Ablation test-case series #2

- Numerical simulation of ablative-material response: code and model comparisons –

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. Introduction

1. **Motivation:** **Why did we start this? -> pure curiosity**
- **How do codes compare? – if same model.**
- **How do models compare? – if different physics implemented.**

2. **Goal**
- **propose problems of increasing complexity until it is agreed that the most-elaborated well-defined problem is formulated**

3. **Method to design a test case**

1 - census on problems of interest

2 - census on code capabilities

3 - draft a proposition of test case (necessarily a compromise)

4 - iterate with the community until the test-case definition is clear and complete

4. **We try our best to propose SOFT test-cases**
- **Simple, Open, Focused, Trouble-free.**

. Introduction

Where are we? Where are we going?

outline

0 – TACOT: Theoretical Ablative Composite for Open Testing created from literature data.
It is a low-density carbon/phenolic.

1st test-case (2011) : 15 participants / 25 codes in the open literature
In-depth analysis only: fixed surface temperature, no recession, 1D.

2nd test-case series (2012) – progress: convective boundary condition & recession

2.1 - 1D numerical test – low heat-flux but recession forced to be zero (non-physical but useful for code developers)

2.2 - 1D state-of-the art design level – low heat-flux (0.45 MW/m²)

2.3 - 1D state-of-the art design level – higher heat-flux (7.7 MW/m²)

2.4 - Comparison of methods to compute recession rates (e.g. B' tables)

3rd test-case series (2013) – progress: 2D & 3D, see presentation by Tom van Eekelen

3.1 - Pseudo-IsoQ axi-symmetric - 2D axi

3.2 - Pseudo-IsoQ with orthotropic material properties (conductivity, permeability, etc) – full 3D

3.3 - Sprite

4th test-case series (2014) – progress: coupling & flight tests

Coupled ground-test problem: IsoQ in ArcJet; Sprite in ArcJet

Coupled or uncoupled flight: tbd.

. TACOT: defined in spreadsheet “TACOT_2.2.xls”

Theoretical Ablative Composite for Open Testing

Elemental composition

o Reinforcement: ex-cellulose carbon fibers, heat treated at 2000 K, density 1600 kg/m^3, length: 1mm, diameter: 10 microns.

o Matrix: ex-novolac/formaldehyde polymer, virgin density 1200 kg/m^3

Architecture

o Random fiber distribution and orientation

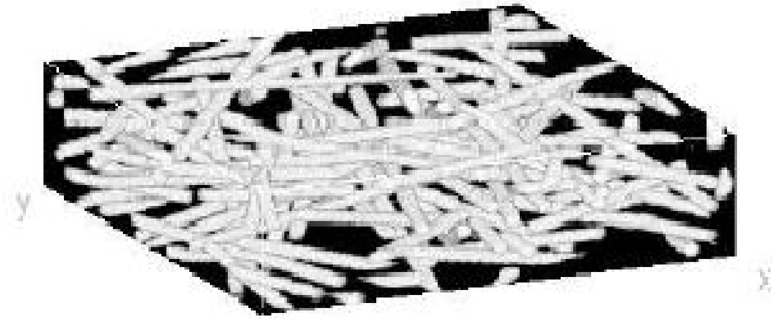
Fiber volume fraction: 10 %

o Fiber-coating matrix

Matrix volume fraction: 10 %

o Initial porosity: 80 %

3D numerical construction of the architecture of TACOT



Properties

o Inspired from open literature data - when available for similar materials

conductivity, heat capacity, pyrolysis gases (composition, decomposition, finite-rate chemistry up to 1644 K)

