Deliverable D-7
TN-5: Booklet with Numerical Ablation Test Cases

Relating and contributing to WP5: Definition of Numerical Test Cases (Booklet)

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Contents

Applicable documents

[AD1] Ablative TPS numerical test cases – mathematical code assessment & improvement. Appendix 1 to AO/1-9091/17/NL/RA, issue 1 rev. 3. Prepared by ESA ESTEC, 2017.

[AD2] Ablative TPS numerical test cases – mathematical code assessment & improvement: Technical, Implementation, Management and Financial Proposal. Prepared by the AblaNTIS consortium in response to ESA AO/1-9091/17/NL/RA, 2017.

[AD3] AblaNTIS: Negotiation meeting minutes and attachments. ref: AblaNTIS_MoM_1, December 2017.

[AD4] AblaNTIS: Kickoff meeting minutes and attachments. ref: AblaNTIS_MoM_2, February 2018.

[AD5] AblaNTIS Deliverable D-1 TN-1: Detailed Work Plan. ref: AblaNTIS_D-1_TN-1, May 2018.

[AD6] AblaNTIS Deliverable D-5 TN-3.2: Plasma Test Report. ref: AblaNTIS_D-5_TN-3.2, July 2020.

[AD7] AblaNTIS Deliverable D-3 TN-2.2: Material Characterisation Test Report. ref: AblaNTIS_D-3_TN-2.2, July 2020.

Reference documents

[RD1] Jean Lachaud, Alexandre Martin, Ioana Cozmuta, and Bernie Laub. Ablation test case 1. In *4th Ablation Workshop*.

[RD2] Jean Lachaud, Alexandre Martin, Tom van Eekelen, and Ioana Cozmuta. Ablation test case 2. In *5th Ablation Workshop*.

[RD3] Jean Lachaud, Alexandre Martin, Tom van Eekelen, and Ioana Cozmuta. Ablation test case 3. In *5th Ablation Workshop*.

[RD4] AblaRadAbla: Plasmatron test preparation and execution. ESA Contract 40001131101/15/NL/RA, ref: TR2v2, prepared by von Karman Institute for Fluid Dynamics, November 2017.

[RD5] `VKI_ZURAM_characterization_v1-5.ods` – prepared by VKI for AblaNTIS activity. OpenOffice spreadsheet file.

[RD6] `DLR_updated_data.ods` – Collection by DLR of several data for ZURAM. OpenOffice spreadsheet file.

[RD7] `TACOT_v3.0.xlsx` – Properties of the Theoretical Ablative Composite for Open Testing (TACOT). Excel Spreadsheet prepared for 6th US Ablation Workshop.

[RD8] `Zuram_aged_data_en.xlsx` – Thermal diffusivity measurements by DLR for ZURAM precharred at different temperatures. Excel spreadsheet file.

[RD9] `LFA_charred_ZURAM_Summary.xlsx` – Summary of LFA results on pre-charred ZURAM prepared by Forschungszentrum Juelich for AblaNTIS activity. Excel spreadsheet file.

[RD10] Mersen. Properties of CALCARB rigid carbon insulation CBCF 18-2000. Manufacturer datasheet.

[RD11] Joan Rico Orero. *Computational study on the effect of the microstructure on macroscopic properties for carbon fiber felts*. Msc thesis, von Karman Institute – Vrije Universiteit Brussel.

[RD12] G Chambre P Reynier. ISA TN-04-2007 – Test case definition for numerical rebuilding within the european ablation working group. October 2007.

1 Introduction

The main objective of Task 5 is the definition of ablation numerical test cases and the edition of a booklet (this document) with detailed descriptions of these test cases for distribution to the community.

In the Detailed Work Plan document (Deliverable 1 – TN-1 [AD5]), a set of 17 numerical test cases have been drawn up, based on:

1. already available data, i.e.
   - the ablation test-case series 1, 2 and 3 of the 4^{th} and 5^{th} Ablation Workshops [RD1, RD2, RD3]
   - the AblaRadAbla Plasmatron tests results [RD4]
2. the preliminary definition of the experimental tests to be performed (cf. Task 3 – Plasma Testing) and the foreseen results

These numerical tests and their naming convention are listed in section 2 of this document.

Two different materials[1,2] are considered in the numerical test cases: CALCARB® and ZURAM®. The material properties required for running the thermal-response codes selected in this project have been identified and a list of "common" input parameters and properties for both materials in the various states (i.e., virgin, char, pyrolysis gas) are detailed in section 3.

Two types of test cases are planned:

1. one-dimensional planar test cases — these tests are purely numerical (there will be no experimental validation) and are intended for code-to-code comparison only;
2. two-dimensional hemispherical test cases — these tests will be compared with the results of Plasmatron runs.

The geometry and the boundary conditions related to these two types of tests are detailed in section 4.

The requested output results as well as the file format (selected to ease code-to-code comparison) are defined in section 5.

[1] Test cases with CALCARB® are designed to allow a step-by-step evolution in the tests complexity, the preform being not subjected to pyrolysis.

[2] Carbon graphite (plug support) and alumina (insulating disk) are also considered behind the specimen in the numerical test cases simulating the 14 experimental test cases

The final section is dedicated to the detailed description of each numerical test case, including:

- the test-case description,
- the corresponding assumptions and simplifications,
- the material properties to be used (referring to the values introduced in section 3),
- the boundary conditions (referring to the values introduced in section 4),
- the requested output results.

Remarks:

1. At the end of this document, an appendix is dedicated to the description of the GitHub repository created to group all the reference data and documents useful for the definition of the numerical test cases. The URL of this repository is: `https://github.com/ablantis/AblaNTIS-test-cases`
2. This document has been evolving along the project:
   - Issue 1 was
     - a collection of initial available data, i.e. the available experimental properties for ZURAM® and some dummy values (from similar materials or from TACOT) where data is limited or missing [AD5]
     - a definition of the test cases that will be rebuilt to see if the models works as expected
   - Issue 2 contains the implementation of
     - the material characterization (WP2)
     - the plasma tests results (WP3)

2 Naming convention of the numerical test cases

As introduced in the Detailed Work Plan document (Deliverable 1 – TN-1 [AD5]), all the test cases (listed in Table 1) follow the naming convention

[Num/Exp]-N-[T/SEB]-[P/Z]

where:

- **Num/Exp**:
  - **Num**, the test case involves code-to-code comparison only. These tests are identical to the US Ablation Workshop test cases with the exception that the ZURAM® material properties are used instead of the "fictitious" material TACOT. Therefore, these tests do not depend in any way on the plasma tests performed within Task 3.
  - **Exp**, the test case includes comparison with tests performed in the Plasmatron. Some of these tests are repetitions of to the tests already performed in AblaRadAbla (cf. Table 3).
- **N**: test case condition number, i.e. one value per combination of heat flux and atmosphere (Nitrogen or Air).
- **T/SEB**:
  - **T**, the surface boundary temperature, pressure and recession rate are predefined functions of time and surface location.
  - **SEB**, the surface boundary conditions are found by satisfying the surface energy balance (SEB), with a convective heat flux that is a function of time and surface location.
- **P/Z**:
  - **P**, the sample material will be CALCARB® .
  - **Z**, the sample material will be ZURAM® .

Together with this short list, the conditions (physical phenomena) that are active in each of the test cases are summarized in Table 2.

An extended description of each numerical test case can be found in section 6 of this document.

Table 1: List of numerical test cases

Numerical test ID	Plasm. exper. ID (or code-to-code)	Geometry	Material (specimen)	Heat flux * [MW/m^2]	Gas	B.C.	Heating duration [s]	max T_w † [K]	P_w [hPa]
Num-1-T-P	code-to-code	1D, planar	CALCARB®	n.a.	n.a.	T_w	120	1500	50
Num-1-T-Z	code-to-code	1D, planar	ZURAM®	n.a.	n.a.	T_w	120	1500	50
Num-2-SEB-Z	code-to-code	1D, planar	ZURAM®	0.5	N_2	SEB	120	n.a.	50
Num-3-SEB-Z	code-to-code	1D, planar	ZURAM®	1.5	Air	SEB	120	n.a.	50
Num-4-SEB-Z	code-to-code	1D, planar	ZURAM®	5.0	Air	SEB	120	n.a.	50
Exp-1-T-P	P-N-50-q300	2D, hemisphere	CALCARB®	0.3	N_2	T_w,$\dot{r}$	80	n.a.	50
Exp-1-SEB-P	P-N-50-q300	2D, hemisphere	CALCARB®	0.3	N_2	SEB	80	n.a.	50
Exp-2-T-Z	Z-A-50-q300	2D, hemisphere	ZURAM®	0.3	Air	T_w,$\dot{r}$	160	n.a.	50
Exp-2-SEB-Z	Z-A-50-q300	2D, hemisphere	ZURAM®	0.3	Air	SEB	160	n.a.	50
Exp-3-T-P	P-N-100-q2500	2D, hemisphere	CALCARB®	2.5	N_2	T_w,$\dot{r}$	30	n.a.	100
Exp-3-SEB-P	P-N-100-q2500	2D, hemisphere	CALCARB®	2.5	N_2	SEB	30	n.a.	100
Exp-3-T-Z	Z-N-100-q2500	2D, hemisphere	ZURAM®	2.5	N_2	T_w,$\dot{r}$	60	n.a.	100
Exp-3-SEB-Z	Z-N-100-q2500	2D, hemisphere	ZURAM®	2.5	N_2	SEB	60	n.a.	100
Exp-4-T-Z	Z-A-100-q2500	2D, hemisphere	ZURAM®	2.5	Air	T_w,$\dot{r}$	90	n.a.	100
Exp-4-SEB-Z	Z-A-100-q2500	2D, hemisphere	ZURAM®	2.5	Air	SEB	90	n.a.	100
Exp-5-T-Z	SS-Z-A	2D, hemisphere	ZURAM®	4.5	Air	T_w,$\dot{r}$ ‡	45	n.a.	25
Exp-5-SEB-Z	SS-Z-A	2D, hemisphere	ZURAM®	4.5	Air	SEB	45	n.a.	25

* Cold-wall heat flux

† The maximum wall temperature T_w is set to 1500 K for the tests Num-1-T-P and Num-1-T-Z. For all the other tests, it was a priori unknown and it has been defined for prescribed-temperature 2D tests (Exp-x-T-x) after experimental test measurements became available.

‡ The recession and the surface temperature may be inaccurately measured.

Table 2: Physical phenomena that are included in the tests

Test ID	2D effects	λ_c	λ_v	Pyrolysis	Convective heat transfer	Oxid.	Subl.	Recession	Shape change	Non-equil.rad. (Potential†)
Num-1-T-P	-	✓	-	-	-	-	-	-	-	-
Num-1-T-Z	-	✓	✓	✓	✓	-	-	-	-	-
Num-2-SEB-Z	-	✓	✓	✓	✓	-	-	-	-	-
Num-3-SEB-Z	-	✓	✓	✓	✓	✓	-	✓	-	-
Num-4-SEB-Z	-	✓	✓	✓	✓	✓	✓	✓	-	-
Exp-1-T-P	✓	✓	-	-	-	-	-	-	-	-
Exp-1-SEB-P	✓	✓	-	-	-	-	-	-	-	-
Exp-2-T-Z	✓	✓	✓	✓	✓	✓	-	-	-	-
Exp-2-SEB-Z	✓	✓	✓	✓	✓	✓	-	-	-	-
Exp-3-T-P	✓	✓	-	-	-	-	-	✓	-	✓
Exp-3-SEB-P	✓	✓	-	-	-	-	-	✓	-	✓
Exp-3-T-Z	✓	✓	✓	✓	✓	-	-	✓	-	-
Exp-3-SEB-Z	✓	✓	✓	✓	✓	-	-	✓	-	-
Exp-4-T-Z	✓	✓	✓	✓	✓	✓	-	✓	-	-
Exp-4-SEB-Z	✓	✓	✓	✓	✓	✓	-	✓	-	-
Exp-5-T-Z	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Exp-5-SEB-Z	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

† The introduction of non-equilibrium radiation in the numerical models is limited to the re-run of tests EXP-3-j-P and EXP-5-j-Z after Plasmatron and characterization tests execution, as mentioned in the Detailed Work Plan document D-1 TN-1 [AD5]

Table 3: List of Plasmatron ablation experiments to be performed. "No. of tests" indicates the total amount of identical tests to be performed; "Repeated" indicates if the test is a repetition of a test performed (either in previous or in the present test campaign); "AbraRad. ref." indicates to which test of the AblaRadAbla TRP [RD4] the present test is linked.

Material	Shape	Flow	Gas	Cold-wall heat flux [MW/m^2]	No. of tests	Repeated	AblaRad. ref.
CALCARB®	Hemisph.	SUB	N_2	0.3	1	No	ZU1
CALCARB®	Hemisph.	SUB	N_2	2.5	1	No	ZU2
ZURAM®	Hemisph.	SUB	Air	0.3	1	Yes	ZU1
ZURAM®	Hemisph.	SUB	N_2	2.5	1	Yes	ZU4
ZURAM®	Hemisph.	SUB	Air	2.5	1	Yes	ZU2
ZURAM®	Hemisph.	SUP	Air	4.6	2	Yes (2 tests)	-

3 Material properties

All samples in the numerical test cases are made of either CALCARB® CBCF 18-2000 , or ZURAM® 18/50 material.

CALCARB® is a carbon fibre preform that can be impregnated with a phenolic resin to prepare ZURAM®. As CALCARB® does not pyrolyse, fewer material properties are required to characterize its behavior.

For ZURAM® (the reference material of the present activity), the list of "common" input parameters and properties set in the Detailed Work Plan document (Deliverable 1 – TN-1 [AD5]) are given in the Table 4.

Table 4: List of necessary input parameters/properties for the thermal-response simulation of charring ablators. The "-" indicates non-applicable quantities, e.g., pyrolysis rate of the material in charred state.

	Property	ZURAM® virgin	ZURAM® char	CALCARB®
Composition	Open porosity	✓	✓	✓
	Volume fractions	✓	✓	✓
	Intrinsic densities	✓	✓	✓
	Elemental composition	✓	✓	-
Chemistry	Overall pyrolysis rate	✓	-	-
Transport	Permeability	✓	✓	✓
	Tortuosity†	✓	✓	✓
Energy	Heat capacity	✓	✓	✓
	Formation enthalpy	✓	✓	-
	Effective conductivity	✓	✓	✓
	Heat of pyrolysis	✓	-	-
	Emissivity	✓	✓	✓

† Tortuosity is not foreseen to be used in any of the codes selected for computing the numerical test cases of this project, but it is given as an indicative value.

The material properties of alumina and graphite are also provided for the modelling of the insulator disk and the holding plug used in the experimental test campaign [AD6]. These materials must be considered in the 2D hemispherical test cases (Exp-x-x-x).

All the material properties listed in this document are also available on the AblaNTIS GitHub repository (see details in the Appendix).

