SACOMAR
Technologies for Safe and Controlled Martian Entry

SPA.2010.3.2-04

EU-Russia Cooperation for Strengthening Space Foundations (SICA)

Re-entry Technologies and Tools

Theme 9 - Space
Activity 9.3 - Cross-Cutting-Activities
Area 9.3.2 - International Cooperation

Deliverable Reference Number: D 4.1
Deliverable Title:

Requirements on Modelling and Simulation

Due date of deliverable: 21st April 2011

Actual submission date: 30th April 2011 (issue 1.0), 30th November 2011 (issue 1.1)

Start date of project: 20th January 2011

Duration: 18 months

Organisation name of lead contractor for this deliverable: TAS-I

Revision #: 1

Project co-funded by the European Commission within the Sixth Framework Programme		
Dissemination Level		
PU	Public	X
PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	

APPROVAL

Title	issue	revision
Requirements on Modelling and Simulation	1	1

Author(s)	date
V. Mareschi	

Approved by	date
C. Chiarelli / E. Gaia	

Table of Contents

List of figures

List of tables

Nomenclature

A, n, Ta	Arrhenius formula parameters
E	Energy
H	Enthalpy
Ma	Mach number
P	Pressure
Q	Heat flux
T	Temperature
x, y, z	Coordinates
Y	Mass fraction
ρ	Density

Subscripts

∞	Free stream
0	Stagnation condition
conv	convective
diff	diffusive
tr	translational
vib	vibrational
w	Wall value

Acronyms

ASTRIUM	EADS Astrium Space Transportation GmbH (EU)
CFD	Computational Fluid Dynamics
CIRA	Italian Aerospace Research Centre
DLR	German Aerospace Centre
HEG	High Enthalpy Facility, DLR, Göttingen
IPG-4	IPM plasmatrons facility
IPM	Institute for Problems in Mechanics (Russia)
IT-2	Hot Shot Facility of TsAGI
ITAM	Institute of Theoretical and Applied Mechanics (Russia)
L2K	Ark-heated facility, DLR, Cologne
TAS-I	Thales Alenia Space Italy
TsAGI	Central Aerohydrodynamic Institute (Russia)
TsNIImash	Central research institute of Machine-Building (Russia)
U-13	TsNIImash plasmatrons facility
WP	Work Package

1 Executive summary

1.1 Scope of the deliverable

- The present document defines the requirements for the modelling, simulation and testing activities to be conducted in the framework of the SACOMAR project.

1.2 Results

A series of guidelines are presented to address partners' activities, data exchange, and to comply with industrial requirements.

1.3 Specific highlights

An overview of currently used models for CO2 flows is given, a series of possible test conditions is suggested, the objectives and standards for numerical simulations are discussed.

1.4 Forms of integration within the work package and with other WPs

In the framework of WP4 this first deliverable, dealing with program requirements, will be the basis for a second activity concerning results' synthesis (WP 4.2).

WP4 will be linked to the modelling, simulation and testing work packages (WP6, WP7, WP5 respectively) throughout the program by giving, in the first phase, inputs about requirements and standards, and in the final phase by collecting and critically analyzing partners' results.

1.5 Problem areas

Physical and chemical models for high speed/high temperature CO2 flows, computational fluid dynamics, experimental tests in ground based facilities.

2 Introduction

This document defines the guidelines for the physical modelling activity (WP6) and numerical/experimental test campaign (WP7, WP5) to be conducted in the framework of the SACOMAR program, focusing on the optimal requirements that various partners contributions are expected to meet.

After a brief description of the program objectives and of the role played by Thales Alenia Space Italia (*TAS-I*), the key aspects defined in the program proposal document [1] will be discussed:

- an overview on the current **physico-chemical modelling** techniques for CO2 high enthalpy flows, including **transport properties**, **gas phase kinetics** and **surface chemistry**, their status and chances for improvement,
- the type of **CFD simulations** needed to gather information about the implementation of the developed models, and the indications to define a standard method for data exchange,
- the requirements on the **experimental activity** to be performed in order to investigate the Martian atmosphere's relevant properties,
- the criteria for the **validation** of numerical simulations results over experimental data, and their use for the **extrapolation to flight** task.

3 The SACOMAR project

Missions to Mars represent today one of the most challenging aspects of space research and technology: up to present only a few programs have been successfully completed (by *NASA*) and there is still a lack of significant knowledge of the planet environment to help and support mission design.

For what concerns the entry phase, the deceleration from hypersonic to low subsonic speed exposes the vehicle to a series of aero-thermal phenomena that must be properly taken into account to minimize design margins: this entails the development of a reliable aerodynamic database for the Martian atmosphere, coming from the joined effort of both theoretical and experimental research.

In this framework, the SACOMAR program aims to promote the study of chemical-physical properties of the Martian atmosphere and the improvement of numerical and experimental tools to investigate the key phenomena of Martian entry aerothermodynamics, involving, for the first time, EU and Russian institutions.

TAS-I will support the partners' activity by providing, in the first phase of the program, a series of high level guidelines to address the experimental test campaign and to define the numerical simulations' objectives and validation strategy. The role played by *TAS-I* in the ongoing EXOMARS project will further help in focusing on the relevant aspects that characterize a modern Mars mission design. This task is also intended to make the program consistent to a series of standards that are normally required in an industrial research and development program.

A synthesis of the results achieved by the modelling, numerical and experimental activities will follow (WP 4.2), together with a correlation of the produced data and the extrapolation of validated models to EXOMARS trajectory.

4 Physico-chemical modelling

This section briefly presents an overview on currently used physico-chemical models of Martian atmosphere, in order to provide a minimal requirement from which a development program should start. The relevant variables to be investigated are presented and discussed.

