulation capability for non-equilibrium ablation phenomenon of earth reentry. Therefore, technical transitions are focused on the research result dissimilation to research scientists of AFRL and national/international conferences of professional societies and follow up through personal interaction. In order to keep abreast with the state-of-the-art progression, an active participation and productive contribution has been maintained with the Joint National Hypersonic Science Center (NHSC) Program by USAF and NASA.

A productive interaction has been maintained with Dr. Roger Kimmel of the Air Vehicles Directorate, Air Force Research Laboratory (AFRL/RBA, 937-255-8295) for the UASF HiFire Program. Collaboration and knowledge sharing interaction on the kinetic models research for nonequlibrium high-temperature gas has consistently been maintained with Dr. D. Gaitonde (937-904-4031) and Mr. E. Josyula (937-904-4044) of AFRL/RBAC.

The concept and potential practical applications of the Gaussian quadrature for local numerical resolution refinement in an isolated high-gradient domain has been regularly exchanged with Dr. M. Roquemore of the Propulsion and Power Directorate of Air Force Research Laboratory (AFRL/RZ), as well as, Dr. Y. Liu and Dr. T. Pulliam of the NASA Ames Research Center.

The new model and computational simulation for plasma micro jet for enhancing ignition and combustion stability has also conveyed to Dr. Biswa Ganguly; an agreement of mutual support for plasma assisted ignition and enhanced combustion stability has been reached in 2010. The present project will provide a direct technical support to the Center of Advanced Power and Energy Conversion of the joint Wright State University and Air Force Research Laboratory (AFRL/RZPE 937-255-6782).

Basic research accomplishment in high-temperature gas kinetic modeling has received attention from NATO nations. A visiting scholar, Fabio Roveda of Bologna University, Italy joined the research team on April 28, 2010 for a period of nine months. His visit with us is fully funded by the Italy government.

New Discoveries

None.