3.1 ZURAM® material properties

Volume fractions of fibers, resin, and gas are[3] [RD5]:

- virgin: $v_{\mathrm{f}} = 0.1299728$, $v_{\mathrm{r}} = 0.1627287$, and $v_{\mathrm{g}} = 0.7072985$
- charred: $v_{\mathrm{f}} = 0.1299728$, $v_{\mathrm{r}} = 0.1008538$, and $v_{\mathrm{g}} = 0.7691734$

Intrinsic densities are $\rho_{\mathrm{f}} = 1577.24$ kg/m^3 for the fibers, and $\rho_{\mathrm{r}} = 1315.07$ kg/m^3 for the resin [RD5]

Average (bulk) density of ZURAM® is then derived from the intrinsic densities and the volume fractions: $\rho_{\mathrm{v}} = 418.998$ kg/m^3 in virgin state, and $\rho_{\mathrm{c}} = 337.628$ kg/m^3 when charred.

Open porosity is

- virgin: $\phi_{\mathrm{v}} = v_{\mathrm{g,virgin}} = 0.7072985$
- charred: $\phi_{\mathrm{c}} = v_{\mathrm{g,charred}} = 0.7691734$

The intermediate values are derived from the density:

$$\phi = \frac{\rho_{\mathrm{v}}\phi_{\mathrm{v}} - \dfrac{\rho_{\mathrm{v}} - \rho}{\rho_{\mathrm{v}} - \rho_{\mathrm{c}}}\left(\rho_{\mathrm{v}}\phi_{\mathrm{v}} - \rho_{\mathrm{c}}\phi_{\mathrm{c}}\right)}{\rho} \tag{1}$$

Permeability is $\kappa_{\mathrm{v}} = 1.06\ 10^{-11}$ m^2 in virgin state, and $\kappa_{\mathrm{c}} = 3.968\ 10^{-8}$ m^2 when charred [RD6]

Tortuosity [4] is $\tau_{\mathrm{v}} = 1.2$ in virgin state, and $\tau_{\mathrm{c}} = 1.1$ when charred [RD7]

Specific heat capacity in [J/(kg.K)] of the solid phase is a function of the temperature T [AD7]:

$$c_p(T) = a + bT + \frac{c}{T} \tag{2}$$

with the following coefficients[5]:

[3] Mass fractions can be derived from volume fractions and intrinsic densities:
0.489259 for fibers and 0.510741 for resin in virgin state
0.607172 for fibers and 0.392828 for resin in charred state.

[4] not used in any of the selected codes, but given as an indicative value

[5] As detailed in the description of the codes (D1–TN-1 [AD5]), for all the three codes, the intermediate states are derived assuming a linear interpolation with the density, between the virgin state and the charred state.

	a	b	c
virgin	1724.514	0.656	-311009.512
charred	1850.384	0.248	-393964.868

Table 5: Coefficients of the heat capacity formula for virgin and charred ZURAM®

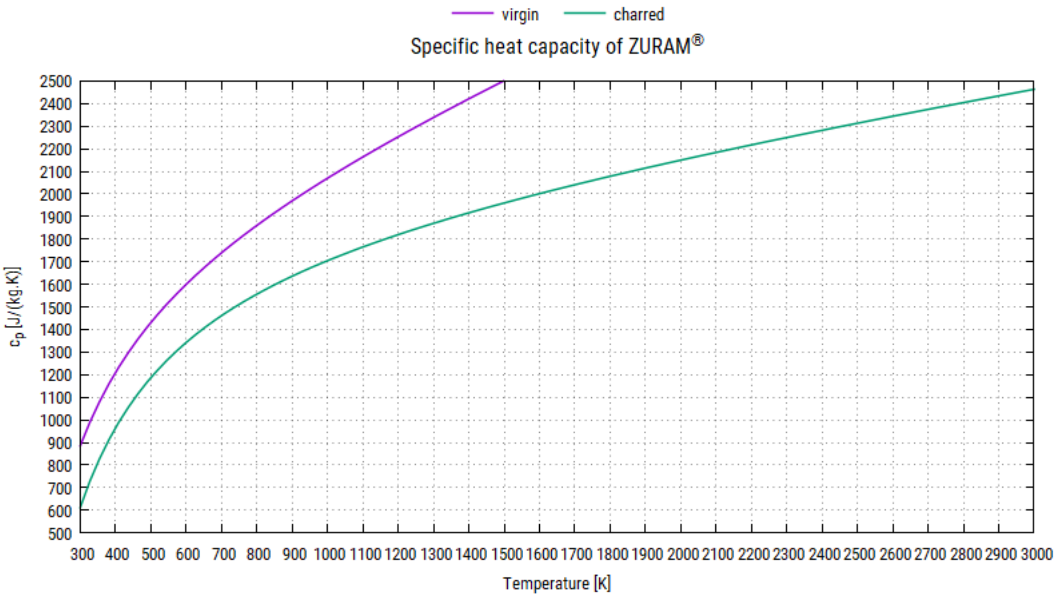


Figure 1: Specific heat capacity of ZURAM® .

Orthotropic thermal conductivity in [W/(m.K)] is defined by two different functions of the temperature T in the virgin and the charred states[6]:

- virgin ZURAM® [RD8]:

$$k(T) = \frac{a}{T} + b \tag{3}$$

with the following coefficients:

[6] As detailed in the description of the codes (D1–TN-1 [AD5]), for all the three codes, the intermediate states are derived assuming a linear interpolation with the density, between the virgin state and the charred state.

	a	b
through-the-thickness (k_{zz})	-31.39	0.2443
in-plane ($k_{xx} = k_{yy}$)	-108.1	0.8784

Table 6: Coefficients of the orthotropic thermal conductivity (virgin ZURAM®)

- charred ZURAM® [AD7] & [RD9]:

$$k(T) = \frac{a}{T} + b + c\,T + d\,T^2 + e\,T^3 \tag{4}$$

with the following coefficients:

	a	b	c	d	e
through-the-thickness (k_{zz})	-56.02	0.3812	$5.354\ 10^{-4}$	$-3.605\ 10^{-7}$	$1.267\ 10^{-10}$
in-plane ($k_{xx} = k_{yy}$)	-470	2.476	$-9.128\ 10^{-4}$	$1.606\ 10^{-7}$	$8.523\ 10^{-11}$

Table 7: Coefficients of the orthotropic thermal conductivity (charred ZURAM®)

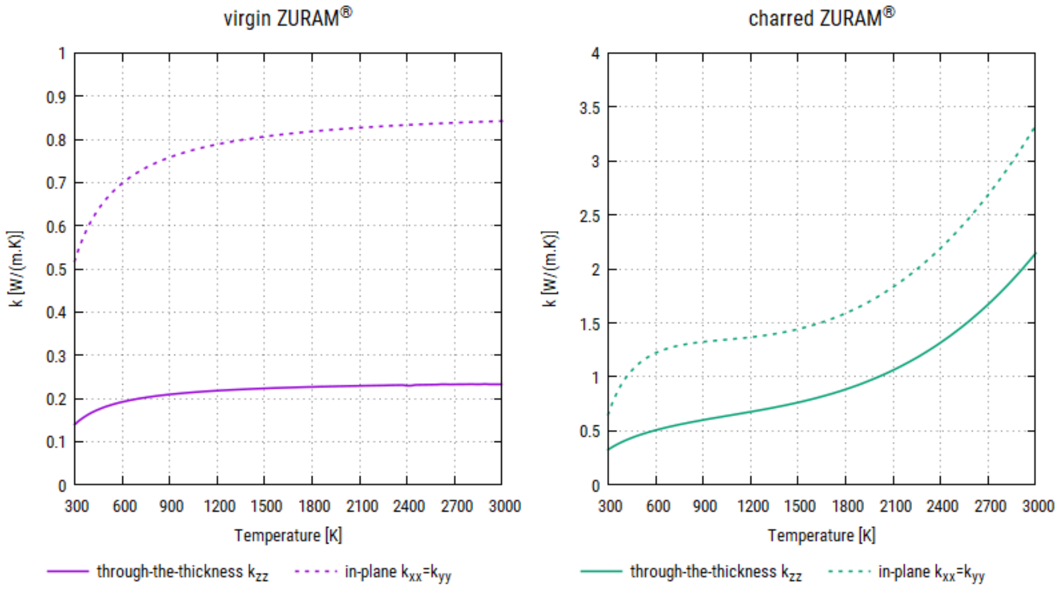


Figure 2: Orthotropic thermal conductivity of ZURAM® .

Emissivity is[7] $\varepsilon_{\mathrm{v}} = 0.8$ in virgin state, and $\varepsilon_{\mathrm{c}} = 0.9$ when charred [RD7].

Formation enthalpy of char at 298 K is set as the reference (zero), so that it is equal to -2.1437 10^6 J/kg for pure phenolic resin, and -1.094878036 10^6 J/kg for virgin ZURAM® [RD5].

Average elemental composition of the pyrolysis gases is [RD5]:

Element	mole fraction	mass fraction	molar mass [g/mol]
C	0.170941536	0.457	12.0107
H	0.722071254	0.162	1.00794
O	0.109687209	0.381	15.999
Total	1	1	4.535818

Table 8: Average elemental composition of the pyrolysis gases for ZURAM®

Pyrolysis kinetics Two pseudo-phases are considered: inert fibers and resin that is decomposing to char. The resin pyrolysis kinetics is characterized by four Arrhenius-type equations and corresponding density loss fractions F_i, such that the pyrolysis gas generation rate, Π, is given by Equation 5 and the rate of change in the extent of reaction, ξ_j, of component j is given by Equation 6.

$$\Pi = -\frac{\partial\left(\varepsilon_m\, \rho_m\right)}{\partial t} = \varepsilon_{m,v}\, \rho_{m,v} \sum_{i=1}^{4} F_i \frac{\partial \xi_i}{\partial t} \tag{5}$$

$$\frac{\partial \xi_i}{\partial t} = \left(1 - \xi_i\right)^{n_i} A_i \exp\frac{-E_i}{RT} \tag{6}$$

where the index v denotes the virgin state (unpyrolysed material), ε_m is the resin volume fraction and ρ_m is the intrinsic density of the resin phase.

The constants in the four Arrhenius rate equations are given in Table 9 [AD7].

[7] As detailed in the description of the codes (D1–TN-1 [AD5]), for all the three codes, the intermediate states are derived assuming a linear interpolation with the density, between the virgin state and the charred state.

reaction	F_i	$\log_{10} A_i$ (A_i in [s^{-1}])	E_i/R [K]	n_i
1	0.035070	5.33	8178.5	4.3
2	0.027687	8.69	16068.4	3.7
3	0.095981	10.6	21612.9	2.57
4	0.221495	11.67	26423.8	4.63

Table 9: Pyrolysis kinetics for ZURAM®

Heat of pyrolysis The heat of pyrolysis is given by the difference between the gas enthalpy and the solid phase enthalpy. A linear evolution of the solid density ρ from the virgin state ρ_v to the charred state ρ_c is assumed, and the heat of pyrolysis H_p is:

$$H_\mathrm{p} = h_\mathrm{g} - \frac{\rho_\mathrm{v}\, h_\mathrm{v} - \rho_\mathrm{c}\, h_\mathrm{c}}{\rho_\mathrm{v} - \rho_\mathrm{c}} \tag{7}$$

where h_g is the gas enthalpy.

3.2 CALCARB® material properties

Average (bulk) density is $\rho = 180$ kg/m^3 [RD10]

Intrinsic density of the fibers is $\rho_\mathrm{f} = 1577$ kg/m^3 [RD5]

Volume fraction is:

- $v_\mathrm{f} = \frac{\rho}{\rho_\mathrm{f}} = 0.11414$ for fibers
- $v_\mathrm{g} = 1 - v_\mathrm{f} = 0.88586$ for gas

Open porosity is $\phi = v_\mathrm{g} = 0.88586$

Permeability is $\kappa = 3.968\ 10^{-8}$ m^2 (same as charred ZURAM® [RD6])

Tortuosity [8] is $\tau = 1.1$ [RD7]

Specific heat capacity (of the solid phase) in [J/(kg.K)] is defined as a function of the temperature T:

$$c_p(T) = 1850 + 0.248\ T - \frac{394000}{T} \tag{8}$$

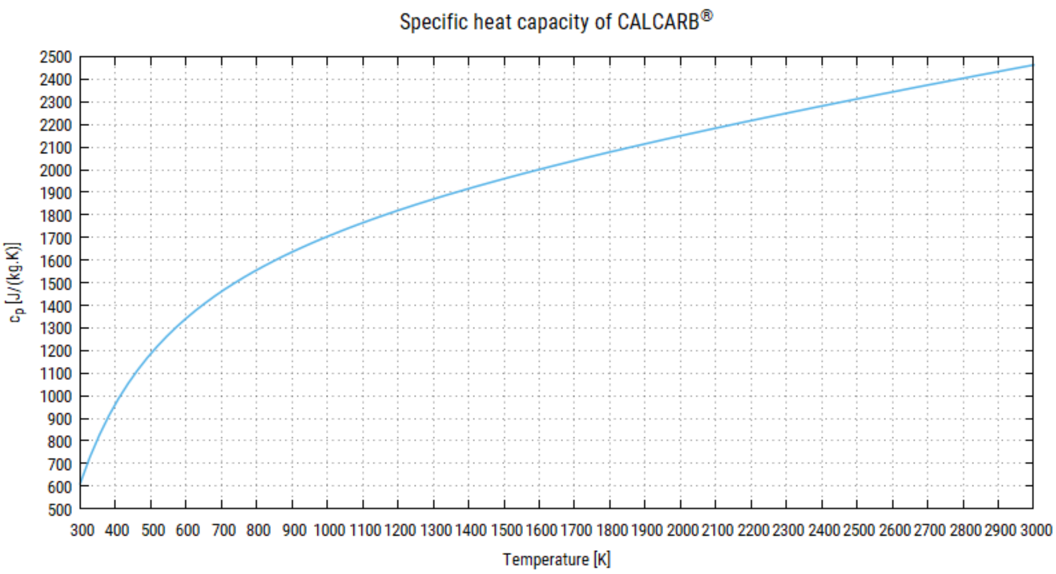


Figure 3: Specific heat capacity of CALCARB® CBCF 18-2000.

[8] not used in any of the selected codes, but given as an indicative value

Thermal conductivity in [W/(m.K)] is defined as:

$$k(T) = a + b\,T + c\,T^2 \tag{9}$$

with the following coefficients:

	a	b	c
through-the-thickness (k_{zz})	0.08187	$0.58175\ 10^{-4}$	$0.425975\ 10^{-7}$
in-plane ($k_{xx} = k_{yy}$)	0.32748	$2.327\ 10^{-4}$	$1.7039\ 10^{-7}$

Table 10: Coefficients of the orthotropic thermal conductivity (CALCARB® CBCF 18-2000)

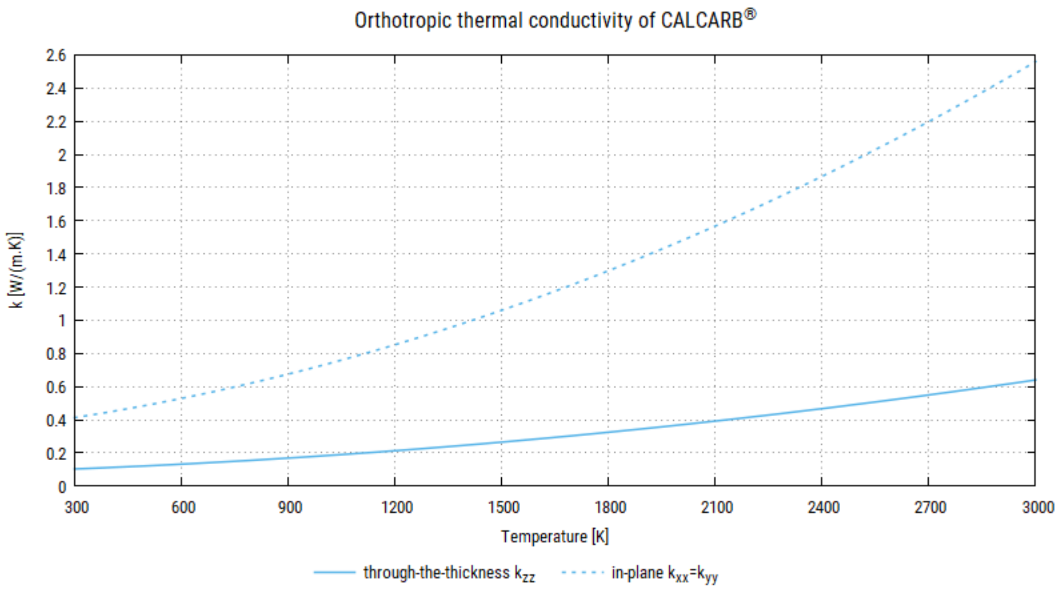


Figure 4: Orthotropic thermal conductivity of CALCARB® CBCF 18-2000

In-plane conductivity $k_{yy} = k_{zz}$ is based on [RD10], while through-the-thickness conductivity k_{zz} is the same divided by 4, according to [RD11].