Major difficulties in modelling Martian atmosphere arise firstly from the fact that the main component (CO2) is a nonlinear polyatomic species, for which there is a lack of sufficiently validated thermal and caloric models. In addition, a typical entry path is characterized by a low pressure/low density environment that drives dissociation and ionization at low temperatures (with respect to Earth) and contributes to raise chemical relaxation times (freezing).

These aspects globally affect wall heat fluxes and surface chemistry, requiring a correct thermodynamic, kinetic, transport and catalysis model.

A detailed review on modelling state of the art will be conducted by *ASTRIUM* in the framework of WP 6.1, and will serve as an input for the entire modelling task.

For species' **thermodynamic properties**, the data published by Capitelli et al. [2] represent an extension over the widely used Gordon-McBride curve fits, and should be used: including a greater number of excited states in the electronic partition function, these data permit calculations up to extremely high temperatures (above 10000 K).

The classical set of coefficients to describe **chemical kinetics** properties of Mars atmosphere, given by Park [3] for an 18-species gas with 33 characteristic reactions, should be updated with Gökçen's data [4] to achieve a 23 species model:

C2, C, N2, N, CO, O, CN, CO2, NO, O2, NCO, CN+, N+, N2+, C+, O+, Ar, Ar+, e-, C2+, O2+, CO+, NO+.

The reduced set obtained by Mitchelltree and Gnoffo [9], which considers 8 species neglecting ionization reactions, is basically derived from Park's work and is particularly suited for economic computations, but it works best for entry velocities about 8 km/s, that is when ionization level is small. Moreover, when radiation or communication blackout effects are investigated, charged species must be taken into account.

In all cases, rate coefficients are calculated with an Arrhenius-like formula. In the framework of the EXOMARS program, a set of characteristic reactions and rate parameters has been produced (Table 1) and can be used by the partners as a reference.

Over the years various sets of parameters to compute these coefficients have been produced for case-specific analyses, however a comparison shows that, at least for the prominent CO2 dissociation reaction, the rates tend to converge to Park's values (Figure 1).

A correct modelling effort is indeed very important in this phase of the program: it should be noted that many of these reaction rates have not been measured in typical Mars entry conditions but are estimated from indirect measurements, and are potential sources of uncertainty. The same applies for the not yet understood effect of thermal nonequilibrium on chemical kinetics and for the relaxation models, developed for air flows and then applied to other mixtures with minimal validation.

The analysis of these problems will be conducted by *DLR AS-RF* (WP 6.3), together with the creation of a library containing the new parameters and the relative documentation.

To account for vibrational nonequilibrium the standard multi-temperature approach (with at least one roto-translational and one vibro-electronic temperature) with the use of Landau-Teller V-T transfer model and Millikan-White relaxation times are normally adopted, using the data of Camac [5] and Park [3]. According to this dataset, the dominant species CO2 and CO are expected to relax very quickly, leading to a small level of thermal nonequilibrium in the shock layer. Nevertheless, since CO2 relaxation has an effect on trim angle of attack, this feature could be further investigated.

An accurate **transport** model is needed to correctly predict diffusion-dominated flow regions (boundary layer), shear stresses and heat fluxes.

Single species transport properties can be computed using collision-integrals based formulations (e.g. Lennard-Jones eventually accounting for Debye shielding for viscosity and modified Eucken relation for thermal conductivity [6]), that are usually preferable over temperature dependent curve fits (Blottner's law) due to the availability of updated collision integrals, e.g. by Wright et al. [7],[8].

For mixture values, besides the classical Wilke's rule, the first order approximation of the Chapman-Enskog relations, given in [6], can be implemented at a relatively low computational cost.

Thermal and pressure diffusion effects are generally small in comparison to ordinary diffusion and could be neglected.

Transport properties of Mars species will be investigated by *TsNIImash* in WP 6.2, and a dataset with the quantities needed in numerical simulations will be created.

Another source of aeroheating uncertainty is catalytic heating in a dissociated CO2 atmosphere, related to the **surface chemical properties**. Catalysis, in which the TPS surface facilitates the recombination of incident species, can be a large contributor to the total heating rate. No fully validated model currently exists to accurately predict the catalytic behaviour of real Mars TPS materials under flight conditions, and thus conservative design assumptions are employed to bound this effect.

Surface chemistry and catalysis models will be studied by *IPM*, as scheduled by WP 6.4.

All the partners will work not only on the development of the models, but also on their implementation in CFD codes: though basic research is a fundamental part of SACOMAR, the program results will be used to perform real case simulations, so attention must be kept in order to provide models that can be easily and, most of all, efficiently, implemented in numerical codes.