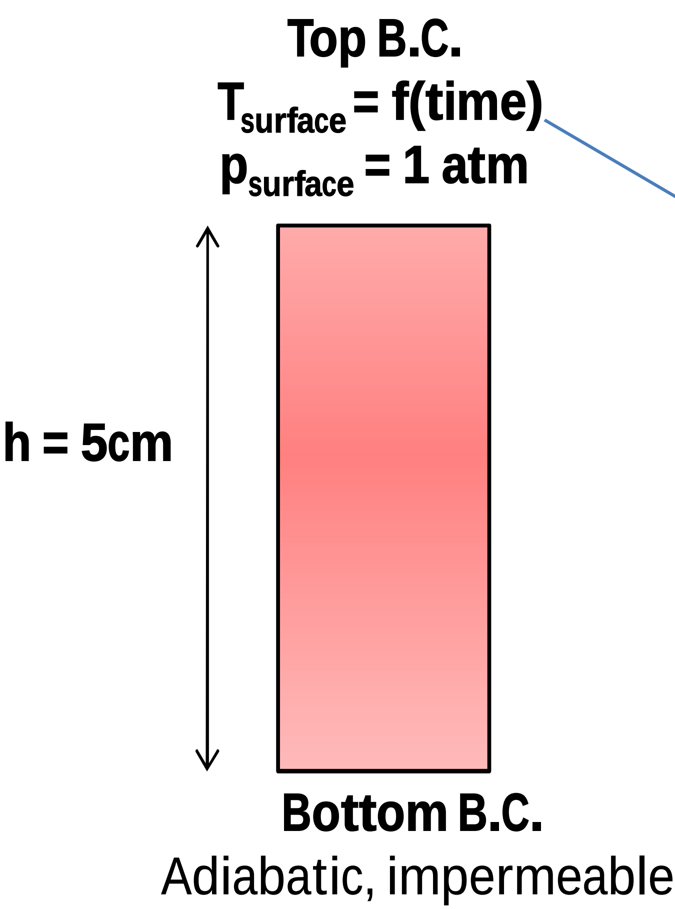
o Derived/computed - when not found in the literature

formation enthalpy of the solid, thermodynamic properties of the pyrolysis gases at equilibrium (CEA database), viscosity, permeability, tortuosity, B’ table for air (CEA database).

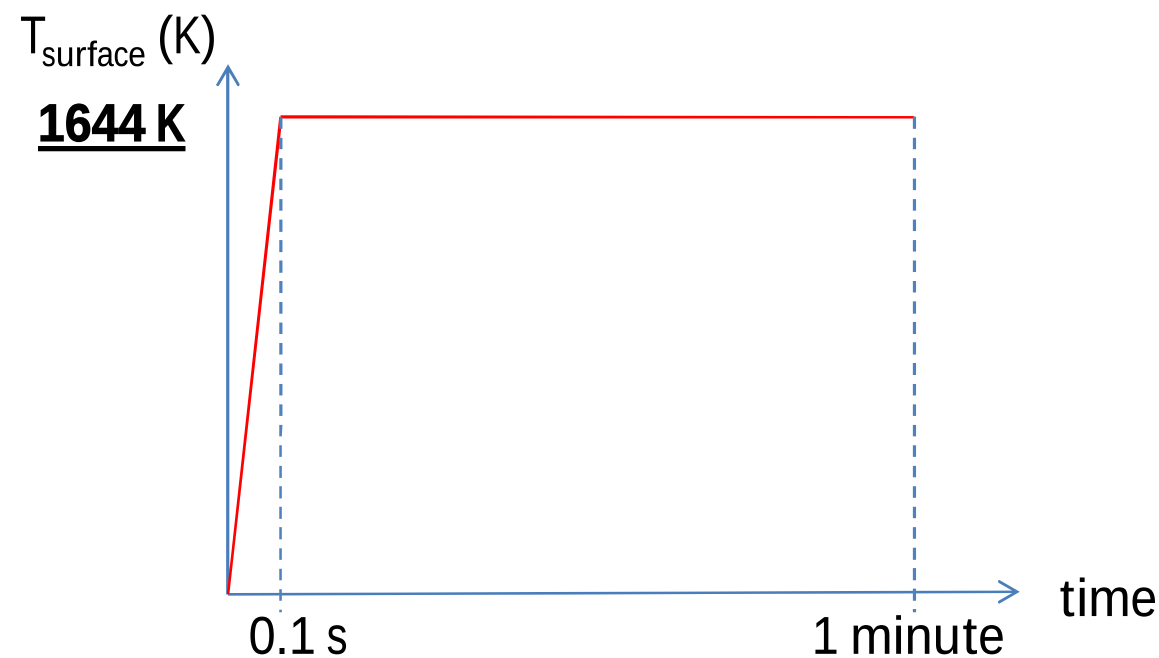
. 1st test case

Quick summary

- ✓ **Objective :** comparison of the "in-depth physics and chemistry"
- ✓ **Simple :** 1D, fixed surface temperature, no recession.
- ✓ FIAT baseline provided