Emissivity is $\varepsilon = 0.90$ [RD7]

3.3 Alumina material properties

Specific heat capacity in J/(kg.K):

$$\begin{aligned} c_p(T) &= 87.4609180616 + 3.1467711444\,T \\ &\quad -3.2471325\ 10^{-3}\,T^2 + 1.1752\ 10^{-6}\,T^3 \end{aligned} \tag{10}$$

Isotropic thermal conductivity in W/(m.K):

$$k(T) = 0.0255089286 + 1.785714\ 10^{-4}\,T \tag{11}$$

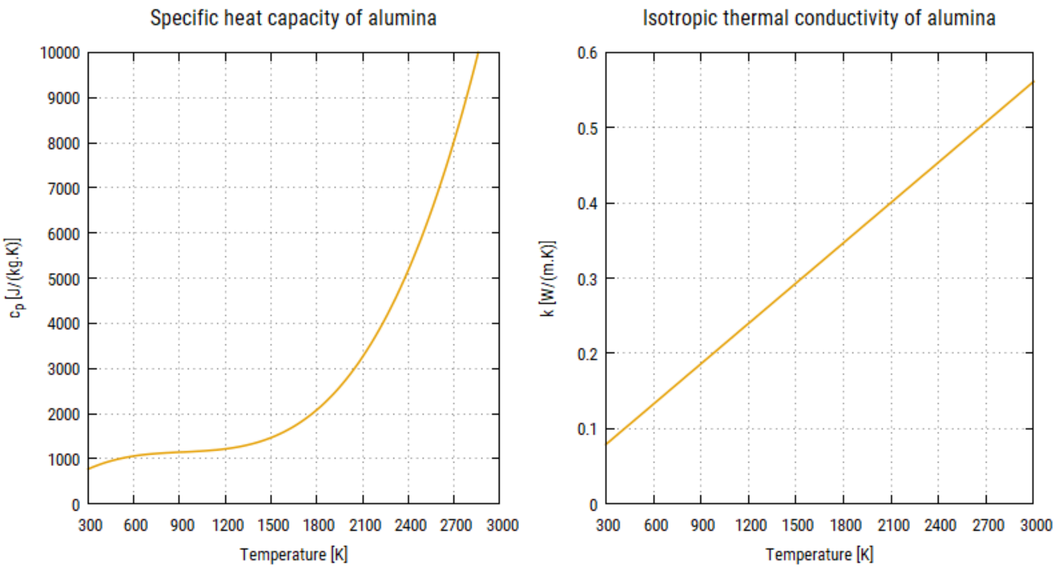


Figure 5: Specific heat capacity and isotropic thermal conductivity of alumina.

Density $\rho = 400$ kg/m^3

Emissivity $\varepsilon = 0.8$

3.4 Graphite material properties

According to [RD12]:

Specific heat capacity in J/(kg.K):

$$c_p(T) = 878.5714286 + 0.305573593\,T + 8.625\ 10^{-4}\,T^2 - 5.01515\ 10^{-7}\,T^3 + 7.72727\ 10^{-11}\,T^4 \quad (12)$$

(best-fitting polynomial of degree 4)

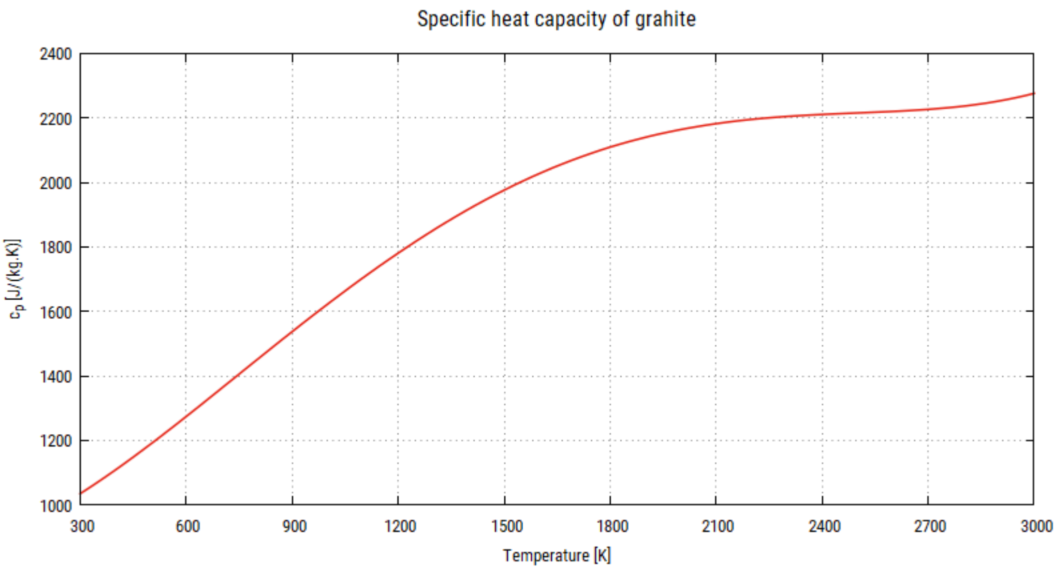


Figure 6: Specific heat capacity of graphite.

Constant isotropic thermalconductivity $k = 92$ W/(m.K)

Density $\rho = 1720$ kg/m^3

Emissivity $\varepsilon = 0.94$

4 Geometry and boundary conditions

Preliminary remark:
In both 1D and 2D axisymmetric models defined hereafter, all the samples are equally oriented such that the "through-the-thickness" direction lies along z-axis. This orientation is consistent with the orthotropic material properties defined in section 3 (more specifically with the effective thermal conductivities k_{xx}, k_{yy}, k_{zz}).

4.1 One-dimensional planar test cases (Num-x-x-x)

4.1.1 Geometry

All the test cases are assumed 1D planar:

- the length of the sample is $L = 50$ mm
- on one side, the sample is heated ($z = 0$)
- the opposite side ($z = L$) and lateral sides are adiabatic and impermeable

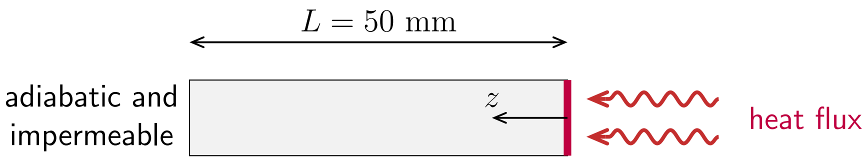


Figure 7: One-dimensional planar numerical test case

4.1.2 Initial conditions

- the initial temperature of the sample is uniform and equal to $T_0 = 300$ K
- the initial composition of the atmosphere is Air (mole fractions: O_2=0.21, N_2=0.79)
- the initial gas pressure is uniform and equal to $P_0 = 5000$ Pa

4.1.3 Boundary conditions

Prescribed wall temperature (Num-1-T-x)
The first type of heating boundary condition is defined by a prescribed wall temperature T_w, with a linear ramp up applied during the first 0.1 s from the initial temperature T_0 to T_w, then constant during the remaining test duration, see Figure 8.

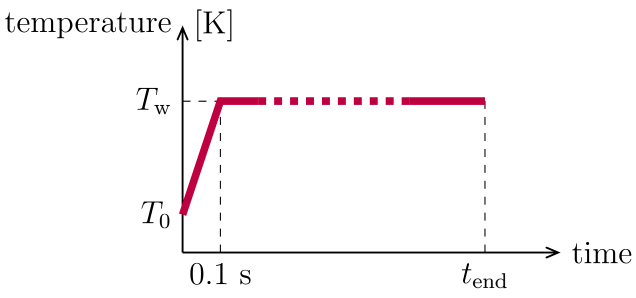


Figure 8: Prescribed wall temperature vs. time

The value of T_w is set to 1500 K for both Num-1-T-P and Num-1-T-Z, and the final time is $t_{end} = 120$ s.

Convective heat flux and re-radiation (Num-x-SEB-Z)

The second type of heating boundary condition is defined by applying a heat flux given by:

$$q_w = \rho_e u_e C_H (H_r - H_w) \tag{13}$$

where $\rho_e u_e C_H$ is the heat transfer coefficient, H_r is the recovery enthalpy and H_w is the gas enthalpy at the wall.

Assuming Prandtl number $\mathrm{Pr} = 1$, the recovery enthalpy is related to the edge enthalpy H_e as follows:

$$H_r = H_e + \frac{u_e^2}{2} \tag{14}$$

The value of the heat transfer coefficient and the recovery enthalpy were evaluated by the means of aero-thermal calculations such that the resulting cold-wall heat flux is approximately:

- low (≈ 0.5 MW/m^2) for the test case Num-2-SEB-Z
- medium (≈ 1.5 MW/m^2) for the test case Num-3-SEB-Z
- high (≈ 5.0 MW/m^2) for the test case Num-4-SEB-Z

The heat transfer coefficient is constant during the heating period (until time $t = 120$ s). After heating, a period of cooling is modelled by setting the heat transfer coefficient to almost zero (0.001 kg/(m^2.s)) with a linear transition during 0.1 s until $t_{\text{end}} = 240$ s, see Figure 9.

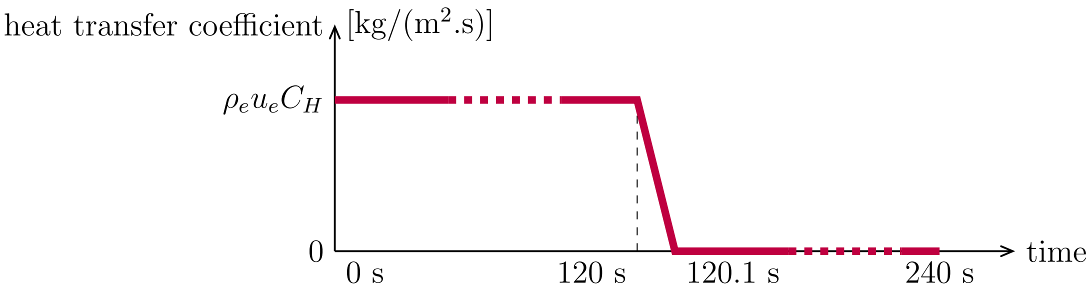


Figure 9: Heat transfer coefficient vs. time

The values of the heat transfer coefficient and the recovery enthalpy for each Num-x-SEB-x test case is summarized in Table 11.

time [s]	Num-2-SEB-Z low (≈ 0.5 MW/m^2) H_r [J/kg]	$\rho_\text{e}u_\text{e}C_\text{H}$ [kg/(m^2.s)]	Num-3-SEB-Z medium (≈ 1.5 MW/m^2) H_r [J/kg]	$\rho_\text{e}u_\text{e}C_\text{H}$ [kg/(m^2.s)]	Num-4-SEB-Z high (≈ 5.0 MW/m^2) H_r [J/kg]	$\rho_\text{e}u_\text{e}C_\text{H}$ [kg/(m^2.s)]
0	9418113.0	0.042617	28172526.	0.065487	2.5e7	0.1872
120	9418113.0	0.042617	28172526.	0.065487	2.5e7	0.1872
120.1	52477.051	0.001	52477.051	0.001	52477.051	0.001
240	52477.051	0.001	52477.051	0.001	52477.051	0.001

Table 11: Heat transfer coefficient and the recovery enthalpy for Num-x-SEB-x test cases

In addition to the applied heat flux, re-radiation is active during the whole test (heating and cooling), considering a view factor equal to 1 and the infinity temperature $T_\infty = T_0 = 300$ K. The emissivity of the virgin/charred material is defined in the material properties, cf. section 3.

Additional boundary conditions

The wall pressure P_w is constant and prescribed equal to 5000 Pa for all 1D test cases.

When required by the test case definition, the recession speed at wall $\dot{r}_\text{w}$ due to ablation must be modelled using the following assumptions:

- The factor for the blowing-correction correlation (CMA-like model) is taken as $\lambda = 0.5$
- Heat and mass transfer coefficients are assumed equal in the boundary layer and $\mathrm{Pr} = \mathrm{Le} = 1$
- The wall enthalpy h_w and dimensionless ablation speed B'_c must be generated with the Mutation++ v1.0.1 open-source library[9] as functions of
  - the wall pressure P_w (in a range 0.001–1 bar)
  - the dimensionless out-gassing parameter B'_g (in the range 0–10)
  - the wall temperature T_w (in the range 300–3500 K)

  These boundary condition must be considered for ZURAM® pyrolysis gas in both air and nitrogen atmospheres.

4.1.4 Thermocouples position

For the purpose of code-to-code comparison, a set of specific locations is defined in order to provide time-dependent results (see section 5).

In the case of the 1D tests, these locations will not be confronted to any physical measurement of an experimental campaign. The locations can therefore be defined a priori without taking care of the exact positioning of thermocouples in any real tested sample.

The coordinates of the thermocouples are provided in the Table 12. They apply for all 1D test cases.

z_1	z_2	z_3	z_4	z_5	z_6	z_7	z_8	z_9
0 mm	1 mm	2 mm	4 mm	8 mm	12 mm	16 mm	24 mm	50 mm

Table 12: Coordinates of virtual thermocouples for one-dimensional planar test cases

It must be underlined that z_1 is located on the heated surface ($z_1 = 0$ in time $t = 0$). Later, it is moving with it when recession occurs, i.e. $z_1 = z_\mathrm{w}$ (like a pyrometer), while other coordinates are fixed (like thermocouples), z_9 being on the left-end surface.

[9] input files for Mutation++ (`*.xml`) and a bash script example to generate these data are available on the AblaNTIS GitHub repository, see Appendix.

4.2 Two-dimensional hemispherical test cases (Exp-x-x-x)

4.2.1 Geometry

Two-dimensional hemispherical samples

All the test samples share the same hemispherical-cylindrical axisymmetric geometry, cf. Figure 10 [AD7].