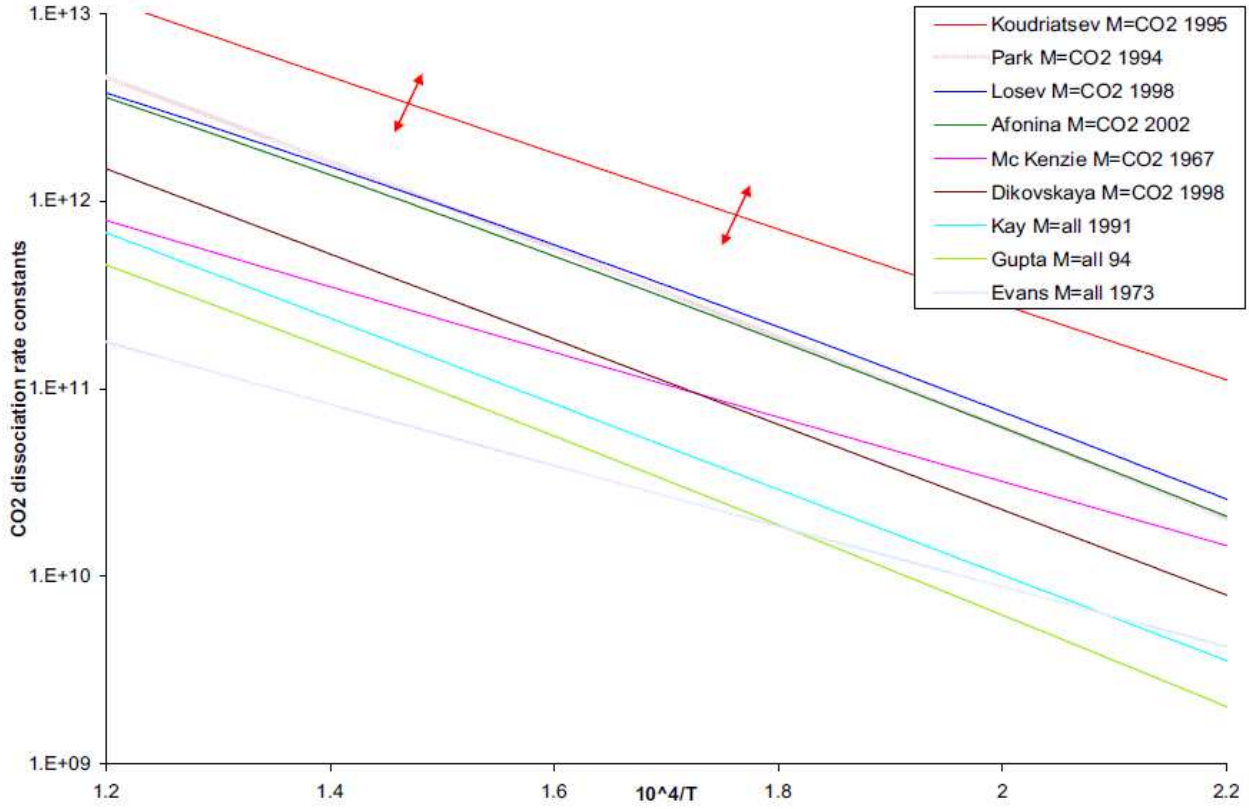


Figure 1: CO_2 dissociation rates from various works (M=colliding partner).

Reaction	*A (cm^3/mol.s)*	*N*	*Ta=E/R (K)*
$C_2 + M = C + C + M$	1.50e+16	0.0	71 600
$N_2 + M = N + N + M$ O/4.286/C/4.286/N/4.286/E/1714.3/	7.00e+21	-1.6	113 200
$CO + M = C + O + M$ O/1.478/C/1.478/N/1.478/AR/0.1	2.30e+20	-1.0	129 000
$CN + M = C + N + M$	2.53e+14	0.0	71 000
$O_2 + M = O + O + M$ O/5./C/5./N/5./	2.00e+21	-1.5	59750
$NO + M = N + O + M$ O/22./C/22./N/22./	5.00e+15	0.0	75500
$CO_2 + M = CO + O + M$ O/2.029/C/2.029/N/2.029/AR/0.1/	6.90e+21	-1.5	63 275
$NCO + M = CO + N + M$	6.30e+16	-0.5	24 000
$C + N_2 = CN + N$	5.24e+13	0.0	22 600
$CN + C = C_2 + N$	5.00e+13	0.0	13 000
$C_2 + N_2 = CN + CN$	1.50e+13	0.0	21 000
$NO + O = N + O_2$	8.40e+12	0.0	19 450
$N_2 + O = NO + N$	6.40e+17	-1.0	38 370
$CO + O = C + O_2$	3.90e+13	-0.18	69 200
$CO + C = C_2 + O$	2.00e+17	-1.0	58 000
$CO + N = CN + O$	1.00e+14	0.0	38 600
$CN + O = NO + C$	1.60e+13	0.1	14 600
$CO_2 + O = O_2 + CO$	2.10e+13	0.0	27 800
$CN + O_2 = NCO + O$	6.60e+12	0.0	-200
$CN + CO_2 = NCO + CO$	4.00e+14	0.0	19 200
$CN + NO = NCO + N$	1.00e+14	0.0	21 200
$CO + NO = NCO + O$	3.80e+17	-0.873	51 600
$CN + CO = NCO + C$	1.50e+16	-0.487	65 800
$N + O = NO^+ + E$	8.80e+08	1.0	31 900
$O + O = O_2^+ + E$	7.10e+02	2.7	80 600
$CO + O = CO^+ + E$	8.80e+08	1.0	33 100
$NO^+ + C = NO + C^+$	1.00e+13	0.0	23 200
$O_2^+ + O = O^+ + O_2$	4.00e+12	-0.09	18 000
$NO^+ + N = O^+ + N_2$	3.40e+13	-1.08	12 800
$NO^+ + O = O_2^+ + N$	7.00e+12	0.29	48 600
$CO + C^+ = CO^+ + C$	1.00e+13	0.0	31 400
$O_2 + C^+ = O_2^+ + C$	1.00e+13	0.0	9 400
$CN^+ + N = CN + N^+$	9.80e+12	0.0	40 700
$C^+ + N_2 = N_2^+ + C$	1.11e+14	-0.11	50 000
$C + N = CN^+ + E$	1.00e+15	1.5	164 440
$N + N = N_2^+ + E$	4.40e+07	1.5	67 500
$N + E = N^+ + E + E$	2.50e+34	-3.82	168 600
$C + E = C^+ + E + E$	3.70e+31	-3.0	130 720
$O + E = O^+ + E + E$	3.90e+33	-3.78	158 500

Table 1: EXOMARS reaction set and Arrhenius parameters.