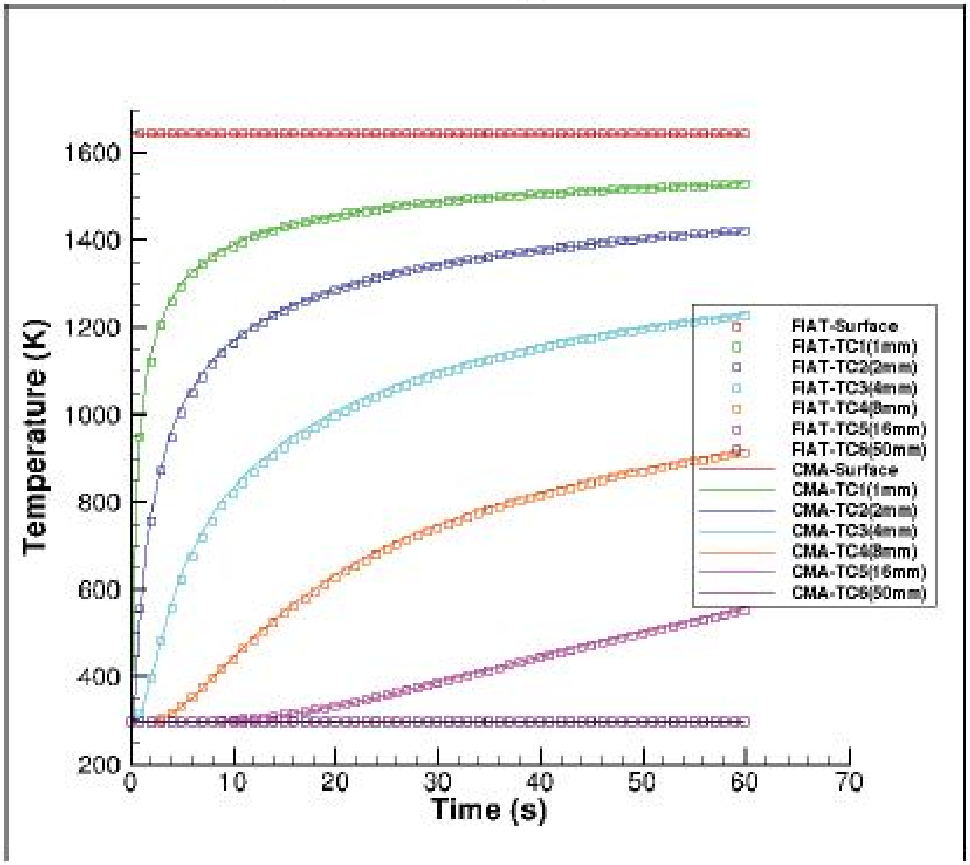
<u>Initial conditions</u>: T=298 K, p= 1 atm, initial gas composition left open (air, Ar, pyrolysis gas, …)