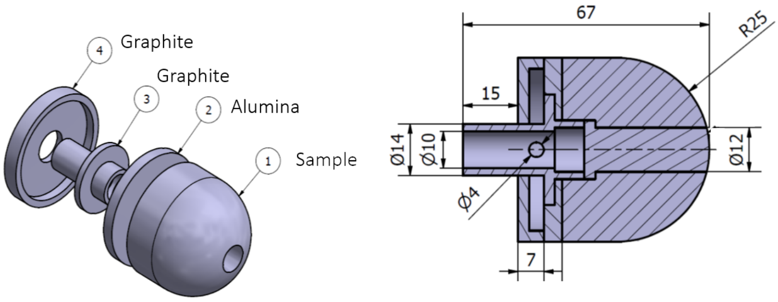


Figure 10: CAD rendering and geometry of the hemispherical sample setup.

- the nose radius is $R = 25$ mm
- the sample length is $L = 40$ mm (nose + cylindrical base)
- during the tests, the samples are supported on a graphite plug
- an insulator disk made of alumina is placed between the sample the graphite plug

A simplified (but realistic) 2D-axisymmetric geometry is used for all 2D numerical test cases, including the holding hole in the back of the sample, the alumina disk insulator and a part of the graphite plug, cf. Figure 11.

4.2.2 Initial conditions

The initial temperature T_0 and initial pressure P_0 are uniform everywhere in the structure, i.e. in the sample, the insulator disk, the plug, but also the surroundings (atmosphere, chamber).

These initial values are test case dependent and equal to the initial measurement for each test, cf Table 13.

The initial composition of the atmosphere is:

- Exp-1-x-P, Exp-3-x-P, Exp-3-x-Z: Nitrogen (mole fraction: N_2=1)
- Exp-2-x-Z, Exp-4-x-Z, Exp-5-x-Z: Air (mole fractions: O_2=0.21, N_2=0.79)

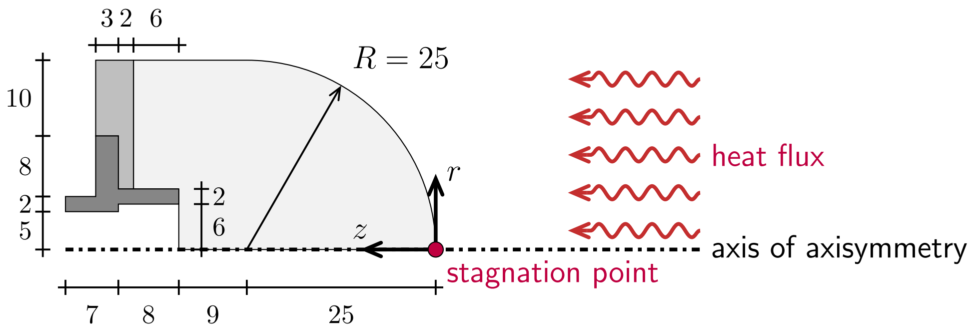


Figure 11: Two-dimensional hemispherical test cases: the sample is in light gray, the graphite holding plug in dark gray, and the alumina insulating disk in medium gray (all the dimensions are in mm).

Test case		T_0 [K]	P_0 [Pa]
Exp-1-x-P		302.45	5014
Exp-2-x-Z		302.85	5417
Exp-3-x-P		301.55	10045
Exp-3-x-Z	part1	309.35	9546
	part2	301.73	10039
Exp-4-x-Z		310.05	10063
Exp-5-x-Z	(-long)	307.25	2674

Table 13: Initial temperature T_0 and initial pressure P_0 for Exp-x-x-x test cases. (Exp-3-x-Z: `part1` is starting from $t = 0$ s, `part2` is starting from $t = 1000$ s)

4.2.3 Boundary conditions

The plug, the insulator disk, and the sample

For the sake of simplicity, perfect thermal contact (infinite thermal contact conductance) and impermeable wall are assumed between the plug, the disk insulator and the sample.

Then, the following zones are defined (cf. Figure 12):

- zones A and B: adiabatic boundary conditions are applied
- zone C: cold-wall boundary conditions are applied, i.e. temperature is prescribed and equal to the initial temperature T_0 (test case dependent) during all the test
- zone D: convective heat flux considering the flux applied on the specimen in P_{theta59} (see Figure 13) is extending to the entire zone D and re-radiation considering $T_\infty = \text{constant} = T_0$

- zone E: heating/cooling boundary conditions detailed in the next sections, either prescribing wall temperature and recession rate (Exp-x-T-x test cases), or computing convective heat flux and re-radiation based on surface energy balance (Exp-x-SEB-x test cases)

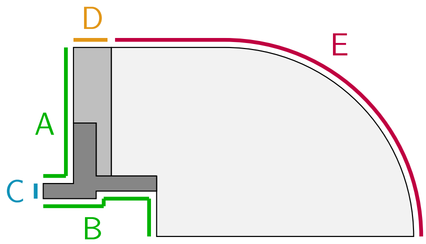


Figure 12: Different zones used for boundary conditions setting.

Prescribed wall temperature and recession rate (Exp-x-T-x)
The first type of boundary conditions is prescribing both:

- the wall temperature T_{w}
- the recession rate $\dot{r}_{\mathrm{w}}$;

The value of T_{w} and $\dot{r}_{\mathrm{w}}$ are test case dependent. They are time dependent, non-uniform and consistent with the experimental measurements [AD6], when both heating and cooling phases were monitored.

For each numerical test case Exp-x-T-x, the exact prescribed temperatures are available in a text file[10] named `surface_temperature.dat` as a table, e.g. Table 14 for Exp-2-T-Z.

The temperatures are provided (in rows) every 0.1 s, from 0 s until the end of the measurements, and (in columns) for 59 angular positions along the surface, for angles $\theta \in [0, 120.96379]$ defined as the angle at the sphere center, cf. Figure 13.

In a second text file[10] named `surface_recession.dat`, the updated polar coordinates of 59 points on the surface of the sample are provided in a similar way, e.g. Table 15 for Exp-2-T-Z.

[10] The `surface_temperature.dat` and `surface_recession.dat` files are available on the GitHub repository (see Appendix), in the 6 following folders:
`Test_case_description\Exp-x-x-x\Exp-i-x-m\Exp-i-T-m\BC_data`
where `i` is `1,2,3,3,4,5` and `m` is `P,Z,P,Z,Z,Z` respectively.

```
Temperature as a function of time and angular position

Angular position
   theta1_[deg]   .........   theta59_[deg]
              0.00000    2.30770    4.61537  ...  120.96376

Time and temperatures for the above positions
  time_[s]   T(theta1)_[K]      .........  T(theta59)_[K]
   0.00000  302.85000  302.85000  302.85000  ...  302.85000
   0.10000  544.31808  539.57029  532.47522  ...  468.93125
   0.20000  616.01582  610.20992  601.63121  ...  484.44698
   0.30000  669.75439  663.18042  653.51341  ...  496.30476
   0.40000  714.01358  706.82749  696.28358  ...  506.26142
   ...
 215.00000  781.65469  779.89241  774.90150  ...  546.25716
```

Table 14: `surface_temperature.dat` file (Exp-2-T-Z)

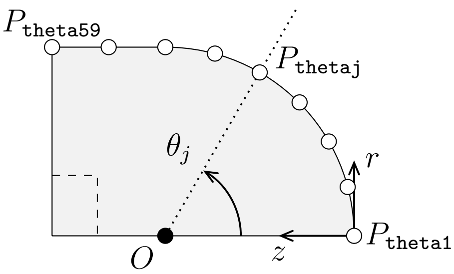


Figure 13: Angular position θ (only some of the 59 points are plot)

Recession at any time $\dot{r}_{\mathrm{w}}$ can be derived from these updated radii. The last definition time can be lower than the final time (defined in the `surface_temperature.dat` file). In such case, the coordinates are assumed to remain constant until the end, e.g. between 153 s and 215 s in the above example. This means there is no more recession over this final period (this happens during the cooling phase).

Convective heat flux and re-radiation (Exp-x-SEB-x)

The second type of boundary conditions is defined by applying a heat flux given by the same Equation 13 – similarly to what is done for 1D test cases.

The evolution in time of the heat transfer coefficient is assumed like in the Figure 9 (1D test cases), but the duration of the heating and cooling phases is test case dependent.

```
Polar coordinates (r,theta) as a function of time

Angular position
   theta1_[deg]   .........   theta59_[deg]
              0.00000    2.30770    4.61537   ...   120.96376

  time_[s]       r1_[mm]    .........       r59_[mm]
   0.00000   25.00000   25.00000   25.00000   ...    29.15476
   0.10000   25.00000   25.00000   25.00000   ...    29.15476
   0.20000   25.00000   25.00000   25.00000   ...    29.15476
   0.30000   25.00000   25.00000   25.00000   ...    29.15476
   0.40000   24.99999   24.99999   24.99999   ...    29.15476
      ...
 153.00000   23.83554   23.83554   23.83554   ...    29.15476
```

Table 15: `surface_recession.dat` file (Exp-2-T-Z)

The value of the heat transfer coefficient and the recovery enthalpy were again evaluated by aero-thermal calculations such that the resulting cold-wall heat flux is approximately matching experimental results.

These calculations led to the Table 16, which provides the evolution in time of the heat transfer coefficient $\rho_{\mathrm{e}} u_{\mathrm{e}} C_{\mathrm{H}}$ and the recovery enthalpy H_{r} at the stagnation point. A linear interpolation of $\rho_{\mathrm{e}} u_{\mathrm{e}} C_{\mathrm{H}}$ and H_{r} is assumed between the definition times indicated in the Table 16.

These parameters allow to compute the applied heat flux at stagnation point at any time $q_{\mathrm{w0}}(t)$. In order to extend the boundary condition definition to the full external surface of the samples, a heat flux distribution function $\varphi(s,t)$ must be define to "weight" the applied flux along the sample surface, so that:

$$q_{\mathrm{w}}(s,t) = \varphi(s,t)\ q_{\mathrm{w0}}(t) \tag{15}$$

A similar approach was used in the test case series 3 of the 5$^{\mathrm{th}}$ Ablation Workshop [RD3], but for another geometry (iso-q specimens).

Introducing such distribution function, the heat transfer coefficient $\rho_{\mathrm{e}} u_{\mathrm{e}} C_{\mathrm{H}}$ can be defined as a function of the curvilinear coordinate s along the specimen surface or the angle θ from 0° at stagnation point to approximately 120°, leading to film coefficient profiles based on CFD computations and illustrated[11] in the Figures 14 to 17.

[11] The exact value of the film coefficient profiles (together with surface pressure profiles) are available as tables on the GitHub repository (see Appendix) in a text file named `p_and_film_vs_theta.dat`

Exp-1-SEB-P			Exp-2-SEB-Z		
time [s]	H_{r} [J/kg]	$\rho_{\mathrm{e}}u_{\mathrm{e}}C_{\mathrm{H}}$ [kg/(m^2.s)]	time [s]	H_{r} [J/kg]	$\rho_{\mathrm{e}}u_{\mathrm{e}}C_{\mathrm{H}}$ [kg/(m^2.s)]
0	6.527 10^6	0.04576	0	7.883 10^6	0.051545
81.0	6.527 10^6	0.04576	160.5	7.883 10^6	0.051545
81.1	53910.	0.0	160.6	52480.	0.0
125.0	53910.	0.0	215.0	52480.	0.0
Exp-3-SEB-P			**Exp-3-SEB-Z**		
time [s]	H_{r} [J/kg]	$\rho_{\mathrm{e}}u_{\mathrm{e}}C_{\mathrm{H}}$ [kg/(m^2.s)]	time [s]	H_{r} [J/kg]	$\rho_{\mathrm{e}}u_{\mathrm{e}}C_{\mathrm{H}}$ [kg/(m^2.s)]
0	48.521 10^6	0.06951	0	48.204 10^6	0.0688
30.5	48.521 10^6	0.06951	5.5	48.204 10^6	0.0688
30.6	53910.	0.0	5.6	52391.	0.0
97.0	53910.	0.0	50.0	52391.	0.0
			1000.1	47.069 10^6	0.06728
			1061.0	47.069 10^6	0.06728
			1061.1	53910.	0.0
			1103.1	53910.	0.0
Exp-4-SEB-Z			**Exp-5-SEB-Z(-long)**		
time [s]	H_{r} [J/kg]	$\rho_{\mathrm{e}}u_{\mathrm{e}}C_{\mathrm{H}}$ [kg/(m^2.s)]	time [s]	H_{r} [J/kg]	$\rho_{\mathrm{e}}u_{\mathrm{e}}C_{\mathrm{H}}$ [kg/(m^2.s)]
0	44.920 10^6	0.07739	0	34.799 10^6	0.1671
90.2	44.920 10^6	0.07739	44.7	34.799 10^6	0.1603
90.3	52480.	0.0	44.8	52480.	0.0
169.0	52480.	0.0	126.0	52480.	0.0

Table 16: Heat transfer coefficient and the recovery enthalpy at the stagnation point for Exp-x-SEB-x test cases

It is worth noting that the hemispherical specimens are subjected to an evolution in time of their surface shape, hence an evolution of the distribution function. However, only the Exp-5-SEB-Z(-long) test case (the only super-sonic test) is subjected to a significant change in shape, so that an evolution in time should be considered. A linear interpolation in time between the initial and the final distributions is assumed (between 0 s and 45 s, cf. Figure 17). For all other test cases, a constant film coefficient profile is assumed.

in the 6 following folders:
`Test_case_description\Exp-x-x-x\Exp-i-x-m\Exp-i-SEB-m\BC_data`
where `i` is `1,2,3,3,4,5` and `m` is `P,Z,P,Z,Z,Z` respectively.

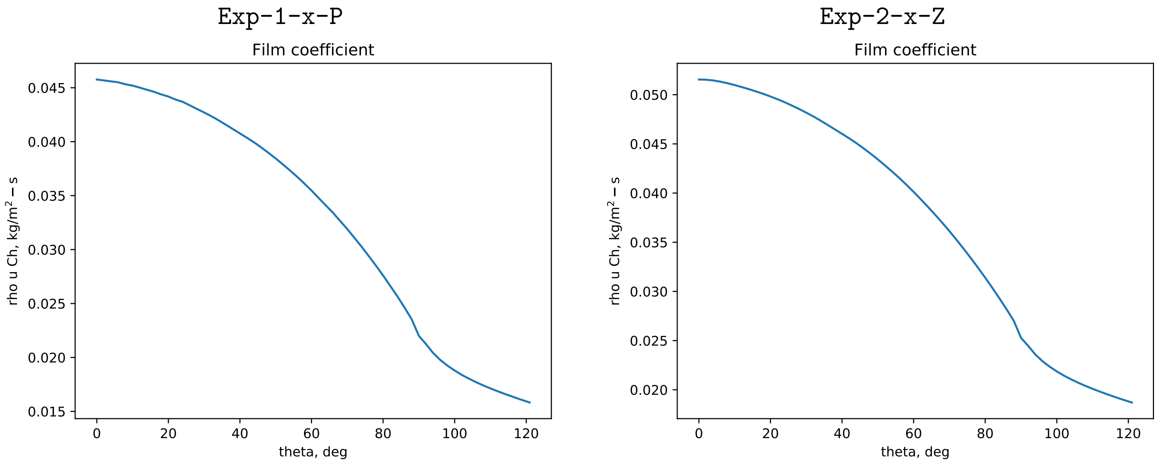


Figure 14: Film coefficient profiles for Exp-1-SEB-P and Exp-2-SEB-Z test cases.

