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Review: Modelling chemical kinetics and convective heating in giant planet entries

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ABSTRACT

A review of the existing chemical kinetics models for H_2/He mixtures and related transport and thermodynamic properties is presented as a pre-requisite towards the development of innovative models based on the state-to-state approach. A survey of the available results obtained during the mission preparation and post-flight analyses of the Galileo mission has been undertaken and a computational matrix has been derived. Different chemical kinetics schemes for hydrogen/helium mixtures have been applied to numerical simulations of the selected points along the entry trajectory. First, a reacting scheme, based on literature data, has been set up for computing the flow-field around the probe at high altitude and comparisons with existing numerical predictions are performed. Then, a macroscopic model derived from a state-to-state model has been constructed and incorporated into a CFD code. Comparisons with existing numerical results from the literature have been performed as well as cross-check comparisons between the predictions provided by the different models in order to evaluate the potential of innovative chemical kinetics models based on the state-to-state approach.

1. Introduction

A review is presented of the literature of hypersonic flows in H_2/He mixtures. Many studies are devoted to understand the behaviour of the Galileo probe during its high speed entry into Jupiter's atmosphere. The lessons learnt, however, have bear on other mission scenarios such as entry into other giant planets (Saturn, Uranus, Neptune) that are listed among the highest-priority science goals for planetary exploration in the decade 2013–2022 [1]. In support of these efforts, strong shock waves have been studied in experimental facilities on ground and many studies have been devoted to their understanding.

A review of the available results obtained during the mission preparation and post-flight analyses has been undertaken to select a computational matrix for the numerical simulations. Preliminary calculations of points along the Galileo entry trajectory have been carried out with state-of-the-art models [2] and comparisons with existing numerical predictions performed [3,4]. As an outcome of the literature review, a new transport model for hydrogen/helium mixtures at high temperature has been integrated in the CFD code TINA [5].

In parallel to the CFD efforts, a state-to-state model for hydrogen/helium mixtures has been developed and a macroscopic reaction scheme suitable for CFD calculations derived [6]. This macroscopic model has been incorporated into TINA and applied to Galileo entry and the results cross-checked with other numerical data from the literature or obtained with different modelling.

The focus of this study is on models for chemical reaction schemes and transport properties relevant to flow-field calculations of Jovian entries, and their impact on the predictions of species distribution and convective heating. Key issues such as radiation and ablation have not been targeted even if they are driving parameters for sizing planetary probe heat shields for entry into giant planet atmospheres.

The paper is organized as follows: sec. 2 reviews the available literature data obtained from shock tube experiments, flight experiments and from numerical calculations; sec. 3 discusses modelling approaches and input data related to the description of thermodynamic, transport and chemical kinetic phenomena in these flows; sec. 4 describes the computational framework used to perform the calculations presented in sec. 5.

2. Available data

2.1. Shock tube data

Among the first to deal with the chemical kinetics of hydrogen/he-

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Nomenclature

Symbols

A	Constant in Arrhenius formulation of reaction rate constant, $cm^3/mol/s$
a_i, b_i, c_i	Blottner coefficients of single species viscosities
$Alt.$	Altitude, km
b	Temperature exponent in Arrhenius formulation of reaction rate constant
B_i	Coefficients for the calculation of the equilibrium constant
E_f/R	Activation temperature in Arrhenius formulation of reaction rate constant, K
k_b	Backward reaction rate constant
k_f	Forward reaction rate constant, $cm^3/mol/s$
K_{eq}	Equilibrium constant
P	Pressure, Pa
Q	Heat flux, MW/m^2
R	Perfect gas constant, J/K
R_n	Nose radius, m
s	Curvilinear abscissa, m
Sc	Schmidt number
T	Temperature, K
T_e	Free electron temperature, K
V	Velocity, km/s

Greek symbols

μ	Shear viscosity, kg/m
ρ	Mass density, kg/m^3

Subscripts

a	Temperature index, can be t, v or e
eq	Equilibrium
i	Species index
t	Translational
v	Vibrational