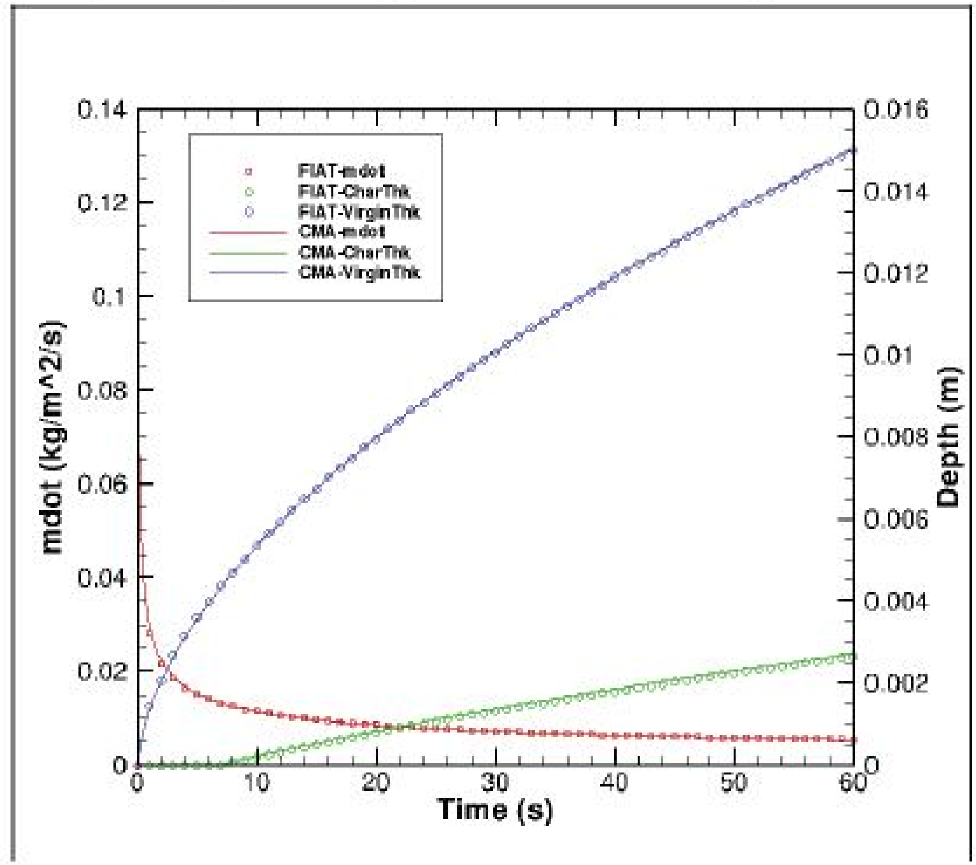
. 1st test case

Quick summary : CMA vs. FIAT baseline – excellent agreement.