5 Experimental study

This section presents the ground-based facilities that will be used during the program's experimental campaign, giving an insight on the requirements of the test samples and on the reference flowfield characteristics.

Different high enthalpy facilities have been made available by program's partners: two short duration high enthalpy facilities (shock tunnel HEG of *DLR AS-RF* and hot shot facility IT-2 of *TsAGI*), two plasmatrons (IPG-4, *IPM* and U-13, *TsNIImash*) and an arc-heated facility (L2K, *DLR AS-WK*).

In this framework it will be possible to investigate a wide range of flight conditions and to accurately measure the relevant parameters of the physico-chemical models, such as, in long duration high enthalpy facilities (IPG-4, U-13, L2K):

- rotational and vibrational temperatures
- species concentration
- flow velocity

and, in short duration facilities (HEG, IT-2):

- relaxation processes.

In order to provide large shock stand-off distances and to obtain as many data as possible in the shock layer region, two flat-faced cylinders, with main axis parallel to flow direction, will be used as test models. Sample diameters are 100 mm and 50 mm (standard ESA geometry for TPS testing) with an 11.5 mm edge radius. Silver coating will be used to simulate a fully catalytic wall and quartz coating for non-catalytic wall. Tests on surfaces with partial catalytic properties are also recommended. All tests will be performed with gas compositions representative of Mars atmosphere.

As a general requirement, flow conditions should be chosen close to a series of anchorage points defined during the long-term EXOMARS program.

In the EXOMARS shallow (sizing) trajectory, six points representing characteristic aero-thermodynamic configurations have been selected for the creation of the ATDB: it will be useful to perform ground tests in similar conditions in order to have data to perform a meaningful cross-check and validation campaign. After a preliminary analysis, six points could be identified as candidates for the experimental campaign: relevant values characterizing these points are given in Table 2.

In Figures 2 and 3 the trajectory and the proposed points are given in term of Mach *vs* time and Pitot pressure *vs* total enthalpy.

According to facilities' performances, and in order to have a sufficient overlap between the measuring capabilities to completely characterize the flowfield, **two** configurations will be selected (WP 5.1) and used in the experimental campaign. Also, test cases must be defined taking into account that the data obtained could be numerically reproduced by means of numerical codes and software modules implemented, and that the tests serve to generate data needed for the validation of single models, reducing at minimum the interactions of other phenomena. In this sense, the use of non-intrusive measurement techniques should be preferred whenever possible.

Design, manufacturing and integration of test models into the facilities will be performed by partners as part of work packages 5.2, 5.3 and 5.4, as well as specific calibration and measurement activities. A report on test results, uncertainties and flow characterization will be delivered by each partner.

point	time [s]	Pitot pressure [mbar]	Total enthalpy [MJ/kg]
1	81	55	13.8
2	104	82	8.5
3	113	82	6.6
4	120	79	5.5
5	131	70	3.8
6	140	62	2.9

Table 2: Experimental campaign candidate points.

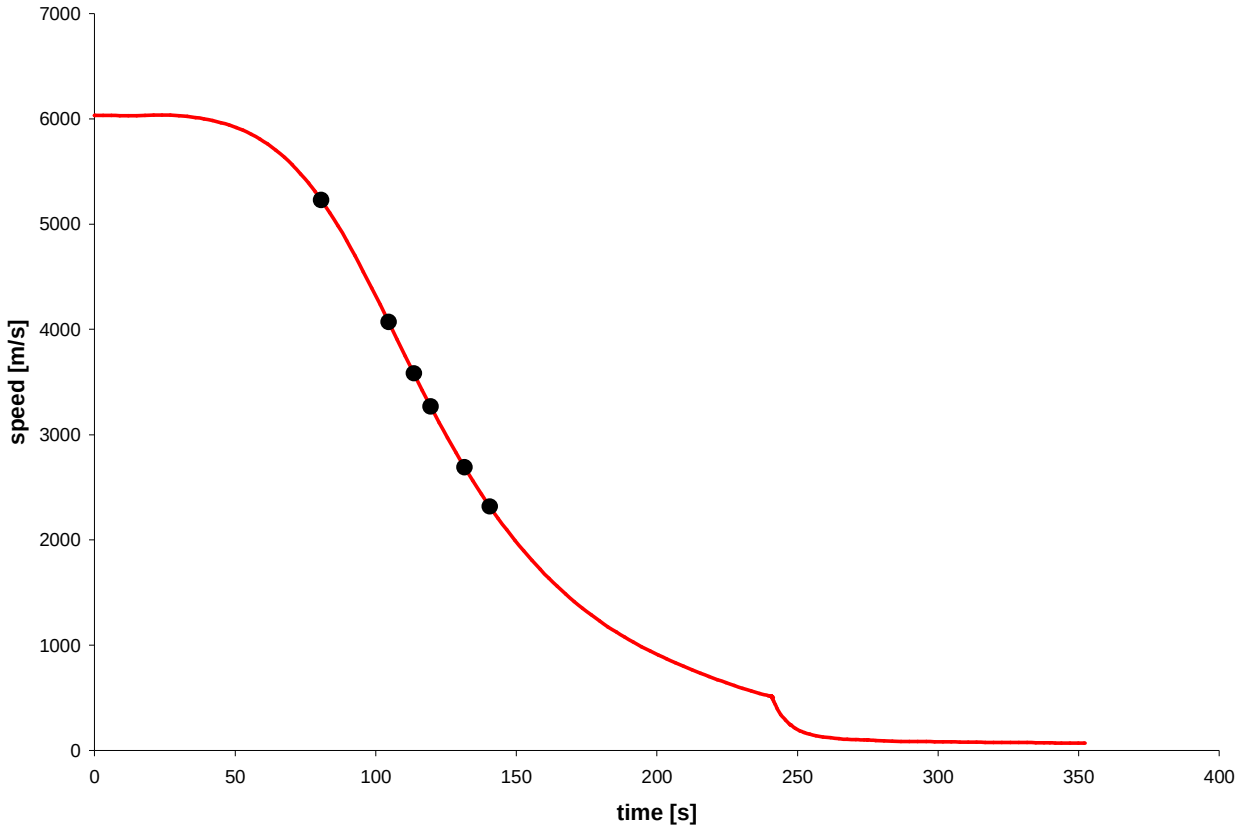


Figure 2: EXOMARS sizing trajectory speed VS time and proposed test points.