Acronyms

ARAD	Analog Resistance Ablation Detector
BL	Boundary layer
CEA	Chemical Equilibrium with Application
CFD	Computational Fluid Dynamics
CFL	Courant-Friedrichs-Lewy
CR	Collisional Radiative
DSMC	Direct Simulation Monte Carlo
EAST	Electric Arc Shock Tube
ESA	European Space Agency
ESTEC	European Space Research and Technology Center
NASA	National Aeronautics and Space Administration
NIR	Near InfraRed
NIST	National Institute of Standards and Technology
PES	Potential Energy Surface
QCT	Quasi-Classical Trajectory
QSS	Quasi Steady State
TPS	Thermal Protection System
VRT	Vibrational Rotational Translational
VSL	Viscous shock-layer
VUV	Vacuum UltraViolet

lium mixtures and therefore atmospheric entry into giant planets, Leibowitz [7] performed experiments in an electric arc driven shock tube with H_2/He mixtures, exploring the range of shock velocities from 13 to 20 km/s. Temporal profiles were obtained for H_β lines and continuum emission. The measurements were interpreted with a kinetic scheme including hydrogen dissociation and a two-step excitation-ionisation mechanism for atomic hydrogen ionisation by atom-atom and electron-atom collisions. In particular, excitation by atom collision was found to govern the ionisation induction time, and excitation by electron collision the relaxation to thermal equilibrium between heavy particles and electrons (ionisation relaxation time). Recommended expressions for the rate constants of the atom excitation processes were then obtained that give the best agreement with the measurements [7,8].

Similar experiments were performed in a mixture richer in H_2 with shock speeds from 26 to 46 km/s [9]. Equilibrium electron densities and ionisation relaxation distances were measured from the Stark broadening of H_β lines and from holographic interferometry.

These two old experiments still represent a significant benchmark for the validation of theoretical models.

Very recently, new shock tube experiments have been carried out at the Electric Arc Shock Tube (EAST) at NASA Ames Research Center [10]. Shock waves with velocities from 20 to 30 km/s were investigated by measuring temporal profiles of the spectral emission radiance in four spectral ranges from the VUV to the NIR; temporal profiles of electron densities were also obtained from Stark analysis of high-resolution Balmer-α line. Quantitative rebuilding of these experimental data, though, remains difficult [11].

2.2. Flight data

Galileo was an unmanned spacecraft sent by NASA to study the planet Jupiter and its moons. It was launched on October 18, 1989. The Galileo Atmospheric Entry Probe arrived in Jupiter's atmosphere on December 7, 1995. The probe descended through 150 km of the top layers of the atmosphere, it collected 58 min of data on the local weather and only stopped transmitting when ambient pressure exceeded 23 atm.

The Galileo Probe shape was a sphere-cone with 22.2 cm nose radius and 44.86 deg cone-half-angle (Fig. 1). The mass of the atmospheric

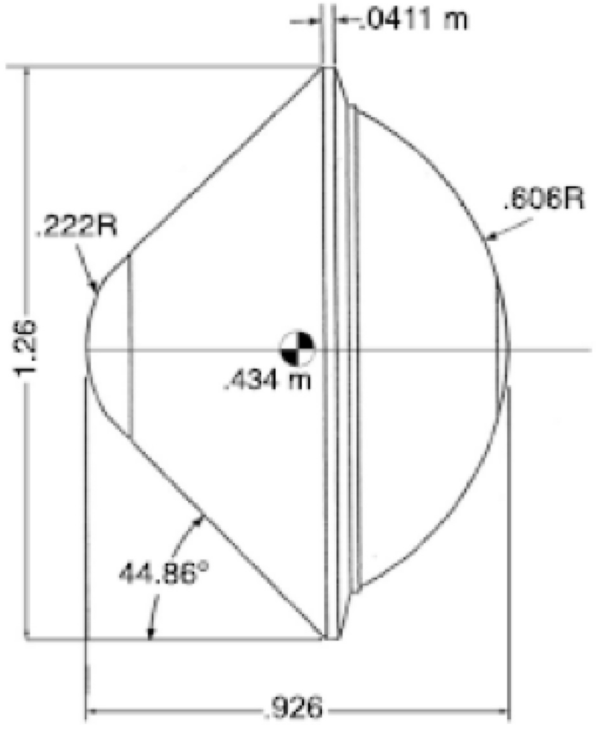

Fig. 1. Scheme of Galileo probe [12].