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Lachaud, Jean R.; Martin, Alexandre; van Eekelen, Tom; and Cozmuta, Ioana, "Ablation Test-Case Series #2. Numerical Simulation of Ablative-Material Response: Code and Model Comparisons" (2012). *Mechanical Engineering Faculty Publications*. 21.
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Notes/Citation Information

Published in the *Proceedings of the 5th Ablation Workshop*, AW05–051, p. 1-9.

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ABLATION TEST-CASE SERIES #2
NUMERICAL SIMULATION OF ABLATIVE-MATERIAL RESPONSE: CODE AND MODEL COMPARISONS
VERSION 2.8, FEBRUARY 6, 2012

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1. PREAMBLE

This test-case series on the numerical simulation of the response of ablative-materials really started out of pure curiosity. Code developers and users were curious to see "how the codes compare" and "what is the effect of the different hypotheses in the models implemented". The objective of these test-case series is to propose problems of increasing complexity until it is agreed that the most-elaborated well-defined problem is formulated. The first test-case was mostly a simple heat transfer problem chosen for its simplicity (it is summarized in section 2.1). The second test-case series goes one step further, with the objective of reaching the state-of-the-art design level. It will require the patience of the industrial participants for whom this second series will still mean "running a basic case", with codes that have already been tested, verified, and validated. It will also require the comprehension of the academic participants for whom it will imply implementing in their codes engineering models, with maybe no other intents than "running the second ablation test-case series" and comparing their codes with design tools.

2. INTRODUCTION

2.1. Summary of the first test-case

The first test case was defined for the 4th Ablation Workshop, 1-3 March 2011, Albuquerque, New Mexico [1]. It was a one-dimensional test case focusing on the in-depth material response - fixed surface temperature and no recession. There were 14 participants (estimated to be about 50% of the community [2]). Three types of material-response codes have been identified:

- Type 1: based on the CMA[3] model or any mathematically equivalent model (heat transfer, pyrolysis, simplified mass transport);
- Type 2: CMA-type + Averaged momentum equation for the transport of the pyrolysis gases;
- Type 3: Higher fidelity codes (chemical/thermal non-equilibrium, etc).

The results had been provided by the participants before the workshop and a summary was presented during the workshop [4]. For type 1 and type 2 codes, differences in the temperature prediction were mostly below 1%. The participants tentatively attributed the differences to slight model differences and implementation and numerical integration errors needing further detailed investigation. The material properties have been interpreted differently by a few participants leading to differences larger than 1%. Codes of type 3 have shown differences and discrepancies that will need further analysis. We propose to thoroughly analyze the first and second test-case series results together at the 5th Ablation Workshop, Feb. 28- March 1, 2012, Lexington, Kentucky (tentative dates).

2.2. Introduction of the second test-case series

The purpose of this document is to define the second test-case series aiming at pushing the comparison further and reaching the state-of-the-art TPS-design level. For consistency with test-case #1 and to limit time-investment, most of the parameters and boundary conditions are unchanged. The main modifications will be to: (1) switch from the fixed surface-temperature boundary condition to a convective boundary condition, and (2) introduce surface recession. Computing the ablation rate to obtain the amount of surface recession is a complicated and still open problem. A traditional B' table will be provided to facilitate the in-depth material-response comparison but other tables/methods may be used. A specific test-case dedicated to the estimation of the ablation rate is also proposed. Therefore, the test-case series #2 includes three traditional ablation tests and one additional test dedicated to the estimation of the ablation rate:

- 2.1: low heating, no recession (targeted surface temperature of about 1644 K, cf. test-case 1) - non-physical intermediate case without recession in preparation for 2.2.
- 2.2: low heating (same as test case 2.1), recession
- 2.3: high heating, recession (targeted surface temperature of about 3000 K)
- 2.4: computation of the ablation rate of TACOT for a temperature range of 300K-4000K and an air pressure of 101325 Pa (1 atm). The B'-table format will be used to enable visual comparison.