In-depth temperatures



Pyrolysis gas blowing rate

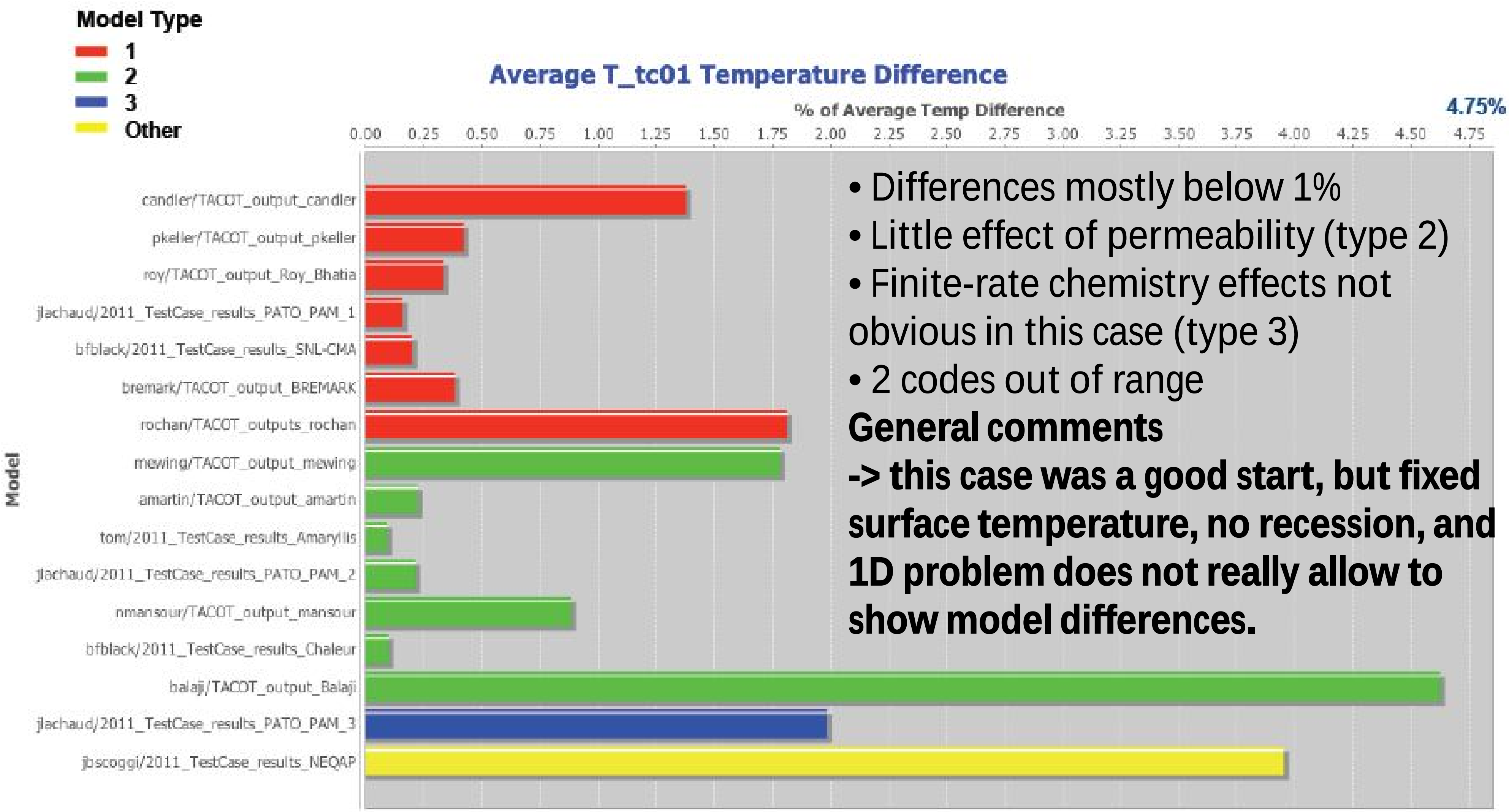


Micah Howard, Dave Kuntz, Ben Blackwell, "Prediction of TACOT decomposition using the CMA code", 4th AF/SNL/NASA workshop, 1-3 March 2011.

Sandia National Laboratories

. 1st test case

Quick summary : 16 code outputs compared to FIAT



- Differences mostly below 1%
- Little effect of permeability (type 2)
- Finite-rate chemistry effects not obvious in this case (type 3)
- 2 codes out of range

General comments

-> this case was a good start, but fixed surface temperature, no recession, and 1D problem does not really allow to show model differences.

Thermal performance database team, “Overview of the inter-calibration results”, 4th AF/SNL/NASA workshop, 1-3 March 2011.

. 2nd series

Introduction

✓ **Objectives**

- reach the state-of-the art design level
- keep as much as possible from test-case 1 – to optimize time investment.

✓ **NEW in 2nd series**

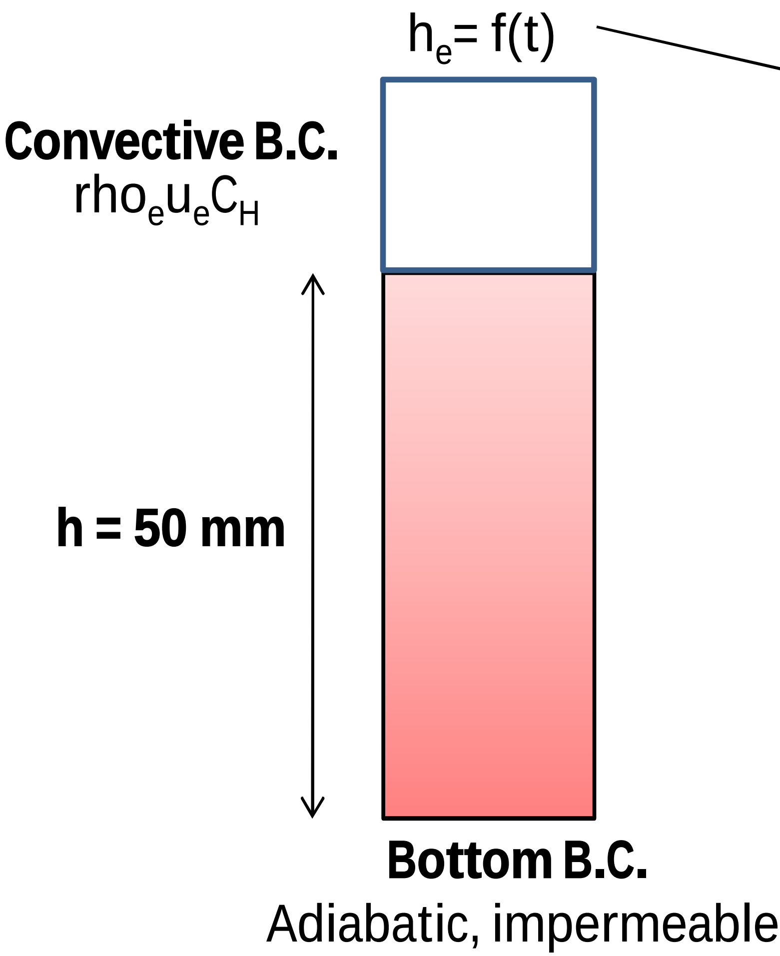
- convective boundary condition (instead of fixed surface temperature)
- surface recession