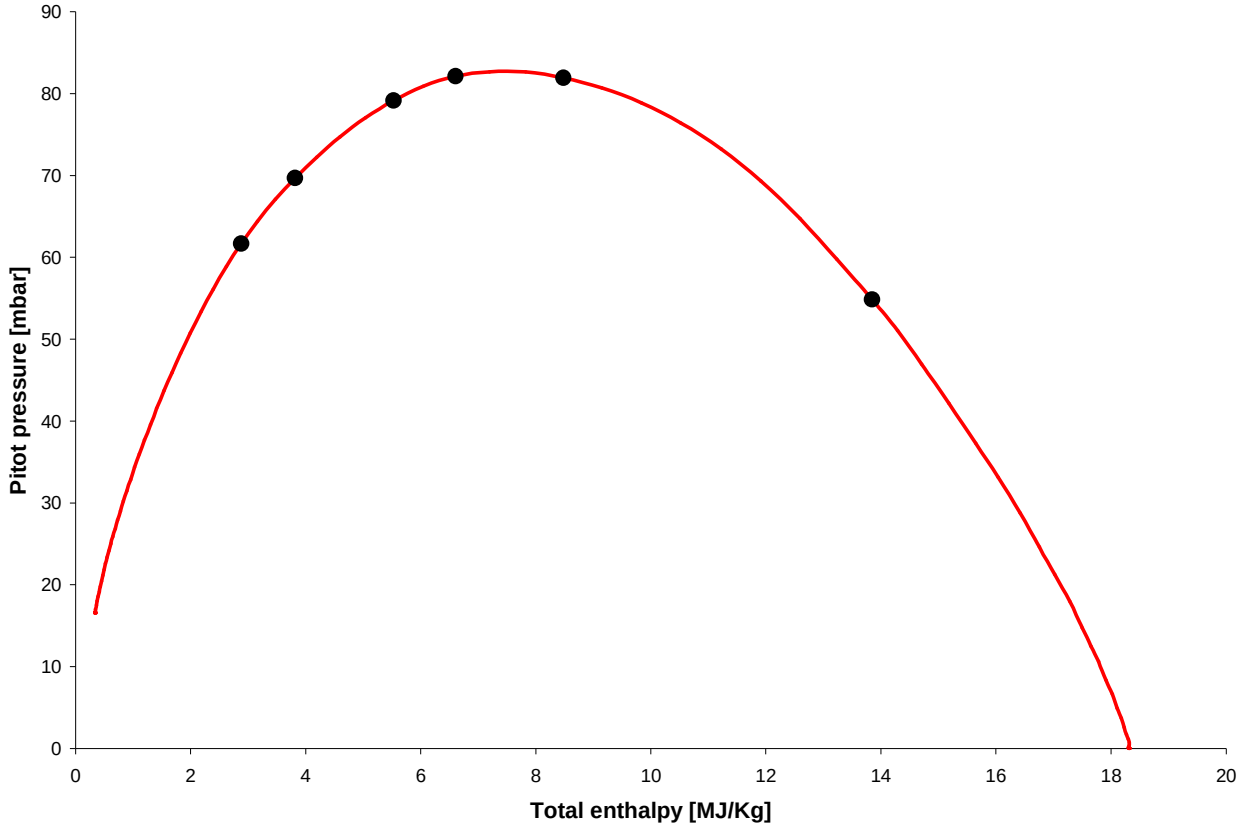


Figure 3: EXOMARS sizing trajectory Pitot pressure VS total enthalpy and proposed points.

6 CFD simulations

Five CFD codes (from *DLR, CIRA, TsNIImash, IPM* and *ITAM*), developed to simulate high enthalpy flows in chemical and vibrational nonequilibrium, will be used to implement the new chemical-physical models, to perform numerical rebuilding of experimental tests and for the ground-to-flight extrapolation process. Four Finite Volumes, differing in space discretization and time integration schemes, and a DSMC solver are available: this fact leaves room for an interesting cross-check campaign to point out performance differences between diverse algorithms.

Referring to the test conditions proposed in the previous section, in Table 3 the free-stream values usually used as input parameters for CFD simulations are given for the six candidate points. The reference composition is 97% CO2 and 3% N2 by mass.

point	time	speed [m/s]	Mach	P∞ [Pa]	T∞ [K]
1	81	5228	22.74	8.72	213.05
2	104	4072	17.32	22.46	222.92
3	113	3581	15.17	29.34	225.07
4	120	3266	13.79	34.22	226.49
5	131	2691	11.29	44.89	229.09
6	140	2317	9.69	53.86	230.79

Table 3: Free stream conditions for candidate test points.

A general requirement regards data exchange: it is important for an efficient management of produced results to have a common type and format for numerical simulations' output files.

For every simulation, the partners should provide:

- a text file containing the CFD method and physical models applied as well as input parameters (free stream temperature, density, speed and pressure) and boundary conditions. An indication of convergence history of sensitive variables should help to compare models' efficiencies.