3. DESCRIPTION OF THE SECOND TEST-CASE SERIES

3.1. Convective boundary-condition test-cases: 2.1, 2.2, and 2.3

The 1D geometry and the theoretical material TACOT of series 1 are re-used. A 1D sample of TACOT of 5 cm is heated on one side for 1 minute (convective boundary condition) at atmospheric pressure with adiabatic boundary condition on the other side. When the heat flux is applied or removed, transitions of 0.1 s (linear ramping) are applied (see figure 1). We will also model the cool-down for 1 minute under the hypothesis that it is a pure radiative cooling.

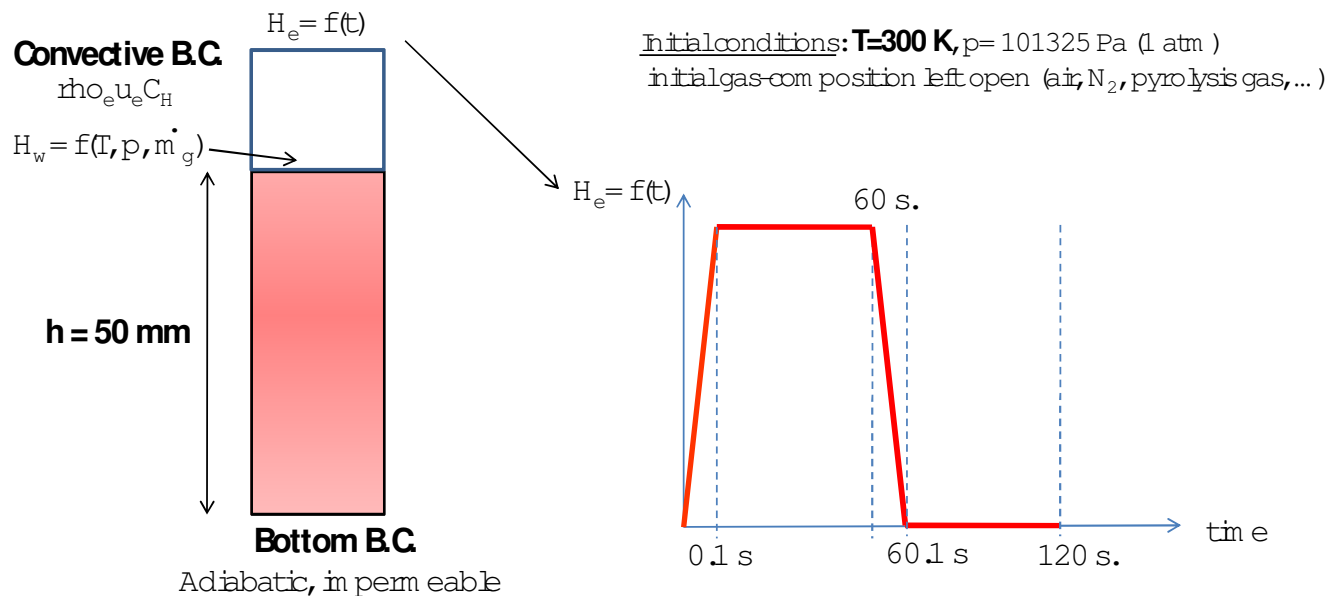


Figure 1: Schematic illustration of the boundary conditions for test-cases 2.1, 2.2, and 2.3

The time-dependent boundary-layer properties are given in table 1.

N.B.: References [3, 5, 6, 2] describing the convective boundary-condition may be obtained from the authors.

Table 1: Summary of the environment properties. Please use linear interpolation during the 0.1s heating and cooling periods (linear ramping).

time (s)	$\rho_e u_e C_H$ ($kg \cdot m^{-2} \cdot s^{-1}$)	h_e ($J \cdot kg^{-1}$)	p_w (Pa)
0	0	0	101325
0.1	0.3	#2.1 & #2.2 : $1.5 \cdot 10^6$ / #2.3: $2.5 \cdot 10^7$	101325
60	0.3	#2.1 & #2.2 : $1.5 \cdot 10^6$ / #2.3: $2.5 \cdot 10^7$	101325
60.1	0	0	101325
120	0	0	101325