✓ **Structure of 2nd series : 4 cases**

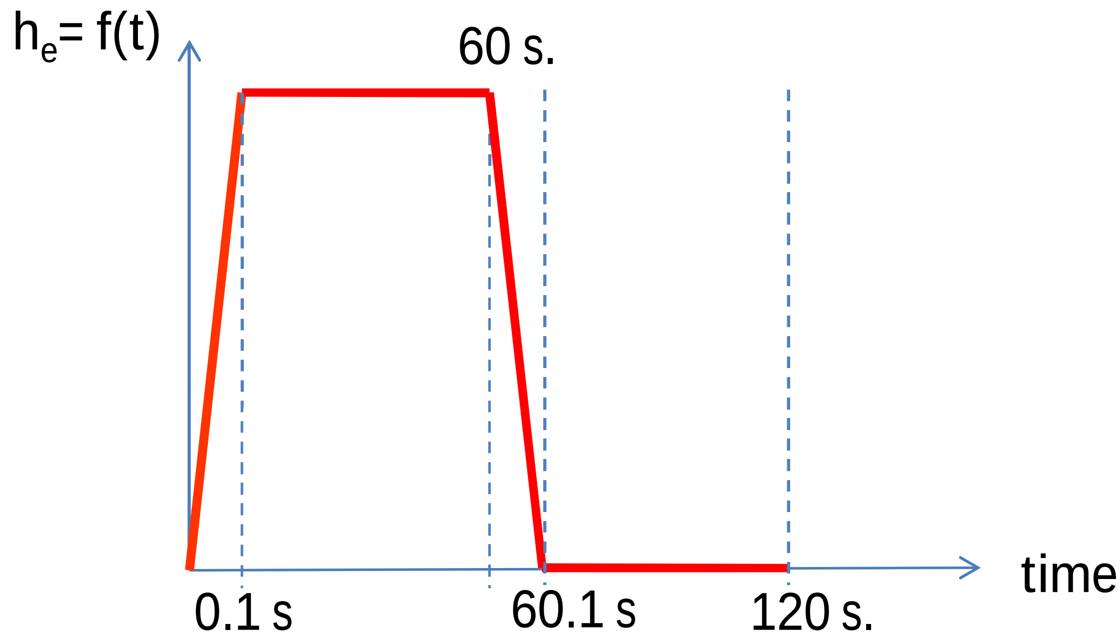
- 3 complementary material-response test-cases
  - ❑ 2.1: low heating, no recession (non-physical intermediate test case found useful by code developers)
  - ❑ 2.2: low heating, recession – should be in the finite-rate chemistry regime for model comparison
  - ❑ 2.3: high heating, recession – should be in the equilibrium chemistry regime
- Specific comparison of methods to compute recession rates (e.g. B’ tables)
  - ❑ 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).

. 2nd series

Definition of 2.1, 2.2, 2.3



Initial conditions: **T=300 K**, p= 101325 Pa (1 atm), air.