- a data file containing surface values, organized with at least these variables:

VARIABLES = {x, y, z, T_w, P_w, Q_tot, Q_conv, Q_diff, Q_vib, Y_[name], Evib_[name]}

The file should be delivered in TECPLOT format, at least version 8 compatible.

- a TECPLOT file with volume data, containing at least:

VARIABLES = {x, y, z, rho, P, Ma, H, T_tr, Tvib_[name], Y_[name], Evib_[name]}

Where:

x,y,z	=	coordinates
Y_[i]	=	i-th species mass fraction
rho	=	density
Evib[i]	=	i-th species vibrational energy
P_w	=	wall pressure
P	=	pressure
H	=	total enthalpy
Ma	=	Mach number
Q_tot, _conv, _diff, _vib	=	total, convective, diffusive, vibrational fluxes
T_w, _tr, _vib[i]	=	wall, translational, vibrational (for i-th molecule) temperature

The details of model implementation in numerical codes will be given in a series of technical reports to be delivered by the partners in the framework of work package 7.1, in particular by *CIRA* (WP 7.1.1), *DLR AS-RF* (WP 7.1.2), *TsNIImash* (WP 7.1.3) and *ITAM* (WP 7.1.4).

Numerical rebuilding of experimental tests will also be described in technical reports: for shock tunnel tests in HEG and IT-2, *ASTRIUM* will give the performances of the TAU code, in predicting both the nozzle and the test chamber flows (WP 7.2). *IPM* and *TsNIImash* will report the simulations of the plasmatrons tests (7.3.1, 7.3.2), and *CIRA* the arc-heated facility L2K tests (WP 7.4).

7 Validation

The SACOMAR program permits to experimentally investigate, in different facilities, a large number of flowfield variables: this represents a big chance for validation of both the physical-numerical models and the measurement techniques.

After a correct calibration of ground facilities a first experiment-to-experiment comparison should be performed to determine measurement uncertainties. A parallel cross-check campaign between numerical simulations (code-to-code) on simple configurations will ensure the correct implementation of the physical models developed in the framework of WP6.

A report containing the status of code to code validation is to be considered as part of the work package 7.1.

Then the comparison between the measured and predicted fluid-dynamic parameters (code-to-experiment) for the reference test-cases will be performed, taking into account experimental and numerical accuracies.

Two reports, focusing on Validation Strategy and Validation Results respectively, will be delivered in the framework of WP2.

It should be noted that the reference configurations proposed in the previous sections refer to trajectory points where continuum assumptions are valid. Being a DSMC solver available (SMILE, from *ITAM*), it would be interesting to identify a third configuration in order to exploit the capabilities of this kind of algorithm to predict rarefied flows. Since experimental tests are not designed to simulate such an environment, a possible comparison would be performed between DSMC and Navier-Stokes solvers in a rarefied/hot hypersonic transition regime (Kn ~ 0.001).

A candidate point can be extracted from the early stage trajectory of EXOMARS (time = 47.93 sec, altitude = 75.42 km). Free-stream conditions for this case are given in Table 4.

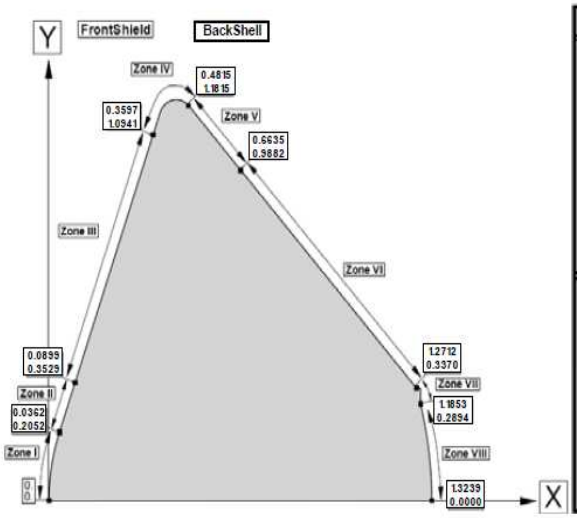
speed [m/s]	Mach	P∞ [Pa]	T∞ [K]	ρ∞ [kg/m^3]
5941.214	30.317	0.951	155.201	3.207·10^-2

Table 4: Transition point free-stream conditions.

8 Extrapolation to flight

Validated models and codes can be used to extrapolate prediction capabilities to real cases. Again, EXOMARS program could provide helpful data for comparison purposes: hereafter some details on the reference shape are given.

The EXOMARS descent module is a classical sphere-cone shaped body, with a 70° front angle and a 47° rear angle, a rounded back cover and a ring close to the base (Figure 4). As discussed, a complete aero-thermo database has been constructed for a reference trajectory.



	Zones	X (m)	Y (m)
Frontshield		0	0
	Zone I - Stagnation Region	0,0362	0,2052
	Zone II - Sphere Cone Junction	0,0362	0,2052
		0,0899	0,3529
	Zone III - Mid-Cone	0,0899	0,3529
		0,3597	1,0941
	Zone IV - Shoulder	0,3597	1,0941
		0,4814	1,1815
BackShell	Zone V - Shoulder / Rear Cone junction	0,4814	1,1815
		0,6635	0,9882
	Zone VI - Rear-Cone	0,6635	0,9882
		1,2712	0,3370
	Zone VII - Rear Cone / Base Junction (ring)	1,2712	0,3370
		1,2853	0,2894
	Zone VIII - Base	1,2853	0,2894
		1,3239	0

Figure 4: EXOMARS descent module geometry.