The initial conditions are: $p_0 = 1$ atm (101325 Pa), $T_0 = 300$ K, sample length: $L_0 = 0.05$ m. The initial gas composition in the material is left open. For type 1 and 2 codes, pyrolysis gas in thermal equilibrium is the usual practice. For type 3 codes, it is suggested to start with air. The time-dependent boundary-layer properties are summarized in table 1. The other boundary-layer assumptions/properties are as follows for the code comparison:

- The factor for the blowing-correction correlation used is the CMA model is taken as $\lambda = 0.5$.
- Heat and mass transfer assumptions in the boundary layer: $Pr = Le = 1$
- Re-radiation is active during the entire analysis [$q_r = \epsilon \sigma (T_w^4 - T_\infty^4)$]. Since it is a 1D case, a view factor of 1 is used. The infinity temperature is chosen to be $T_\infty = 300$ K .

Important notes on the recession rate and on the wall enthalpy:

- 2.1: Please read the wall enthalpy (h_w) from the B' table provided in the TACOT_2.2.xls spreadsheet for code comparison and set recession to zero (i.e. $B'c = 0$). Please use an equivalent method if you do not use B' tables. The objective of this test case is to prepare as much as possible for 2.2 but without recession, to avoid mixing boundary-condition and mesh-motion issues during the comparison. It should be outlined that this case is not really physical as the actual wall enthalpy without recession is not equal to the wall enthalpy with recession (different content in carbon in the gas phase). However, it was agreed that this "numerical" test-case is important for code comparison in preparation of 2.2.
- 2.2: Please use the B'c table provided in the TACOT_2.2.xls file for code comparison or other methods for model comparison.
- 2.3: Idem.

3.2. Ablation-rate test-case: 2.4

The goal of this test-case 2.4 is to compare codes and methods used to compute the ablation rate of the material TACOT. To keep the work load reasonable, we will focus on the following conditions: $p = 1$ atm; $T = 300-4000$ K; under air. B' table (or methods using the same theory) are commonly used - please refer to the literature for definition of B' and B' tables [3, 2, 7]. In this test-case 2.4, we propose two levels of comparison: 2.4.1 and 2.4.2.

- 2.4.1: The first level of comparison consists in comparing B'-table generation algorithms using the following constraints:
 - Air (in mol fractions): $O_2 = 0.21$, $N_2 = 0.79$
 - Pyrolysis gas (in mol fractions): $C = 0.206$ / $H = 0.679$ / $O = 0.115$
 - Equal diffusion coefficients, frozen chemistry in the boundary layer, no erosion/failure, CEA database (please use the last version of the CEA2 thermodynamics table: cea092004.inp).
 - Mixture (25 species): C; H; O; N; CH₄; CN; CO; CO₂; C₂; C₂H; C₂H₂, acetylene; C₃; C₄; C₄H₂, butadiyne; C₅; HCN; H₂; H₂O; N₂; CH₂OH; CNN; CNC; CNCOCN; C₆H₆; HNC.
- 2.4.2: For the second level of comparison, which is more a model comparison than a code comparison, we propose to fix only the following parameters:

- Air (in mol fractions): O2=0.21, N2=0.79
- Pyrolysis gas (in mol fractions): C=0.206 / H=0.679 / O=0.115 (species may be used for finite-rate chemistry)

In other words, for the second level of comparison, the database is open (CEA, JANAF, etc), the boundary layer conditions are open, finite-rate chemistry may be used, etc...

For visual comparison, the usual B'-table plots (B'c= f(T, B'g)) should be used for both 2.4.1 and 2.4.2 if possible. To keep the data load reasonable, we suggest focus on the following conditions: p= 1 atm; T=300-4000K. An example of plot is presented in figure 2. The B' table using the CEA database and a reduced set of 25 species is included in the spreadsheet TACOT_2.2.xls. To enable comparison, we suggest to use the B'g values of the spreadsheet.