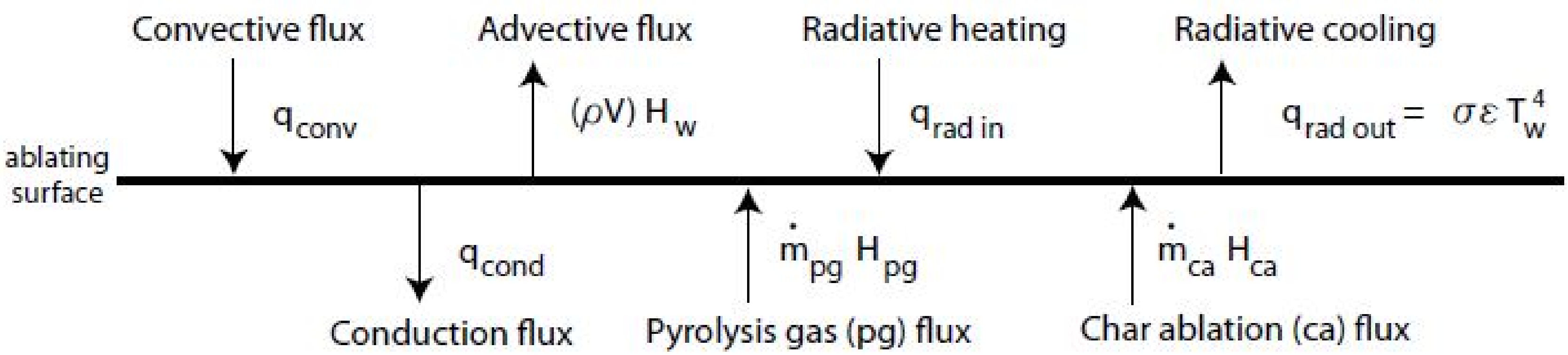


time (s)	$\rho_e u_e C_H$ $(kg \cdot m^{-2} \cdot s^{-1})$	h_e $(J \cdot kg^{-1})$	p_w (Pa)
0	0	0	101325
0.1	0.3	#2.1 & #2.2 : $1.5 \cdot 10^6$ / #2.3: $2.5 \cdot 10^7$	101325
60	0.3	#2.1 & #2.2 : $1.5 \cdot 10^6$ / #2.3: $2.5 \cdot 10^7$	101325
60.1	0	0	101325
120	0	0	101325

References describing the convective boundary condition as implemented in CMA (and still used in most of the design codes) are made available. $q_{conv} = rho_e u_e C'_H (h_e - h_w)$
This does not mean that the CMA model must be used.

. 2nd series

Surface energy balance at the wall as implemented in CMA



$$\boxed{\begin{aligned} q_{conv} - (\rho V)h_w + q_{rad,in} - q_{rad,out} - q_{cond} \\ + \dot m_{pg}h_{pg} + \dot m_{ca}h_{ca} = 0 \end{aligned}}$$

From CFD

2 unknowns

- mass loss rate (kg/m²/s)

-> Will provide the recession rate

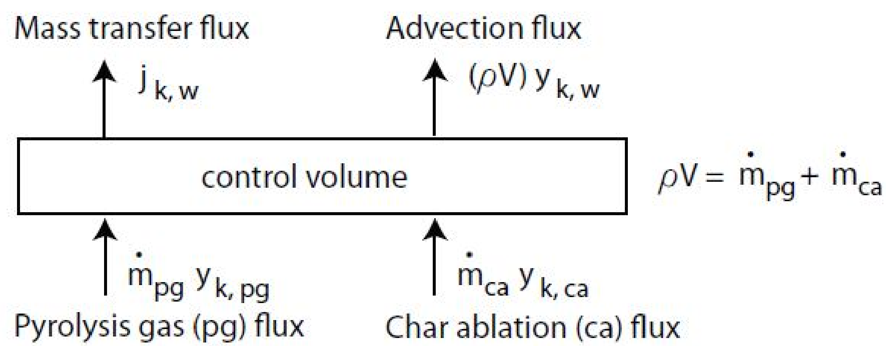
$v_{ablation} = \dot m_{ca} / \rho_{char}$

- h_w

. 2^{nd} series

Mass balance at the wall and B' tables: a simplified description

- Evaluation of the surface recession velocity (ablation)
  - Equilibrium chemistry is assumed in a control volume close to the wall (gas-gas & gas-solid)
  - Mass transport in the boundary layer and element conservation dictate the ablation rate
  - This problem can be solved *a priori*, knowing the elemental composition of the pyrolysis gas ($Y_{k,pg}$), the pyroloysis gas flux ($\dot{m}_{pg}$), the wall temperature (T_w) and pressure (p_w) $\rightarrow \dot{m}_{ca}$, h_w



e.g.
$p_w = 1$
$B'_g = 10$
$T_w = 1000$
↓
$B'_c = 0.1$
h_w=1e6

p_w	B'_g	B'_c	T_w	h_w
1	10	10	3000	3e6
1	10	1	2000	2e6
1	10	0.1	1000	1e6
1	0.1	10	3300	3.4e6
1	0.1	1	2200	2.4e6
1	0.1	0.1	1100	1.3e6
0.1	0.1	0.1	2800	2.5e6

- "B' tables " may be generated when $Y_{k,pg}$ are constant.

By definition: $B'_i = \dot{m}_i / (rho_e\, u_e\, C_M)$, where rho_e and u_e are the boundary layer edge density and velocity, and C_M is the mass Stanton number.

For this test case series, a B' table is provided for the nominal elemental composition of the pyrolysis gases.

For an extensive description, please see:

Moyer, C. B., Rindal, R. A., "An analysis of the coupled chemically reacting boundary layer and the charring ablator", NASA CR-1061, 1968.