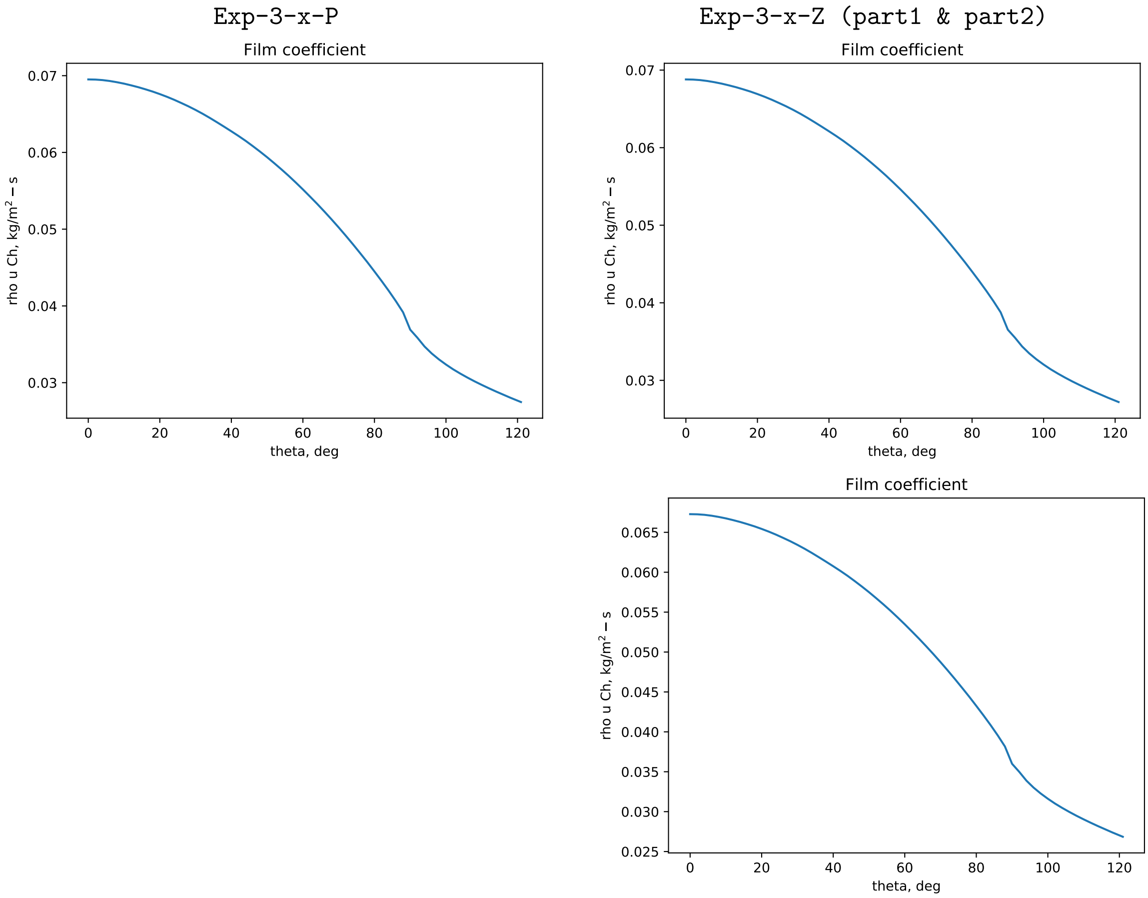


Figure 15: Film coefficient profiles for Exp-3-SEB-P and Exp-3-SEB-Z test cases. (`part1` is starting from $t = 0$ s, `part2` is starting from $t = 1000$ s)

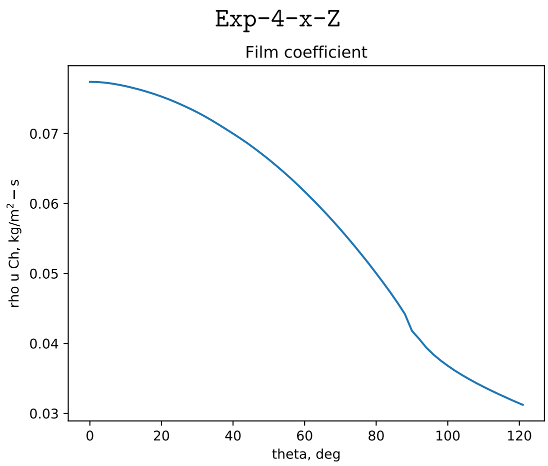


Figure 16: Film coefficient profile for Exp-4-SEB-Z test case.

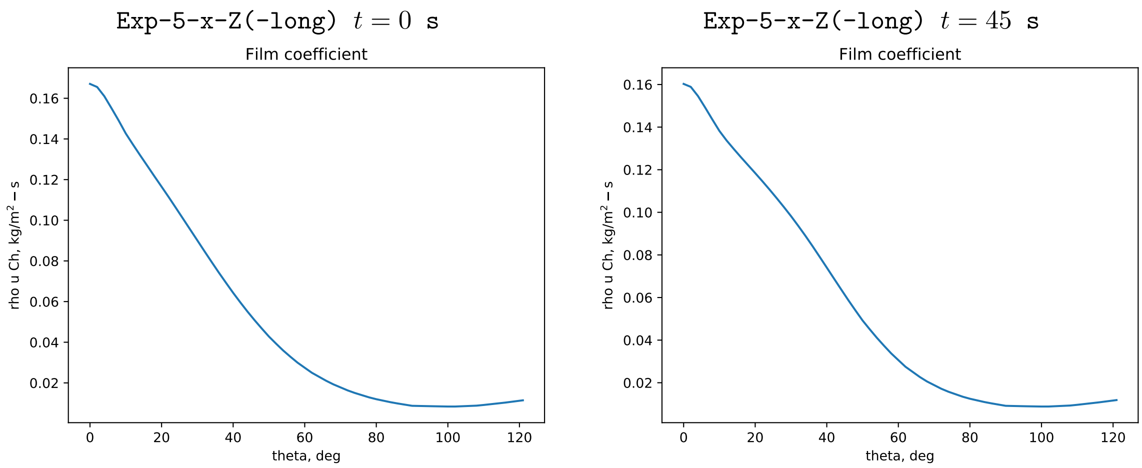


Figure 17: Film coefficient profiles for Exp-5-SEB-Z(-long) test case at times $t = 0$ s and $t = 45$ s.

In addition to this applied heat flux, re-radiation is active during the whole test, considering a view factor equal to 1 and the infinity temperature equals to the initial temperature $T_\infty = T_0$ (test case dependent, cf. Table 13). The emissivity of the virgin/charred material is defined in the material properties, cf. section 3.

Additional boundary conditions

The wall pressure P_w is prescribed during the test. Its value is case dependent and non uniform along the specimen surface. Like the film coefficient profiles, the pressure based on CFD computations is defined[12] as a function of the angle θ (from 0° at stagnation point to approximately 120°), cf. Figures 18 to 21. These profiles are constant in time for most of the test cases, but varying for the only Exp-5-SEB-Z(-long) test case.

When required by the test case definition, the recession speed at wall $\dot{r}_{\mathrm{w}}$ due to ablation must be modelled using the following assumptions:

- The factor for the blowing-correction correlation (CMA model) is taken as $\lambda = 0.5$
- Heat and mass transfer assumptions in the boundary layer are: $\mathrm{Pr} = \mathrm{Le} = 1$
- The wall enthalpy h_{w} and dimensionless ablation speed B'_{c} are provided as tables in the `Bprime_tables.txt` file as function of
  - the wall pressure P_{w} (in a range 0.001–1 bar)
  - the dimensionless out-gassing parameter B'_{g} (in the range 0–10)
  - the wall temperature T_{w} (in the range 300–3500 K)

  These tables are available for ZURAM® pyrolysis gas in both air and nitrogen atmospheres.

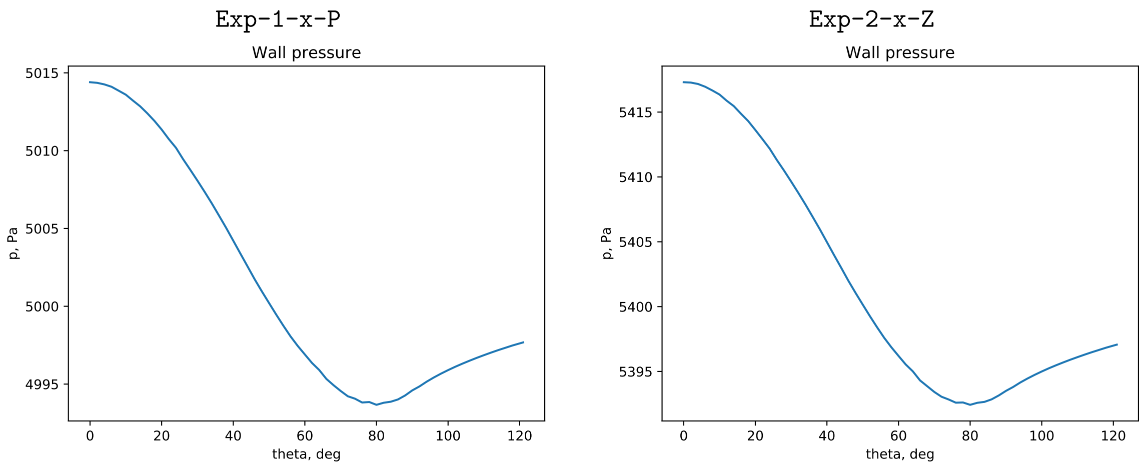


Figure 18: Pressure profiles for Exp-1-SEB-P and Exp-2-SEB-Z test cases.

[12] The exact value of the surface pressure profiles (together with film coefficient profiles) are available as tables on the GitHub repository (see Appendix) in a text file named `p_and_film_vs_theta.dat` in the 6 following folders:
`Test_case_description\Exp-x-x-x\Exp-i-x-m\Exp-i-SEB-m\BC_data`
where `i` is `1,2,3,3,4,5` and `m` is `P,Z,P,Z,Z,Z` respectively.

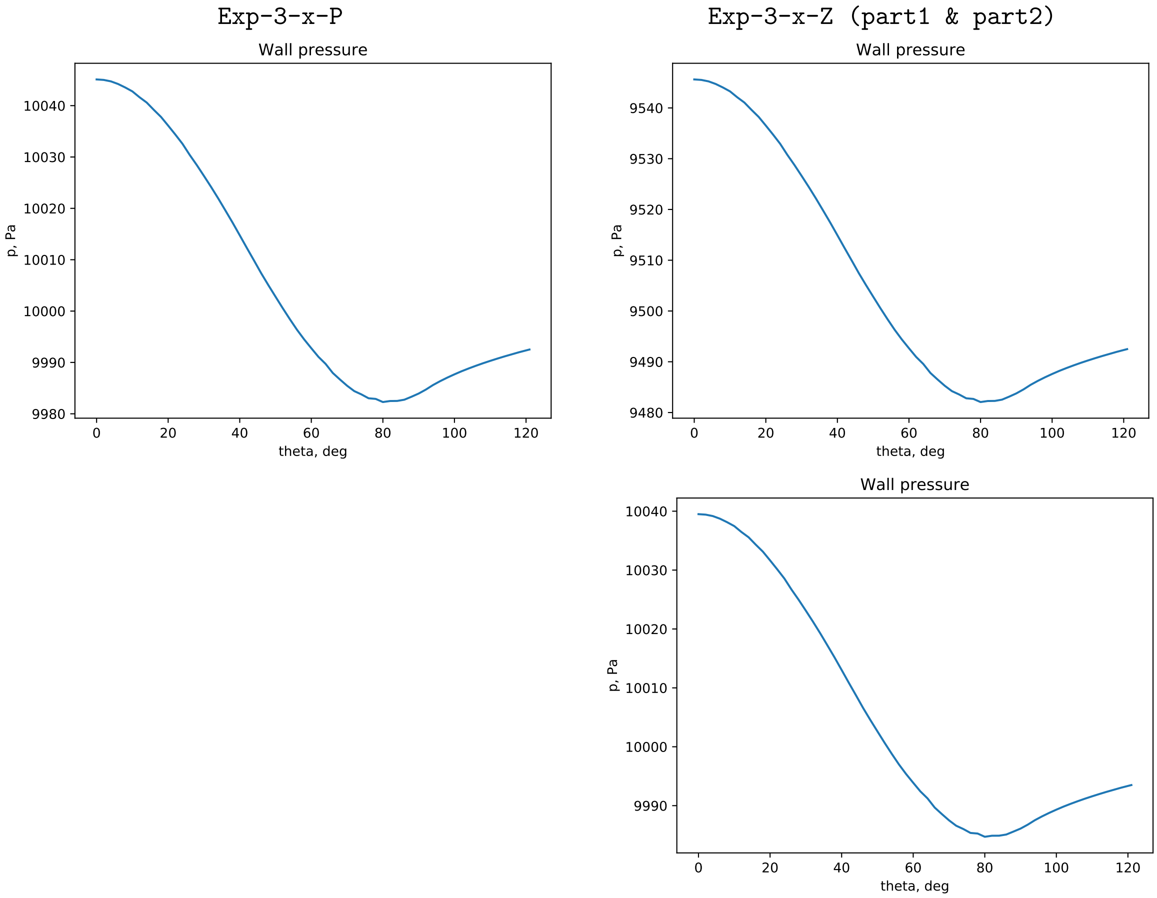


Figure 19: Pressure profiles for Exp-3-SEB-P and Exp-3-SEB-Z test cases.
(`part1` is starting from $t = 0$ s, `part2` is starting from $t = 1000$ s)

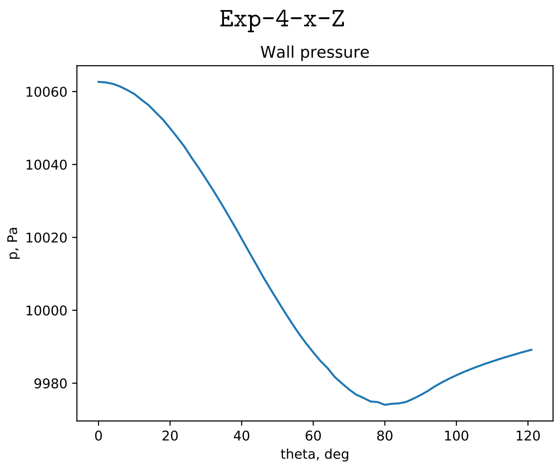


Figure 20: Pressure profile for Exp-4-SEB-Z test case.