4. MATERIAL DATA

The material properties for this test-case series are provided and explained in the spreadsheet TACOT_2.2.xls. Recent updates:

- B' table updated (July 28, 2011)
- Equilibrium properties of the pyrolysis gases up to 4000K (June 2011)

5. CODE OUTPUT AND COMPARISON OF THE RESULTS

An output frequency of 0.1 s will be used for file exchange. Two types of data are required for comparison of the results:

- Type1: temperature response.

It was found more convenient to use probed values (thermocouples) than temperature profiles. The probed values locations from the initial top surface are: $x_1(t) = x_w(t)$: moving top surface (i.e., x_1 follows the surface if recession); $x_2 = 1$; $x_3 = 2$; $x_4 = 4$; $x_5 = 8$; $x_6 = 12$; $x_7 = 16$; $x_8 = 24$; $x_9 = 50\text{mm}$ (x_9 is the bottom surface). $T_1 = T_w$ can be seen as a pyrometer measurement and T_2, T_3, \dots, T_9 as fixed thermocouples.
- Type2: pyrolysis and ablation response (blowing rates, recession, pyrolysis zone)
 - Blowing rates: we suggest to plot $\dot{m}_g(x = x_w)$ (value at the top surface) and \dot{m}_c
 - Pyrolysis zone: we will use again (as in the first test case) the following quantities: virgin 98 % and char 2 % to estimate the location of the pyrolysis and char fronts. The thresholds are defined as: $\rho_v(98\%) = \rho_c + 0.98(\rho_v - \rho_c)$; $\rho_c(2\%) = \rho_c + 0.02(\rho_v - \rho_c)$. For simplicity of the analysis, we suggest to output these quantities with respect to the initial top surface.
 - Recession: we suggest to plot the location of the receding surface with respect to the initial top surface (i.e., total recession = $50 - x_w$)

Output format desired (for analysis by the Thermal Performance Database (TPDB) team)

time (s)	Tw (K)	T2 (K)	T3 (K)	T4 (K)	T5 (K)	T6 (K)	T7 (K)	...
0	3.000e3	3.000e3	3.000e3	3.000e3	3.000e3	3.000e3	3.000e3	...
0.1	9.651e3	3.225e3	3.000e3	3.000e3	3.000e3	3.000e3	3.000e3	...
0.2	1.076e3	3.956e3	3.039e3	3.000e3	3.000e3	3.000e3	3.000e3	...
etc.

Table 2: Output format for the temperature file - please name it: CodeName_Energy_TestCase_2.1.txt

6. PRELIMINARY RESULTS

It has been decided to use CMA as a baseline for visual comparison for test cases 2.1, 2.2, and 2.3. CMA results will be provided by October 2011. In the meantime, **preliminary** results are provided in the following figures. Please do not give them more credit than they deserve and use them for sanity check rather than for comparison.

time (s)	m_dot_g (kg/m2/s)	m_dot_c (kg/m2/s)	Virgin 98%	Char 2%	recession (m)
0	0	0	0	0	0
0.1	5.063e-3	0	0	0	0
0.2	1.340e-2	0	1.781e-4	2.130e-5	0
etc.

Table 3: Output format for the pyrolysis and ablation-response file - Please name it: CodeName_Mass_TestCase_2.1.txt

7. ACKNOWLEDGMENTS

The test-case definition and the material database have been tested using several codes and will now remain unchanged for this second test-case series. We would like to thank you in advance for any comment that will help to improve the clarity of this document. Please send your comments to the authors. The authors would like to thank: Julien de Muelenaere (VKI) for generating the TACOT_2.2 B' table and proposing the reduced set of 25 species; Jonathan Wiebenga (University of Michigan) for testing the test-cases using MOPAR; Bennie Blackwell (Blackwell Consulting) and Micah Howard (SANDIA) for constructive discussions on B' table generation; Bernie Laub (NASA Ames) for his comments on test-case 2.1. that helped clarifying (hopefully) its very limited scope; Jean-Marc Dupillier (EADS Astrium) for his numerous constructive comments on the TACOT database and on the test-case series.