TAS-I will perform this task by using an in-house developed numerical code, in which the validated models could be implemented. The code is a 2D/3D explicit finite volumes solver for the Navier-Stokes equations in chemical and vibrational nonequilibrium.

Convective fluxes are evaluated using an upwind Flux-Difference Splitting technique, and second order accuracy in space and time is obtained using an ENO-like scheme. Diffusive fluxes are computed using a centred scheme.

Different models could be used to describe the chemical-physical properties of the gas. Species transport coefficients can be obtained from collision integrals or from curve-fits, mixture values from classical rules or from Chapman-Enskog theory in the first non vanishing approximation in terms of Sonine polynomials. All diatomic species, including ions, can be assumed to be in vibrational non-equilibrium and the vibrational energy relaxation mechanism is the V-T transfer. Various spectroscopic routines can be used to calculate emission and absorption coefficients if a radiation analysis is to be performed, and the radiative flux can be computed either by the tangent slab or the spherical harmonics P1 methods.

Conjugate heat transfer problems can be studied since the code is coupled to a thermal response solver allowing for ablation and surface recession phenomena.

9 Conclusions

The SACOMAR program will gain from the joined effort of basic and applied science, following the ambitious goal of producing a series of validated models for the Mars atmosphere.

Detailed methods to describe thermodynamics, kinetic, and transport properties of Martian atmosphere will be developed and implemented in modern numerical solvers. Then experimental tests in both long- and short-duration high enthalpy facilities will produce data to perform a wide range validation campaign.

Two continuum regime configurations derived from the experience gained by *TAS-I* in the EXOMARS program will be used as a reference for experiment-to-experiment and code-to-experiment comparisons, using standard test samples. A third transitional regime configuration will serve as a test case to have an insight on different simulation approaches.

A common format for data exchange and a rigid schedule for deliverables will finally ensure an easy and proficient program management.

10 References

[1] SACOMAR, *Technologies for Safe and Controlled Martian Entry*, Project Proposal, Part B.

[2] Capitelli et al., "*High-Temperature Thermodynamic Properties on Mars Atmosphere Components"*, AIAA 2004-2378.

[3] *Park, Howe, Jaffe, Candler, "Review of Chemical-Kinetic Problems of Future NASA Missions, II: Mars Entries", Journal of Thermophysics and Heat Transfer, 8, No. 1, 1994.*

[4] Gökçen, *"N2-CH4-Ar Chemical Kinetic Model for Simulations of Atmospheric Entry to Titan"*, AIAA 2004-2469.

[5] Camac, "*CO2 Relaxation Processes in Shock Waves*," Fundamental Phenomena in Hypersonic Flow, Cornell University Press, 1964.

[6] Gupta, Yos, Thompson, Lee, "*A Review of Rates and Thermodynamic and Transport Properties for an 11-Species Air Model for Chemical and Thermal Nonequilibrium Calculations to 30000 K*", NASA-RP-1232, 1990.

[7] Wright, Bose, Palmer, Levin, "*Recommended Collision Integrals for Transport Property Computations - Part 1: Air Species*", AIAA JOURNAL, 43, no. 12, 2005.

[8] Wright, Hwang, Schwenke, "*Recommended Collision Integrals for Transport Property Computations - Part 2: Mars and Venus Entries*", AIAA JOURNAL, 45, no. 1, 2007.

[9] Mitchelltree, Gnoffo, "*Wake Flow About a MESUR Mars Entry Vehicle*", 1994-1958.

11 Appendix

A preliminary simulation of the trajectory points discussed in Sections 5 and 6 have been conducted with the TAS-I CFD solver. The flowfield around the EXOMARS front shield at zero angle of attack has been reconstructed using a 2D axial symmetric configuration.

The simulation uses the Mitchelltree-Gnoffo chemical model considering the following 8 species:

species	weight [g/mol]	formation enthalpy [KJ/mol]	characteristic vibration temperature [K] *(molecules only)*
O	15.9994	15426422.24	
N	14.0067	33611800.07	
C	12.0107	24760105.57	
NO	30.0061	2992388.21	2741.61
CO	28.0101	-18776666.27	3124.03
O_2	31.9988	0.0	2275.10
N_2	28.0134	0.0	3395.80
CO_2	44.0095	-18298076.55	960.76

Vibrational energies are computed for each molecular species using the infinite harmonic oscillator hypothesis, and allowed to relax according to the Landau-Teller V-T transfer model, where relaxation time is computed with the Millikan-White formula. Vibrational equilibrium is assumed in the free-stream.

Single species transport properties are derived from Wright collision integrals, while mixture values are evaluated with Wilke's rule. Mass diffusion fluxes are obtained with the Stefan-Maxwell relation.

For the computations presented here a non-catalytic wall in radiative equilibrium is assumed.

A plot of the roto-translational temperature along the stagnation streamline is reported in Figure 5, giving an estimate of shock stand-off distances for the six points. Stagnation mass fractions of prominent species are given in Figures 6.