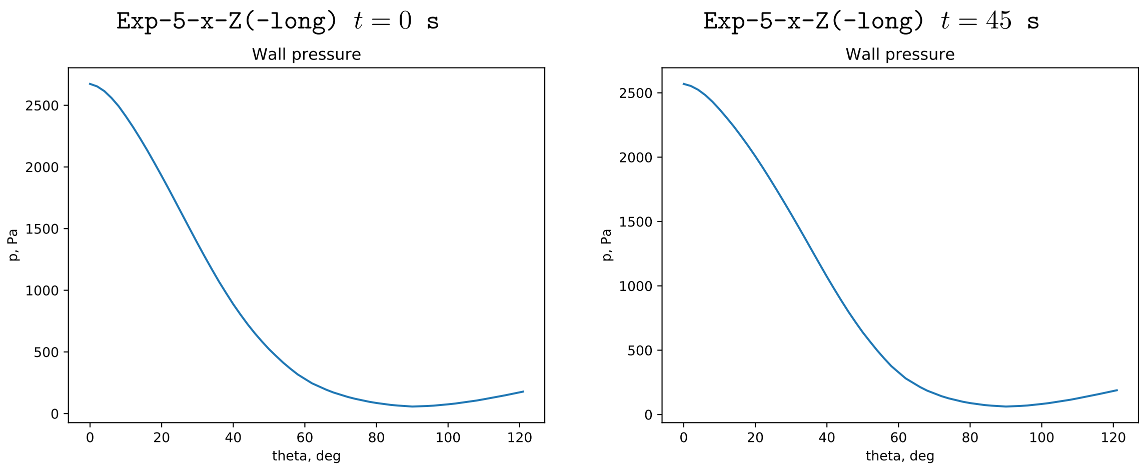


Figure 21: Pressure profiles for Exp-5-SEB-Z(-long) test case at times $t = 0$ s and $t = 45$ s.

4.2.4 Position of the thermocouples

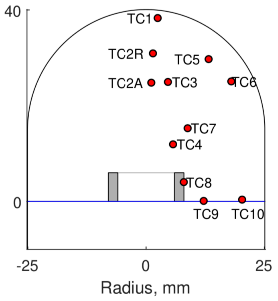
For both code-to-code and code-to-experiments comparisons, a set of specific locations are defined in order to provide time-dependent results (see section 5).

The exact positioning of the thermocouples was measured by tomographic analysis [AD6] and is summarized for all numerical test cases in the tables and sketches below (see Figures 22–27).

In addition to these real thermocouples, a virtual one called TC_0 is located on recession point ($r = z = 0$ in time $t = 0$). Later, it is moving with it when recession occurs, i.e. $r = 0$ and $z = z_\mathrm{w}$ (like a pyrometer), while other coordinates are fixed (like real thermocouples).

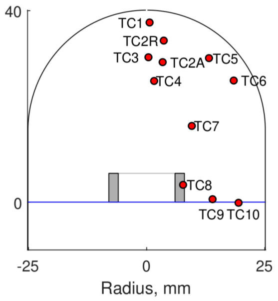
Notes:

1. In the tables from [AD6], the "axial" position was measured from the bottom circular base of the specimen, not from the nose. Therefore, the (r, z) coordinates in the numerical test cases can be computed as (all in mm):
   - z coordinate is $z = 40 -$ "axial"
   - r coordinate is $r =$ "radial"
2. Some thermocouples are not positioned within the hemispherical sample, but slightly in the graphite plug or the alumina disc. They are highlighted in the tables below.



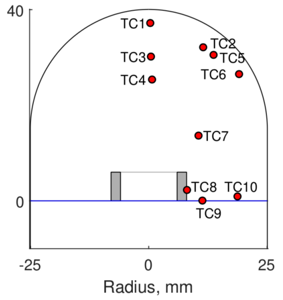
ID:	T1	T2A	T3	T4	T5	T6	T7	T8	T9	T10	T2R
type:	K	K	K	K	K	K	K	K	K	K	K
axial:	38.31	24.81	24.96	11.94	29.73	25.08	15.30	4.05	0.12	0.39	30.93
x pos:	1.94	1.09	0.49	-0.90	11.30	-17.99	7.39	-7.89	-11.82	-12.99	-1.30
y pos:	1.50	0.15	4.59	-5.63	6.85	0.67	-4.75	-1.15	-2.86	-15.58	0.65
radial:	2.46	1.10	4.62	5.70	13.21	18.00	8.78	7.97	12.17	20.29	1.45

Figure 22: Position of the thermocouples in EXP-1-x-P test case



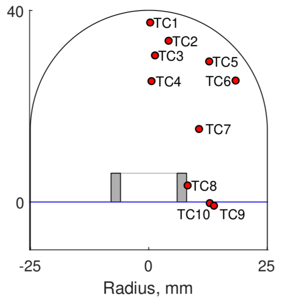
ID:	T1	T2A	T3	T4	T5	T6	T7	T8	T9	T10	T2R
type:	K	K	K	K	K	K	K	K	K	K	K
axial:	37.53	29.25	30.27	25.32	30.09	25.41	15.93	3.60	0.60	-0.15	33.75
x pos:	0.41	-0.39	0.18	1.58	10.32	-18.04	8.97	-7.59	-9.25	-8.98	-0.11
y pos:	0.47	3.36	0.34	0.15	-8.21	3.75	3.31	1.36	10.44	17.25	-3.62
radial:	0.62	3.39	0.38	1.59	13.19	18.43	9.56	7.71	13.95	19.45	3.62

Figure 23: Position of the thermocouples in EXP-2-x-Z test case



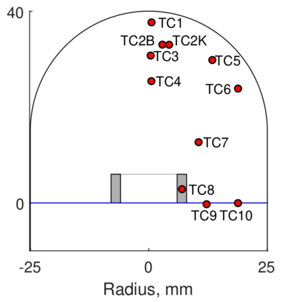
ID:	T1	T2	T3	T4	T5	T6	T7	T8	T9	T10
type:	B	B	K	K	K	K	K	K	K	K
axial:	37.20	32.13	30.18	25.38	30.54	26.52	13.65	2.28	0.06	0.93
x pos:	0.32	-10.57	-0.34	0.32	11.48	-19.06	9.25	-0.33	-9.33	-9.72
y pos:	-0.01	4.53	0.32	0.63	7.46	-0.84	-5.00	-8.08	-6.44	-16.03
radial:	0.32	11.50	0.47	0.70	13.69	19.08	10.51	8.08	11.34	18.75

Figure 24: Position of the thermocouples in EXP-3-x-P test case



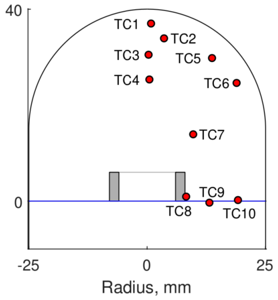
ID:	T1	T2	T3	T4	T5	T6	T7	T8	T9	T10
type:	B	B	K	K	K	K	K	K	K	K
axial:	37.50	33.69	30.63	25.26	29.37	25.38	15.24	3.45	-0.78	-0.24
x pos:	-0.20	-2.54	-1.25	-0.52	4.42	0.89	-6.88	-8.04	-4.46	-9.95
y pos:	0.23	-3.34	0.44	0.27	-11.98	18.33	-8.10	1.69	13.03	8.20
radial:	0.31	4.20	1.32	0.59	12.77	18.35	10.62	8.21	13.77	12.90

Figure 25: Position of the thermocouples in EXP-3-x-Z test case



ID:	T1	T2B	T3	T4	T5	T6	T7	T8	T9	T10	T2K
type:	B	B	K	K	K	K	K	K	K	K	K
axial:	37.71	33.06	30.78	25.44	29.85	23.88	12.69	2.88	-0.27	-0.03	33.03
x pos:	-0.45	0.66	0.09	-0.35	12.00	-18.86	8.89	-6.35	-11.77	-11.62	-0.21
y pos:	0.39	-2.80	0.40	0.43	6.03	0.40	-5.65	-3.02	-3.27	-14.85	4.31
radial:	0.60	2.88	0.41	0.56	13.44	18.87	10.53	7.03	12.22	18.86	4.31

Figure 26: Position of the thermocouples in EXP-4-x-Z test case



ID:	T1	T2	T3	T4	T5	T6	T7	T8	T9	T10
type:	B	B	K	K	K	K	K	K	K	K
axial:	37.02	33.93	30.51	25.35	29.82	24.63	13.92	0.93	-0.33	0.21
x pos:	0.81	0.24	-0.01	0.47	10.31	-18.76	8.99	-6.68	-11.81	-9.59
y pos:	0.15	-3.60	0.27	0.05	9.00	-2.32	-3.76	-4.85	-5.81	-16.64
radial:	0.82	3.61	0.27	0.47	13.69	18.90	9.74	8.25	13.16	19.20

Figure 27: Position of the thermocouples in EXP-5-x-Z test case

5 Output results and file format

File naming convention is `CodeName_Quantity_TestID.txt` where:

- `CodeName` is the code name, i.e. `Amaryllis`, `MABLE`, or `PATO`
- `Quantity` is related to the type of result, `Energy` for thermal response, `Density`, `Mass`, and `Recession` for the pyrolysis and ablation response
- `TestID` refers to the identification of the test as defined in the section 6, e.g. `Num-3-SEB-Z` or `Exp-5-T-Z`

Time sampling The output frequency is 1 s, starting at time $t = 0$ s, ending at the final time t_{end} which is test case dependent (see Table 17):

- for 1-D test cases, the final time is 120 s or 240 s
- for 2-D test cases, the final time is:
  - the time provided in the prescribed temperatures data files (cf. `BC_data/surface_temperature.dat`)
  - the end of heating-up + 100 s for Exp-x-SEB-x test cases

Test cases		t_{end} [s] xxx-x-T-x	xxx-x-SEB-x
Num-1-T-x		120	
Num-x-SEB-Z			240
Exp-1-x-P		125	181
Exp-2-x-Z		215	260
Exp-3-x-P		97	130
Exp-3-x-Z	part1	50	105
	part2	1103	1161
Exp-4-x-Z		169	190
Exp-5-x-Z	(-long)	126	145

Table 17: Final time t_{end} for all numerical test cases

5.1 Thermal response

The result files should be named as `CodeName_Energy_TestID.txt`. The results are the temperature [K] at the specific locations (thermocouples) defined in the Table 12 and in section 4.2.4, for 1D and 2D test cases, respectively. The results will be supplied in ASCII files, according to the following format:

time (s)	Tw (K)	T2 (K)	T3 (K)	T4 (K)	T5 (K)	...
0.0	3.000e2	3.000e2	3.000e2	3.000e2	3.000e2	...
1.0	9.651e2	3.225e2	3.000e2	3.000e2	3.000e2	...
2.0	1.076e3	3.956e2	3.039e2	3.000e2	3.000e2	...
etc.						

Table 18: Output format for the `CodeName_Energy_TestID.txt` files

5.2 Pyrolysis and ablation response

For each numerical test case involving pyrolysis and/or recession phenomena, three result files (in 1-D) or two result files (in 2-D) should be provided and named:

1. `CodeName_Density_TestID.txt`

The results are the density [kg/m^3] at the specific locations (thermocouples) defined in the Table 12 and in section 4.2.4, for 1D and 2D test cases, respectively.

The results will be supplied in ASCII files, according to the following format:

time (s)	rhow (kg/m3)	rho2 (kg/m3)	rho3 (kg/m3)	rho4 (kg/m3)	rho5 (kg/m3)	...
0.0	4.300e2	4.300e2	4.300e2	4.300e2	4.300e2	...
1.0	4.287e2	4.300e2	4.300e2	4.300e2	4.300e2	...
2.0	4.255e3	4.300e2	4.300e2	4.300e2	4.300e2	...
etc.						

Table 19: Output format for the `CodeName_Density_TestID.txt` files

2. `CodeName_Mass_TestID.txt`

Note: This file is only required for <u>1D numerical test cases</u> (Num-x-x-x).

The results are:

- blowing rates $\dot{m}_g$ [kg/(m^{2}s)] and $\dot{m}_c$ [kg/(m^{2}s)] at the outer surface;
- mass ratio: the ratio of the total mass $m(t)$ to the initial total mass $m(t_0)$ of the specimen [-];

The results will be supplied in ASCII files, according to the following format:

```
time      m_dot_g      m_dot_c         m/m0
 (s)    (kg/m2/s)    (kg/m2/s)          (-)
 0.0 0.00000e+00 0.00000e+00 1.00000e+00
 1.0 2.96958e-02 0.00000e+00 9.97795e-01
 2.0 2.17060e-02 0.00000e+00 9.96592e-01
etc.
```

Table 20: Output format for the `CodeName_Mass_TestID.txt` files

3. `CodeName_Recession_TestID.txt`

The results are:

- Pyrolysis zone, i.e. the depth [mm] of the “almost” virgin (98 %) front $z_{\rho_{v^*}}$ and the ”almost” charred (2 %) front $z_{\rho_{c^*}}$, the thresholds being defined as:

$$\rho_{v^*} = \rho_c + 0.98(\rho_v - \rho_c) = 417.3706 \text{ kg/m}^3 \tag{16}$$

$$\rho_{c^*} = \rho_c + 0.02(\rho_v - \rho_c) = 339.2554 \text{ kg/m}^3 \tag{17}$$

  where the densities ρ_i are the ones of the composite material (not the intrinsic densities of the virgin/charred resin).
  For the sake of simplicity, the depth of these two fronts is measured from the initial outer surface.
  In 2D test cases, these two fronts are only measured along the axis of symmetry (depth from the recession point).

- Surface recession, i.e. the coordinate(s) [mm] of some reference points on the receding surface:
  - In 1D test cases, the reference point is simply on the external heated surface, and the required output is the z-coordinate of the recession surface.
  - In 2D test cases, the reference points are defined as the intersection P_j between the recession surface and straight lines from the center O of the hemisphere circular base pointing in the direction θ_j (see Figure 28), where $\theta_j \in \{0°, 15°, 30°, 45°, 60°, 75°, 90°\}$.
    Two additional points – P_A and P_B – are defined to track the surface geometry evolution in the cylindrical part at mid-length of the cylinder ($z_A = 0.0325$ m) and at the ”bottom” surface ($z_B = 0.04$ m), respectively (see Figure 28).

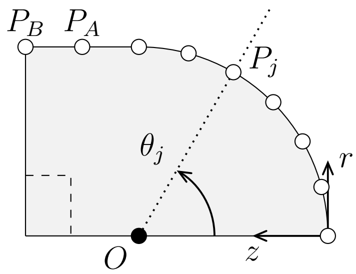


Figure 28: Position of the recession measurement points (for the 2D hemisphere test cases)

The results will be supplied in ASCII files, according to the following format:

For the 1D test cases:

time	z_virg98	z_char2	z_0
(s)	(m)	(m)	(m)
0.0	0	0	0
1.0	0	0	0
2.0	1.781e-4	2.130e-5	0
etc.			

Table 21: Output format for the `CodeName_Recession_TestID.txt` files (1D test cases).

For the 2D test cases:

- both r- and z-coordinates are required for $P_{15°}$, $P_{30°}$, $P_{45°}$, $P_{60°}$ and $P_{75°}$
- only the z-coordinate of $P_{0°}$ and the r-coordinate of $P_{90°}$, P_A and P_B make sense

time	z_virg98	z_char2	z_0	r_15	z_15	...	r_90	r_A	r_B
(s)	(m)	(m)	(m)	(m)	(m)	...	(m)	(m)	(m)
0.0	0	0	0	6.470e-1	8.852e-2	...	2.5e-3	2.5e-3	2.5e-3
1.0	0	0	0	6.470e-1	8.852e-2	...	2.5e-3	2.5e-3	2.5e-3
2.0	1.781e-4	2.130e-5	0	6.470e-1	8.852e-2	...	2.5e-3	2.5e-3	2.5e-3
etc.									

Table 22: Output format for the `CodeName_Recession_TestID.txt` files (2D test cases).

6 Detailed description of the numerical test cases

6.1 1D planar test cases

Num-1-T-P

This test is a simple 1D thermal analysis test with imposed boundary conditions. Because CALCARB® is used, the pyrolysis effect and gas mass flow are not present, and it is the simplest test one can perform with a thermal response code. The goal of this test is to complete the Num-x-x-x series, and prepare a CALCARB® thermal model, which is also used in the test campaign.

