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BOOST-PHASE DISCRIMINATION RESEARCH ACTIVITIES

FINAL REPORT

DAVID M. COOPER
GEORGE S. DEIWERT

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MOFFETT FIELD, CA 94035

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19. ABSTRACT (Continue on reverse if necessary and identify by block number) Theoretical research in Aerothermodynamics and Computational Chemistry has been performed. The Aerothermodynamics research focused on the hard-body and rocket plume flows. Analytical real gas models to describe finite rate chemistry were developed and incorporated into the three-dimensional flow codes. New numerical algorithms capable of treating multi-species reacting gas equations and treating flows with large gradients were also developed. The Computational Chemistry research focused on the determination of spectral radiative intensity factors, transport properties and reaction rates. Ab-initio solutions to the Schrodinger equation provided potential energy curves transition moments (radiative probabilities and strengths) and potential energy surfaces. These surfaces were then coupled with classical particle reactive trajectories to compute reaction cross-sections and rates.			
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BOOST-PHASE DISCRIMINATION RESEARCH ACTIVITIES

David M. Cooper
George S. Deiwert

NASA Ames Research Center
Moffett Field, CA 94035
(415) 694-6213

In a multi-tiered ballistic missile defense (BMD) system, the boost-phase is highly leveraged because of the greater effectiveness of a single kill. In order to increase the effectiveness of a BMD, it is therefore of extreme importance to understand in detail the observable phenomena associated with a booster and any methods by which boosters might be more quickly and confidently recognized, tracked, and ultimately destroyed. The objective of this task was to assist in this detailed understanding by 1.) developing computer codes capable of simulating flow fields around hard-bodies as well as the flow within and around rocket plumes; and 2.) providing the atomic and molecular chemistry database necessary to accurately predict the properties (including radiative intensity signals of these hot interacting flow fields.

Theoretical research in Aerothermodynamics and Computational Chemistry was performed. The Aerothermodynamics research concentrated on developing the capability to simulate the combined hard-body flow-field and exhaust plume rocket-propelled missiles. This involved the development of appropriate two- and three-dimensional flow solvers coupled with realistic chemistry models for these hard-body configurations with propulsive plumes. The coupling of proper chemistry models with a reliable flow solver allows an accurate assessment of the importance of flow-field fluid dynamics on the distribution of chemical species, their temperatures and thereby the radiation signatures. The efforts of this part of the study were aimed at these two aspects.

Nozzle/plume flow codes which simulate flow past the hard-body and include fully coupled interaction between the plume and external flow field, have been developed and applied to the altitude flight regime and speeds of interest for boost phase detection studies. The codes treated both equilibrium and perfect air for fully three dimensional configurations (1-3), and chemically reacting hydrogen-air mixtures for axisymmetric flows (4). A three-dimensional adaptive grid capability was developed (5) which permitted efficient and accurate flow-field simulations. These simulations were performed for a Titan 2nd stage configuration for altitudes up to 60 km and nozzle-to-free-stream pressure ratios of several thousand. The effect of altitude, pressure ratio and hard-body interaction on the fluid dynamic aspects of the plume flow-field (temperature, structure, etc.) have been assessed.

In addition to these studies, a non-equilibrium radiation code (NEQAIR) (6) was enhanced to treat arbitrary gaseous mixtures, including hydrogen and carbonaceous species, to provide detailed spectral resolution from the vacuum UV to the far IR wavelengths, and to include the effects of self-absorption. This code was, in turn, used to identify the spectral signature in the nose stagnation region of missile hard-body (7) as predicted by a new two-dimensional flow code (8,9) for air

in thermo-chemical non-equilibrium. These highly successful studies were performed beyond the initial scope of the proposed research.

The Computational Chemistry research focused on determining the atomic and molecular database necessary to compute the hot flow-fields around vehicles traveling at all speeds and the flow in and around rocket plumes at any altitude of interest. The database generated during this task includes real gas properties for both high and low density flows under equilibrium and non-equilibrium conditions and focused on the following areas:

1. Data required to predict both the equilibrium and non-equilibrium spectral radiative intensity for wavelengths between the UV and near IR;
2. Data required as inputs for the Navier-Stokes equations, Monte Carlo and Molecular Dynamics methods to solve for the vehicle and plume flow-fields. This data included transport properties, collision cross-sections, and reaction rate cross-sections.

Radiative transition probabilities have been determined for the First Positive, Second Positive, Wu-Benesch, and Infrared systems of N_2 , the First Negative, Second Negative, and Meinel Systems of N_2^+ , the Beta, Delta, and Gamma systems of NO, and the First Negative and Second Negative systems of O_2^+ (10). Results have also been obtained on systems of OH, AlO, ZrO, HCl, AlBr, AlH, AlF, and AlCl.

Reaction rate constants for the following reactions involving air species have been calculated and compared with experimental data (10):

1. $N_2 + O \rightarrow NO + N$
2. $O_2 + N \rightarrow NO + O$
3. $NO + N \rightarrow N_2 + O$
4. $NO + O \rightarrow O_2 + N$

Potential energy curves and collision integrals have been calculated for ground state interactions of N-N, O-O, N-O⁺, N-N⁺, and O-O⁺. All nine of the collision integrals needed to determine transport properties to second order have been calculated and tabulated for translational temperatures from 250 to 100,000 K. Plots summarizing the calculated potential energy curves and transport properties are given in publication 10.

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PERSONNEL:

Dr. David M. Cooper
Dr. George S. Deiwert
Dr. Richard L. Jaffe
Dr. Stephen R. Langhoff
Dr. Harry Partridge III
Dr. William J. Feiereisen
Dr. Ethiraj Venkatapathy
Dr. Chul Park
Dr. Graham Candler
Dr. Seung-Ho Lee
Dr. M. Jahed Djomehri
Mr. James Stallcop
Mr. Eugene Levin

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