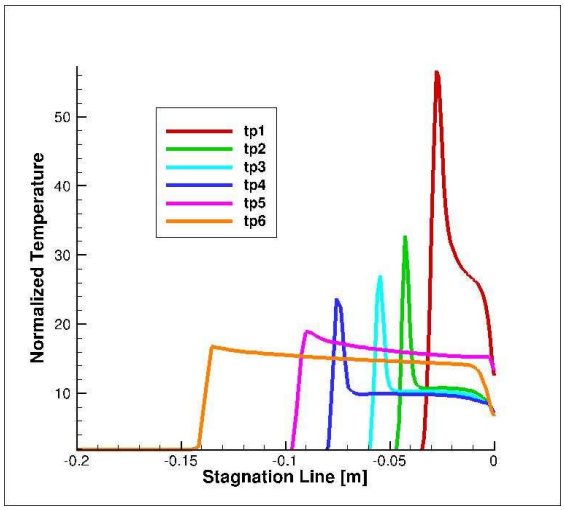


Figure 5: stagnation temperature for trajectory points (*tp*) as in Table 3

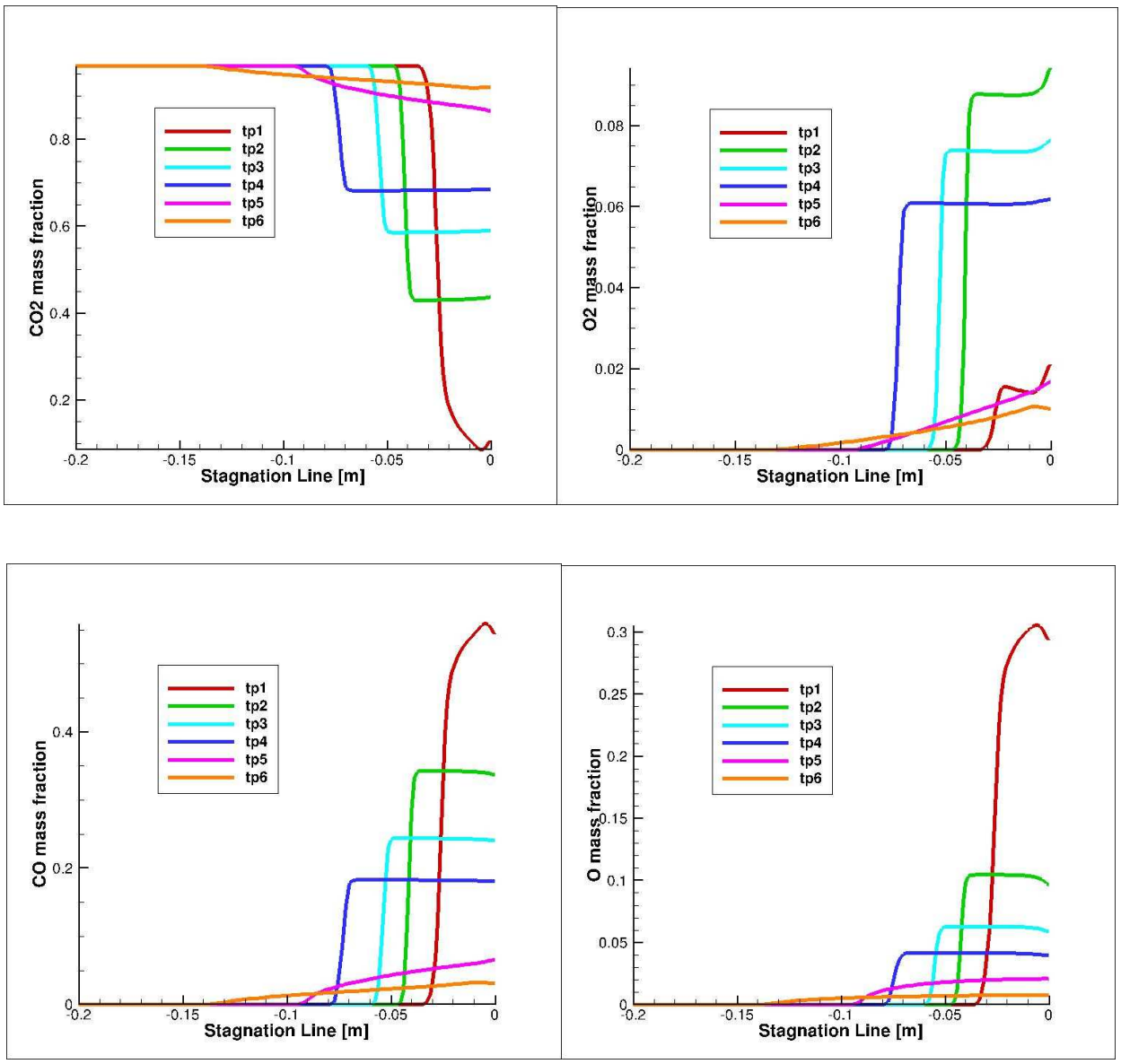


Figure 6: CO_2, O_2, CO and O mass fractions

Considering the concentration gradients predicted by this analysis, together with facilities' performances, the trajectory point 2 could be selected for an investigation of the dissociation-recombination regime.

A set of the aero-thermodynamic characteristic values that could be used in numerical simulations, completing that already given in Tables 2 and 3, is presented in Table 5.

point	tp1	tp2	tp3	tp4	tp5	tp6
time [s]	81	104	113	120	131	140
Mach	22.74	17.32	15.17	13.79	11.29	9.69
density [Kg/m^3]	2.14·10^-4	5.26·10^-4	6.81·10^-4	7.89·10^-4	1.02·10^-3	1.22·10^-3
pressure [Pa]	8.72	22.46	29.34	34.22	44.89	53.86
temperature [K]	213.05	222.92	225.07	226.49	229.09	230.79
speed [m/s]	5228	4072	3581	3266	2691	2317
angle of attack	0°					
free-stream composition	97% CO2, 3% N2					
free-stream vibrational energies	equilibrium					
free stream γ (Cp/Cv)	1.295					
wall	non catalytic – radiative equilibrium (ε=0.85)					
Knudsen	1.45·10^-4	5.97·10^-5	4.61·10^-5	3.98·10^-5	3.07·10^-5	2.58·10^-5
Reynolds	2.27·10^5	4.22·10^5	4.78·10^5	5.03·10^5	533·10^5	5.44·10^5

Table 5