Included physical phenomena:

- ✓ λ_c

Numerical test conditions:

Test ID	Num-1-T-P
Plasmatron test name	–
Geometry	1D planar
Material	CALCARB®
Cold-wall heat flux	–
Gas	–
BC	T_w
Duration	120 s
Max T_w	1500 K
P_w	5000 Pa

Requested output results:

- ✓ thermal response

Num-1-T-Z

This numerical example comes from the 4^{th} Ablation Work Shop [RD1] for code comparison. The goal of this 1D example is to test the basic functionalities of a charring-ablator code, while at the same time avoiding the interaction between the balance equations on the one side and boundary conditions and mesh deformation (due to ablation) on the other. The example tests heat transfer, pyrolysis decomposition and unidirectional gas transfer.

Included physical phenomena:

- ✓ λ_{c}
- ✓ λ_{v}
- ✓ pyrolysis
- ✓ convective heat transfer

Numerical test conditions:

Test ID	Num-1-T-Z
Plasmatron test name	–
Geometry	1D planar
Material	ZURAM®
Cold-wall heat flux	–
Gas	–
BC	T_{w}
Duration	120 s
Max T_{w}	1500 K
P_{w}	5000 Pa

Requested output results:

- ✓ thermal response
- ✓ density (at TCs location)
- ✓ blowing rate
- ✓ pyrolysis zone
- ✓ mass

Num-2-SEB-Z

During the 5th Ablation Workshop [RD2], the simple numerical test Num-1-T-Z was extended, in order to include all relevant phenomena for charring ablators, defining tests of increasing complexity Num-x-SEB-Z. This test uses the SEB, but not yet surface ablation, thus modelling only the interaction between the balance equations and the boundary conditions. After heating phase, this test also include a cooling phase.

Included physical phenomena:

- ✓ λ_c
- ✓ λ_v
- ✓ pyrolysis
- ✓ convective heat transfer

Numerical test conditions:

Test ID	Num-2-SEB-Z
Plasmatron test name	–
Geometry	1D planar
Material	ZURAM®
Cold-wall heat flux	0.5 MW/m^2
Gas	N_2
BC	SEB
Duration	120 s + 120 s
Est. max T_w	$\approx$ 1500 K
P_w	5000 Pa

Requested output results:

- ✓ thermal response
- ✓ density (at TCs location)
- ✓ blowing rate
- ✓ pyrolysis zone
- ✓ mass

Num-3-SEB-Z

In the second numerical test of the 5^{th} Ablation Workshop the surface recession was added, and all the phenomena were therefore activated. The recession rate was still moderate, in order for the code developers to find problems with the interaction between mesh deformation (due to recession) and the solution of the balance equations. After heating phase, this test also include a cooling phase.

Included physical phenomena:

- ✓ λ_c
- ✓ λ_v
- ✓ pyrolysis
- ✓ convective heat transfer
- ✓ oxidation
- ✓ recession

Numerical test conditions:

Test ID	Num-3-SEB-Z
Plasmatron test name	–
Geometry	1D planar
Material	ZURAM®
Cold-wall heat flux	1.5 MW/m^2
Gas	Air
BC	SEB
Duration	120 s + 120 s
Est. max T_w	$\approx$ 1500 K
P_w	5000 Pa

Requested output results:

- ✓ thermal response
- ✓ density (at TCs location)
- ✓ blowing rate
- ✓ pyrolysis zone
- ✓ surface recession
- ✓ mass

Num-4-SEB-Z

In the final numerical test of the 5^{th} Ablation Workshop, all phenomena were activated and the heat flux was chosen such to be representative of a high heat flux condition with high ablation (sublimation regime). This example tests the interaction between all phenomena of a thermal response code for charring ablators. After heating phase, this test also include a cooling phase.

Included physical phenomena:

- ✓ λ_c
- ✓ λ_v
- ✓ pyrolysis
- ✓ convective heat transfer
- ✓ oxidation
- ✓ sublimation
- ✓ recession

Numerical test conditions:

Test ID	Num-4-SEB-Z
Plasmatron test name	–
Geometry	1D planar
Material	ZURAM®
Cold-wall heat flux	5.0 MW/m^2
Gas	Air
BC	SEB
Duration	120 s + 120 s
Est. max T_w	$\approx$ 3000 K
P_w	5000 Pa

Requested output results:

- ✓ thermal response
- ✓ density (at TCs location)
- ✓ blowing rate
- ✓ pyrolysis zone
- ✓ surface recession
- ✓ mass

6.2 2D axisymmetric test cases – Low heat flux

Exp-1-T-P/Exp-1-SEB-P

The objective is to test the CALCARB® for low heat flux conditions in Nitrogen environment. No recession takes place and the only variables are the thermal properties of CALCARB® . Two types of boundary conditions are tested, allowing the separation of boundary conditions from the volume balance equations.

Included physical phenomena:

- ✓ 2D effects
- ✓ λ_{c}

Numerical tests conditions:

Test ID	Exp-1-T-P
Plasmatron test name	P-N-50-q300
Geometry	2D hemisphere
Material	CALCARB®
Cold-wall heat flux	0.3 MW/m^2
Gas	N_2
BC	T_{w}, $\dot{r}_{\mathrm{w}}$
Duration	heating $\approx$ 80 s + cooling $\approx$ 45 s
Est. max T_{w}	$\approx$ 1500 K
Est. P_{w}	$\approx$ 5000 Pa

Test ID	Exp-1-SEB-P
Plasmatron test name	P-N-50-q300
Geometry	2D hemisphere
Material	CALCARB®
Cold-wall heat flux	0.3 MW/m^2
Gas	N_2
BC	SEB
Duration	heating $\approx$ 80 s + cooling $\approx$ 100 s
Est. max T_{w}	$\approx$ 1500 K
Est. P_{w}	$\approx$ 5000 Pa

Requested output results:

- ✓ thermal response

Exp-2-T-Z/Exp-2-SEB-Z

A fully instrumented set of tests with ZURAM® in Air environment and low heat flux levels is performed. This is adding the effect of pyrolysis and oxidation at the surface, w.r.t. to the previous tests. Two types of boundary conditions are tested, allowing the separation of boundary conditions from the volume balance equations.

Included physical phenomena:

- ✓ 2D effects
- ✓ λ_c
- ✓ λ_v
- ✓ pyrolysis
- ✓ convective heat transfer
- ✓ oxidation

Numerical tests conditions:

Test ID	Exp-2-T-Z
Plasmatron test name	Z-A-50-q300
Geometry	2D hemisphere
Material	ZURAM®
Cold-wall heat flux	0.3 MW/m^2
Gas	Air
BC	T_w, $\dot{r}_\mathrm{w}$
Duration	≈ 160 s + cooling
Duration	heating ≈ 160 s + cooling ≈ 55 s
Est. max T_w	≈ 1500 K
Est. P_w	≈ 5000 Pa

Test ID	Exp-2-SEB-Z
Plasmatron test name	Z-A-50-q300
Geometry	2D hemisphere
Material	ZURAM®
Cold-wall heat flux	0.3 MW/m^2
Gas	Air
BC	SEB
Duration	heating ≈ 160 s + cooling ≈ 100 s
Est. max T_w	≈ 1500 K
Est. P_w	≈ 5000 Pa

Requested output results:

- ✓ thermal response
- ✓ density (at TCs location)
- ✓ blowing rate
- ✓ pyrolysis zone
- ✓ surface recession
- ✓ mass

6.3 2D hemispherical test cases – High heat flux

Exp-3-T-P/Exp-3-SEB-P

Included physical phenomena:

- ✓ 2D effects
- ✓ λ_c
- ✓ non-equilibrium radiation (re-run with higher fidelity internal radiation model)

Numerical tests conditions:

Test ID	Exp-3-T-P
Plasmatron test name	P-N-100-q2500
Geometry	2D hemisphere
Material	CALCARB®
Cold-wall heat flux	2.5 MW/m^2
Gas	N_2
BC	T_w, $\dot{r}_w$
Duration	heating ≈ 30 s
	+ cooling ≈ 65 s
Est. max T_w	≈ 2500 K
Est. P_w	≈ 10000 Pa

Test ID	Exp-3-SEB-P
Plasmatron test name	P-N-100-q2500
Geometry	2D hemisphere
Material	CALCARB®
Cold-wall heat flux	2.5 MW/m^2
Gas	N_2
BC	SEB
Duration	heating ≈ 30 s
	+ cooling ≈ 100 s
Est. max T_w	≈ 2500 K
Est. P_w	≈ 10000 Pa

Requested output results:

- ✓ thermal response

Exp-3-T-Z/Exp-3-SEB-Z

A fully instrumented set of tests with ZURAM® in an N_2 environment and high heat flux levels is performed. This is adding the pyrolysis effect, w.r.t. to the Exp-3-x-P tests. Two types of boundary conditions are tested, allowing the separation of boundary conditions from the volume balance equations.

Included physical phenomena:

- ✓ 2D effects
- ✓ λ_c
- ✓ λ_v
- ✓ pyrolysis
- ✓ convective heat transfer

Numerical tests conditions:

Test ID	Exp-3-T-Z
Plasmatron test name	Z-N-100-q2500
Geometry	2D hemisphere
Material	ZURAM®
Cold-wall heat flux	2.5 $\mathrm{MW/m^2}$
Gas	N_2
BC	T_w, $\dot{r}_\mathrm{w}$
Duration	part 1: heating $\approx$ 5 s
	+ cooling $\rightarrow$1000 s
	part 2: heating $\approx$ 60 s
	+ cooling $\approx$ 40 s
Est. max T_w	$\approx$ 2500 K
Est. P_w	$\approx$ 10000 Pa

Test ID	Exp-3-SEB-Z
Plasmatron test name	Z-N-100-q2500
Geometry	2D hemisphere
Material	ZURAM®
Cold-wall heat flux	2.5 $\mathrm{MW/m^2}$
Gas	N_2
BC	SEB
Duration	part 1: heating $\approx$ 5 s
	+ cooling $\rightarrow$1000 s
	part 2: heating $\approx$ 60 s
	+ cooling $\approx$ 100 s
Est. max T_w	$\approx$ 2500 K
Est. P_w	$\approx$ 10000 Pa

Requested output results:

- ✓ thermal response
- ✓ density (at TCs location)
- ✓ blowing rate
- ✓ pyrolysis zone
- ✓ surface recession
- ✓ mass

Exp-4-T-Z/Exp-4-SEB-Z

This set of tests (high heat flux level), extends the Exp-3-x-Z tests to include oxidation due to the Air environment. Two types of boundary conditions are tested, allowing the separation of boundary conditions from the volume balance equations.

Included physical phenomena:

- ✓ 2D effects
- ✓ λ_c
- ✓ λ_v
- ✓ pyrolysis
- ✓ convective heat transfer
- ✓ oxidation
- ✓ recession

Numerical tests conditions:

Test ID	Exp-4-T-Z
Plasmatron test name	Z-A-100-q2500
Geometry	2D hemisphere
Material	ZURAM®
Cold-wall heat flux	2.5 MW/m^2
Gas	Air
BC	T_w, $\dot{r}_w$
Duration	heating ≈ 90 s + cooling ≈ 80 s
Est. max T_w	≈ 2500 K
Est. P_w	≈ 10000 Pa

Test ID	Exp-4-SEB-Z
Plasmatron test name	Z-A-100-q2500
Geometry	2D hemisphere
Material	ZURAM®
Cold-wall heat flux	2.5 MW/m^2
Gas	Air
BC	SEB
Duration	heating ≈ 90 s + cooling ≈ 100 s
Est. max T_w	≈ 2500 K
Est. P_w	≈ 10000 Pa

Requested output results:

- ✓ thermal response
- ✓ density (at TCs location)
- ✓ blowing rate
- ✓ pyrolysis zone
- ✓ surface recession
- ✓ mass

6.4 2D hemispherical test cases – Supersonic conditions

Exp-5-T-Z/Exp-5-SEB-Z

These tests extend the range of the flow to supersonic conditions. This is resulting in higher heat flux levels and higher recession rates leading to shape change of the sample surface. These tests include all the phenomena that can be modelled in the thermal response codes.

Included physical phenomena:

- ✓ 2D effects
- ✓ λ_{c}
- ✓ λ_{v}
- ✓ pyrolysis
- ✓ convective heat transfer
- ✓ oxidation
- ✓ sublimation
- ✓ recession
- ✓ shape change
- ✓ non-equilibrium radiation (re-run with higher fidelity internal radiation model)

Numerical tests conditions:

Test ID	Exp-5-T-Z
Plasmatron test name	Z-A-25-q4500-sup (45s)
Geometry	2D hemisphere
Material	ZURAM®
Cold-wall heat flux	4.5 MW/m^2
Gas	Air
BC	T_{w}, $\dot{r}_{\mathrm{w}}$
Duration	heating ≈ 45 s + cooling ≈ 80 s
Est. max T_{w}	≈ 2750 K
Est. P_{w}	≈ 2500 Pa

Test ID	Exp-5-SEB-Z
Plasmatron test name	Z-A-25-q4500-sup (45s)
Geometry	2D hemisphere
Material	ZURAM®
Cold-wall heat flux	4.5 MW/m^2
Gas	Air
BC	SEB
Duration	heating ≈ 45 s + cooling ≈ 100 s
Est. max T_{w}	≈ 2750 K
Est. P_{w}	≈ 2500 Pa

Requested output results:

- ✓ thermal response
- ✓ density (at TCs location)
- ✓ blowing rate
- ✓ pyrolysis zone
- ✓ surface recession
- ✓ mass

APPENDIX: AblaNTIS GitHub repository

A GitHub repository has been created to group all the reference data and documents. The URL of this repository is: `https://github.com/ablantis/AblaNTIS-test-cases`

The repository contains several folders described in the following sections:

Bprime and pyrolysis gas dataset

Folder and sub-folders structure:

```
Bprime_and_pyrogas_dataset
├──carbonPhenolInAir
│   ├──Plots
│   └──Tab_carbonPhenolInAir_AblaNTIS
├──carbonPhenolInNitrogen
│   ├──Plots
│   └──Tab_carbonPhenolInNitrogen_AblaNTIS
└──Pyrogas
    ├──Thermal_cond
    │   ├──Plots
    │   └──Pyrogas_AblaNTIS
    └──Viscosity
        ├──Plots
        └──Pyrogas_AblaNTIS
```

The contents of this folder is detailed in a `readme.txt` file:

```
    /\   | |   | |        | \ | |__   __|_   _|/ ____|
   /  \  | |__ | | __ _|  \| |  | |    | | | (___
  / /\ \ | '_ \| |/ _` | . ` |  | |    | |  \___ \
 / ____ \| |_) | | (_| | |\  |  | |   _| |_ ____) |
/_/    \_\_.__/|_|\__,_|_| \_|  |_|  |_____|_____/

PYROLYSIS GAS AND B'-TABLE DATASET

This folder contains the B' tables and the transport properties for
the official pyrolysis gas of AblaNTIS (mole frc. C:0.171, H:0.722,
O:0.107).
All the data have been generate with the Mutation++ v1.0.1 that can be
cloned from https://github.com/mutationpp/Mutationpp

Content descriptions:

   * carbonPhenolInAir_AblaNTIS.xml: Mutation++ mixture of Air+Pyrogas
   for B' table generation.

   * carbonPhenolInNitrogen_AblaNTIS.xml: Mutation++ mixture of
   Nitrogen+Pyrogas for B' table generation.
```

```
* bprime_VKI_bash.sh: Example bash script to generate B' tables
using either carbonPhenolInAir_AblaNTIS.xml or
carbonPhenolInNitrogen_AblaNTIS.xml.

* carbonPhenolInAir: contains B' tables for Air+Pyrogas generated
using carbonPhenolInAir_AblaNTIS.xml and some plots of part of the
data.

* carbonPhenolInNitrogen: contains B' tables for Nitrogen+Pyrogas
generated using carbonPhenolInNitrogen_AblaNTIS.xml and some plots
of part of the data.

* Pyrogas: contains the generated transport properties for the
AblaNTIS pyrogas and some plots.
```

Material dataset

Folder and sub-folders structure:

```
Material_dataset
└──Insulators
```

The root folder contains an OpenOffice spreadsheet detailing the properties of ZURAM® and CALCARB® CBCF 18-2000 (`Tacot_Zuram_Calcarb_database_v4.3.1.ods`).