8. REFERENCES

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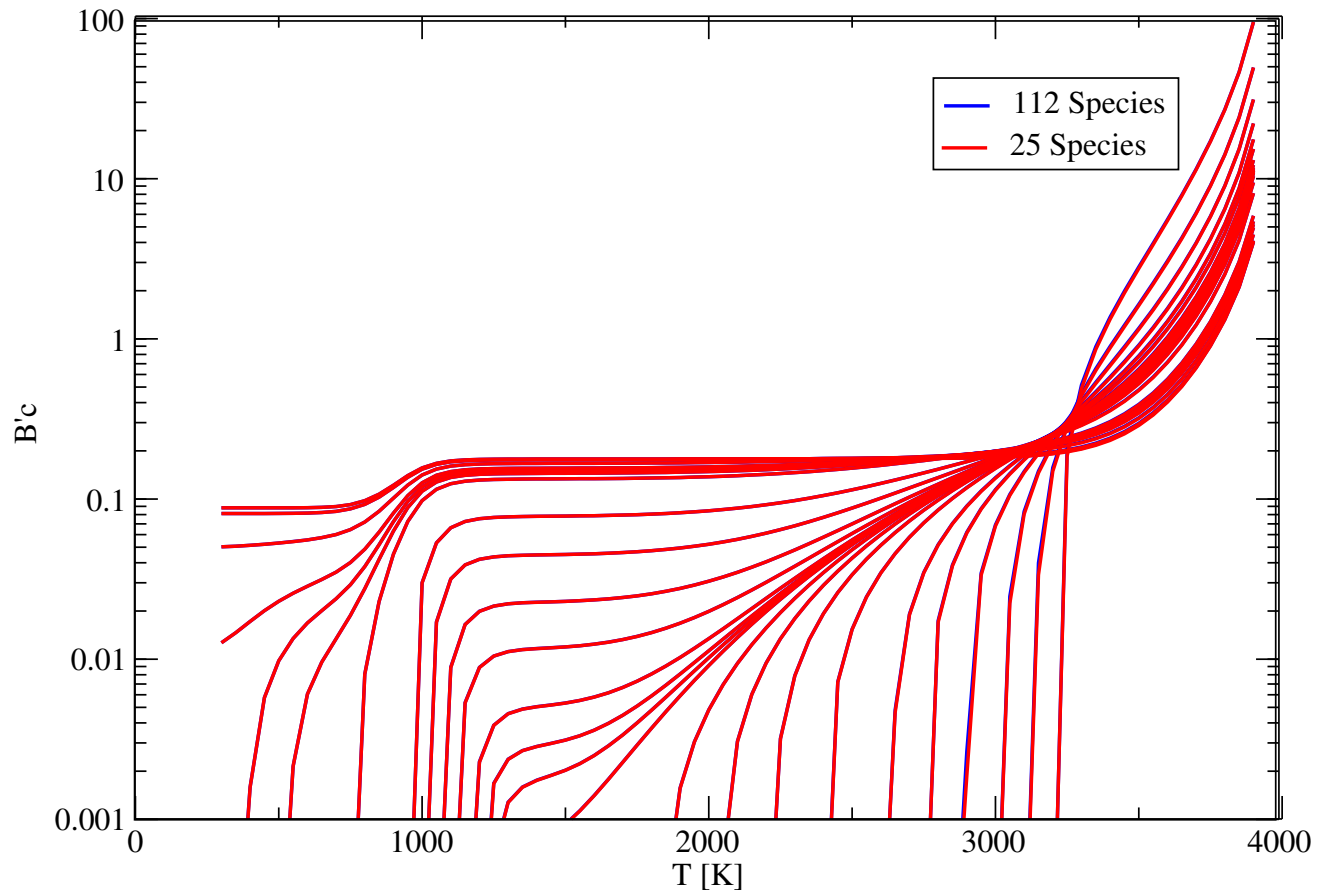


Figure 2: B' table comparison for the 25-species mixture suggested and a 112-species mixture using the CEA database [Computed with Mutation-B' by J. de Muelenaere [7]]. The 25-species B' table is provided in the TACOT_2.2.xls spreadsheet.