The `Insulators` sub-folder contains two `.txt` files detailing thermal properties of alumina and graphite.

Refs

Folder and sub-folders structure:

```
Refs
├──DLR_data
├──Docs
└──VKI_data
```

These folders contains several reference documents, among others:

- `ZURAM® material data_update.xlsx` [RD6]
- `TACOT_3.0.xls` [RD7]
- `Zuram_aged_data_en.xlsx` [RD8]
- `calcarb_brochure.pdf` [RD10]

Test case description

Folder and sub-folders structure:

```
Test_case_description
├──Exp-x-x-x
│   ├──Exp-1-x-P
│   │   ├──Exp-1-SEB-P
│   │   │   └──BC_data
│   │   ├──Exp-1-T-P
│   │   │   └──BC_data
│   │   └──TC_meas_data
│   ├──Exp-2-x-Z
│   │   ├──Exp-2-SEB-Z
│   │   │   └──BC_data
│   │   ├──Exp-2-T-Z
│   │   │   └──BC_data
│   │   └──TC_meas_data
│   ├──Exp-3-x-P
│   │   ├──Exp-3-SEB-P
│   │   │   └──BC_data
│   │   ├──Exp-3-T-P
│   │   │   └──BC_data
│   │   └──TC_meas_data
│   ├──Exp-3-x-Z
│   │   ├──Exp-3-SEB-Z
│   │   │   └──BC_data
│   │   ├──Exp-3-T-Z
│   │   │   └──BC_data
│   │   └──TC_meas_data
│   ├──Exp-4-x-Z
│   │   ├──Exp-4-SEB-Z
│   │   │   └──BC_data
│   │   ├──Exp-4-T-Z
│   │   │   └──BC_data
│   │   └──TC_meas_data
│   ├──Exp-5-x-Z-long
│   │   ├──Exp-5-SEB-Z-long
│   │   │   └──BC_data
│   │   ├──Exp-5-T-Z-long
│   │   │   └──BC_data
│   │   └──TC_meas_data
│   └──Exp-5-x-Z-short
│       ├──Exp-5-T-Z-short
│       │   └──BC_data
│       └──TC_meas_data
└──Num-x-x-x
```

This folder contains sets of input data for the numerical test cases simulations.

Num-x-x-x subfolder mainly contains the `AblaNTIS_1D_environment_conditions.txt` file where are listed the tests duration, the boundary conditions (T_w, P_w, H_r, $\rho_\mathrm{e} u_\mathrm{e} C_\mathrm{H}$) for all the 1-D planar test cases:

```
          _     _       _   _ ------- -----  -----
    /\   | |   | |     | \ | |__   __|_   _|/ ____|
   /  \  | |__ | | __ _|  \| |  | |    | | | (___
  / /\ \ | '_ \| |/ _` | . ` |  | |    | |  \___ \
 / ____ \| |_) | | (_| | |\  |  | |   _| |_ ____) |
/_/    \_\_.__/|_|\__,_|_| \_|  |_|  |_____|_____/

Surface boundary conditions for the 1D test cases


----------------------------
 Nomenclature
----------------------------
Tw     -- Surface temperature
Pw     -- Surface pressure
Hr     -- Recovery enthalpy
CH     -- Heat transfer coefficient = rho_e*u_e*StH

StH    -- Stanton number for heat transfer
h_e    -- Edge gas enthalpy
u_e    -- Edge gas flow speed
rho_e  -- Edge gas density
P_e    -- Edge gas pressure


----------------------------
 Notes
----------------------------
- Surface properties are linearly interpolated between tabulated values
- Where appropriate, edge gas properties are provided to help ensure
  that the calculated recovery enthalpy is consistant with the
  calculated
  surface gas enthalpy.
-- Edge properties were calculated with Mutation++ version ?.? using
the
   'air_5' mixture
-- Recovery enthalpy is calculated using, Hr = h_e + u_e^2/2


%%%%%%%%%%%%%
% Num-1-T-P %
%%%%%%%%%%%%%
Total test duration:  120 s
```

```
--------------------
 Surface conditions
--------------------
Time [s],  Tw [K], Pw [Pa]
0,            300,    5000
0.01,        1500,    5000
120,         1500,    5000


%%%%%%%%%%%%%
% Num-1-T-Z %
%%%%%%%%%%%%%
Total test duration:  120 s

--------------------
 Surface conditions
--------------------
Time [s],  Tw [K], Pw [Pa]
0,            300,    5000
0.01,        1500,    5000
120,         1500,    5000


%%%%%%%%%%%%%%%
% Num-2-SEB-Z %
%%%%%%%%%%%%%%%
Total test duration:   240 s
Edge gas composition:  Nitrogen

--------------------
 Surface conditions
--------------------
Time [s], Pw [Pa],  Hr [J/kg], CH [kg/m^2/s]
0,           5000,  9418113.0,      0.042617
120,         5000,  9418113.0,      0.042617
120.1,       5000,  52477.051,      0.001
240,         5000,  52477.051,      0.001

---------------------------------------------------
 Edge gas properties (supplementary information)
---------------------------------------------------
Time [s], P_e [Pa],  T_e [K], u_e [m/s]
0,           5000,     4455,      41.5
120,         5000,     4455,      41.5
120.1,       5000,      350,       0.0
240,         5000,      350,       0.0


%%%%%%%%%%%%%%%
% Num-3-SEB-Z %
```

```
%%%%%%%%%%%%%%%
Total test duration:   240 s
Edge gas composition:  air_5

-------------------
 Surface conditions
-------------------
Time [s], Pw [Pa],  Hr [J/kg], CH [kg/m^2/s]
0,            5000,  28172526.,      0.065487
120,          5000,  28172526.,      0.065487
120.1,        5000,  52477.051,      0.001
240,          5000,  52477.051,      0.001

-------------------------------------------------
 Edge gas properties (supplementary information)
-------------------------------------------------
Time [s], P_e [Pa],  T_e [K], u_e [m/s]
0,             5000,     6148,     142.5
120,           5000,     6148,     142.5
120.1,         5000,      350,       0.0
240,           5000,      350,       0.0


%%%%%%%%%%%%%%%
% Num-4-SEB-Z %
%%%%%%%%%%%%%%%
Total test duration:   240 s
Edge gas composition:  air_5

-------------------
 Surface conditions
-------------------
Time [s], Pw [Pa],  Hr [J/kg], CH [kg/m^2/s]
0,            5000,      2.5e7,      0.1872
120,          5000,      2.5e7,      0.1872
120.1,        5000,  52477.051,      0.001
240,          5000,  52477.051,      0.001

-------------------------------------------------
 Edge gas properties (supplementary information)
-------------------------------------------------
Time [s], P_e [Pa],  T_e [K], u_e [m/s]
0,             5000,        ?,         ?
120,           5000,        ?,         ?
120.1,         5000,      350,       0.0
240,           5000,      350,       0.0
```

Exp-x-x-x subfolder contains similar data for all the 2-D axi-symmetric test cases. There is a general file `AblaNTIS_2D_environment_conditions.txt`:

```
          _     _       _   _ _______ _____  _____ 
    /\   | |   | |     | \ | |__   __|_   _|/ ____|
   /  \  | |__ | | __ _|  \| |  | |    | | | (___  
  / /\ \ | '_ \| |/ _` | . ` |  | |    | |  \___ \ 
 / ____ \| |_) | | (_| | |\  |  | |   _| |_ ____) |
/_/    \_\_.__/|_|\__,_|_| \_|  |_|  |_____|_____/ 

Boundary and initial conditions for the 2D experimental test cases


----------------------------
 Nomenclature
----------------------------
Pw     -- Surface pressure at stagnation point
H0     -- Total enthalpy of edge gas (h_e + u_e^2/2)
CH     -- Heat transfer coefficient (rho_e*u_e*StH) at stagnation point
Ti     -- Initial sample temperature (initial temperature of the TC
raising the least in each specific case)

h_e    -- Edge gas enthalpy
u_e    -- Edge gas flow speed
rho_e  -- Edge gas density
h_w    -- Wall enthalpy
StH    -- Stanton number for heat transfer (heat_flux/(H0-hw))


----------------------------
 Notes
----------------------------
- "Total test duration" includes both the heating (plasma on) and the
cooling (plasma off) and corresponds to the time for which
thermocouple measurement data are provided.
- The provided "total enthalpy" was used for the computation of the CH
(provided for each test in the specific test-case folder) through CFD
simulations w/ hot wall (isothermal at the measured steady-state
experimental wall temperature) and w/o ablation.
- The distribution of CH and Pw along the surface are provided for
each Exp-x-SEB-x case in the specific "BC_data" folder.

%%%%%%%%%%%%%
% Exp-1-x-P %
%%%%%%%%%%%%%
Plasmatron-test name: P-N-50-q300
Total test duration: 125 s
Gas: Nitrogen
Ti [K]: 302.45
```

```
--------------------
 Surface conditions
--------------------
Time_[s]   Plasma_heat_on/off   CH_[kg/m^2/s]   Pw_[Pa]   H0_[MJ/kg]
0.0        ON                   4.576e-2        5014      6.527
81.1       OFF                  0.0             5014      5.391e-2
125      OFF                  0.0             5014      5.391e-2


%%%%%%%%%%%%%
% Exp-2-x-Z %
%%%%%%%%%%%%%
Plasmatron-test name: Z-A-50-q300
Total test duration: 215 s
Gas: Air
Ti [K]: 302.85

--------------------
 Surface conditions
--------------------
Time_[s]   Plasma_heat_on/off   CH_[kg/m^2/s]   Pw_[Pa]   H0_[MJ/kg]
0.0        ON                   5.1545e-2       5417      7.883
160.6      OFF                  0.0             5417      5.248e-2
215        OFF                  0.0             5417      5.248e-2


%%%%%%%%%%%%%
% Exp-3-x-P %
%%%%%%%%%%%%%
Plasmatron-test name: P-N-100-q2500
Total test duration: 97 s
Gas: Nitrogen
Ti [K]: 301.55

--------------------
 Surface conditions
--------------------
Time_[s]   Plasma_heat_on/off   CH_[kg/m^2/s]   Pw_[Pa]   H0_[MJ/kg]
0.0        ON                   6.951e-2        10045     48.521
30.6       OFF                  0.0             10045     5.391e-2
97         OFF                  0.0             10045     5.391e-2


%%%%%%%%%%%%%
% Exp-3-x-Z %
%%%%%%%%%%%%%
Plasmatron-test name: Z-N-100-q2500
Total test duration: 1103 s (i.e., 50 s + cooldown + 103 s)
Gas: Nitrogen
```

```
Ti_part1 [K]: 309.35

-------------------
 Surface conditions
-------------------
Time_[s]   Plasma_heat_on/off   CH_[kg/m^2/s]   Pw_[Pa]   H0_[MJ/kg]
0.0        ON                   6.880e-2        9546      48.204
5.6        OFF                  0.0             9546      5.391e-2
50         OFF                  0.0             9546      5.391e-2
1000.1     ON                   6.728e-2        10039     47.069
1061.1     OFF                  0.0             10039     5.391e-2
1103.1     OFF                  0.0             10039     5.391e-2


%%%%%%%%%%%%%
% Exp-4-x-Z %
%%%%%%%%%%%%%
Plasmatron-test name: Z-A-100-q2500
Total test duration: 169 s
Gas: Air
Ti [K]: 310.05

-------------------
 Surface conditions
-------------------
Time_[s]   Plasma_heat_on/off   CH_[kg/m^2/s]   Pw_[Pa]   H0_[MJ/kg]
0.0        ON                   7.739e-2        10063     44.920
90.3       OFF                  0.0             10063     5.248e-2
169        OFF                  0.0             10063     5.248e-2


%%%%%%%%%%%%%%%%%%
% Exp-5-x-Z-long %
%%%%%%%%%%%%%%%%%%
Plasmatron-test name: Z-A-25-q4500-sup (45s)
Total test duration: 126 s
Gas: Air
Ti [K]: 307.25
Note: for this test the CH and the Pw (at stagnation and its
distribution) are provided also for the final shape. Check the test
case description booklet for the details on how to handle this in the
numerical test case.

-------------------
 Surface conditions
-------------------
Time_[s]   Plasma_heat_on/off   CH_[kg/m^2/s]   Pw_[Pa]   H0_[MJ/kg]
0.0        ON                   1.671e-1        2674      34.799
44.7       ON                   1.603e-1        2569      34.799
44.8       OFF                  0.0             550       5.248e-2
```

```
126        OFF                  0.0             550      5.248e-2


%%%%%%%%%%%%%%%%%%%%
% Exp-5-x-Z-short %
%%%%%%%%%%%%%%%%%%%%
Plasmatron-test name: Z-A-25-q4500-sup (20 s)
Total test duration: 120 s
Gas: Air
Ti [K]: 293.65
Note: This test is not officially part of the AblaNTIS numerical
tests. The experiment was an exact repetition of the 45-s test. The CH
for the ablated shape at 20 s hasn't been computed. The Surface and
initial conditions are provideed only for completeness.

--------------------
 Surface conditions
--------------------
Time_[s]   Plasma_heat_on/off   CH_[kg/m^2/s]   Pw_[Pa]  H0_[MJ/kg]
0.0        ON                   1.671e-1        2674     34.799
20.1       OFF                  0.0             550      5.248e-2
120        OFF                  0.0             550      5.248e-2
```

Then, for each experiment, one sub-folder divided into 3 sub-folders, e.g. for Exp-4-x-Z:

```
│   ├──Exp-4-x-Z
│   │   ├──Exp-4-SEB-Z
│   │   │   └──BC_data
│   │   ├──Exp-4-T-Z
│   │   │   └──BC_data
│   │   └──TC_meas_data
```

- the `Exp-x-SEB-x` folder is related to the data for SEB type boundary conditions: the pressure profile and the film coefficient profile are available in the `p_and_film_vs_theta.dat` text file (and a plot of each one is available in corresponding `.pdf` files)
- the `Exp-x-T-x` folder is related to the data for T_{w} and $\dot{r}_{\mathrm{w}}$ type boundary conditions: surface temperature and surface recession are are available in the `.dat` text files
- the `TC_meas_data` folder contains thermocouples records and temperature evolution at the stagnation point