. 2nd series:

Test-case 2.4 : computation of ablation rates (e.g. B' tables)

✓ **Goal:** compare codes and methods used to compute ablation rates

✓ **Focus to keep work load reasonable:** material TACOT (char is pure graphite); p= 1 atm; T=300-4000K; under air.

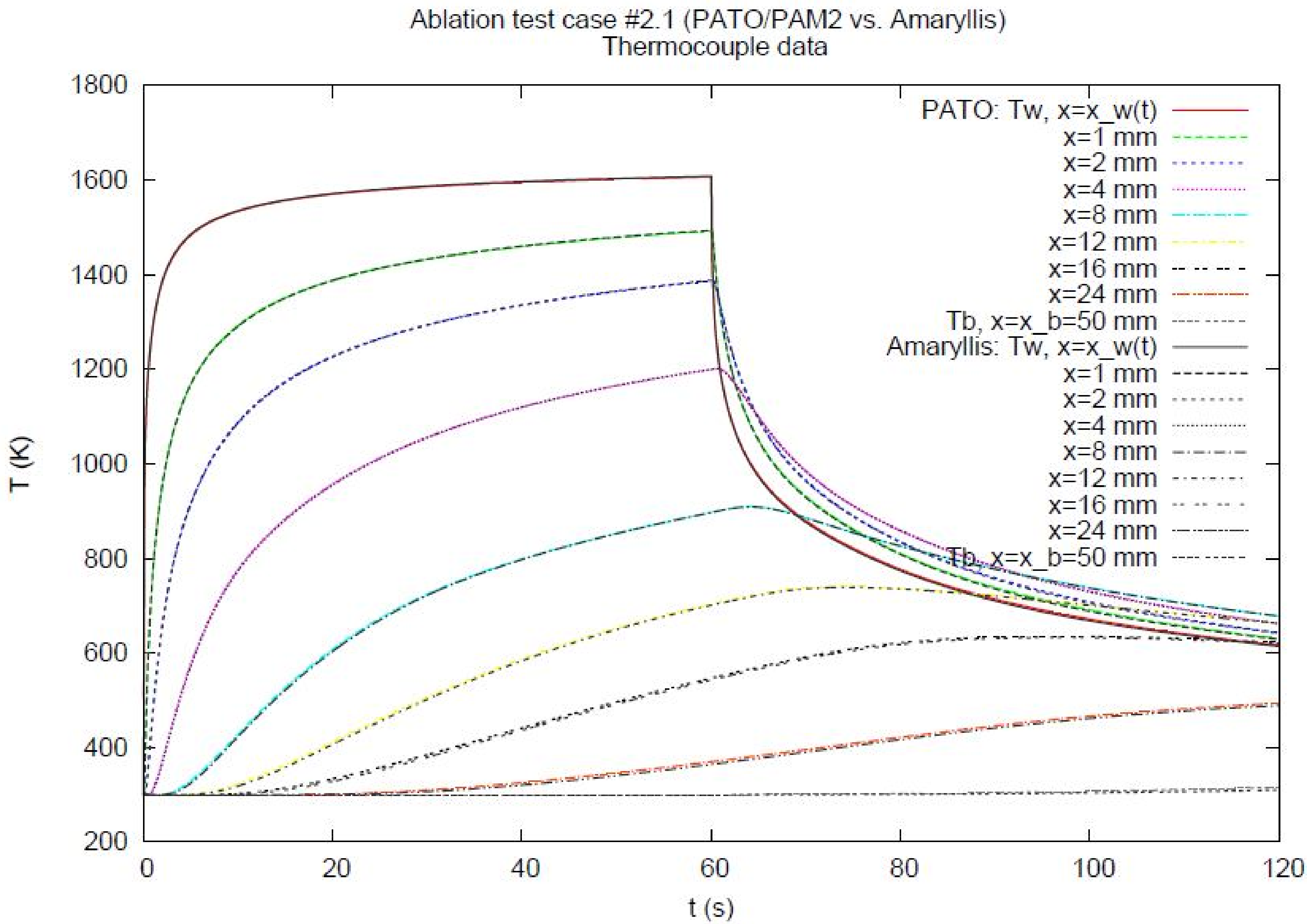
✓ **2 levels of comparison:**

- 2.4.1: comparison of B'-table generation algorithms with the following constraints:
  - Air (in mol fractions): O2=0.21, N2=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 or failure, CEA database, equilibrium chemistry.
  - 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: model comparison with no constraints.

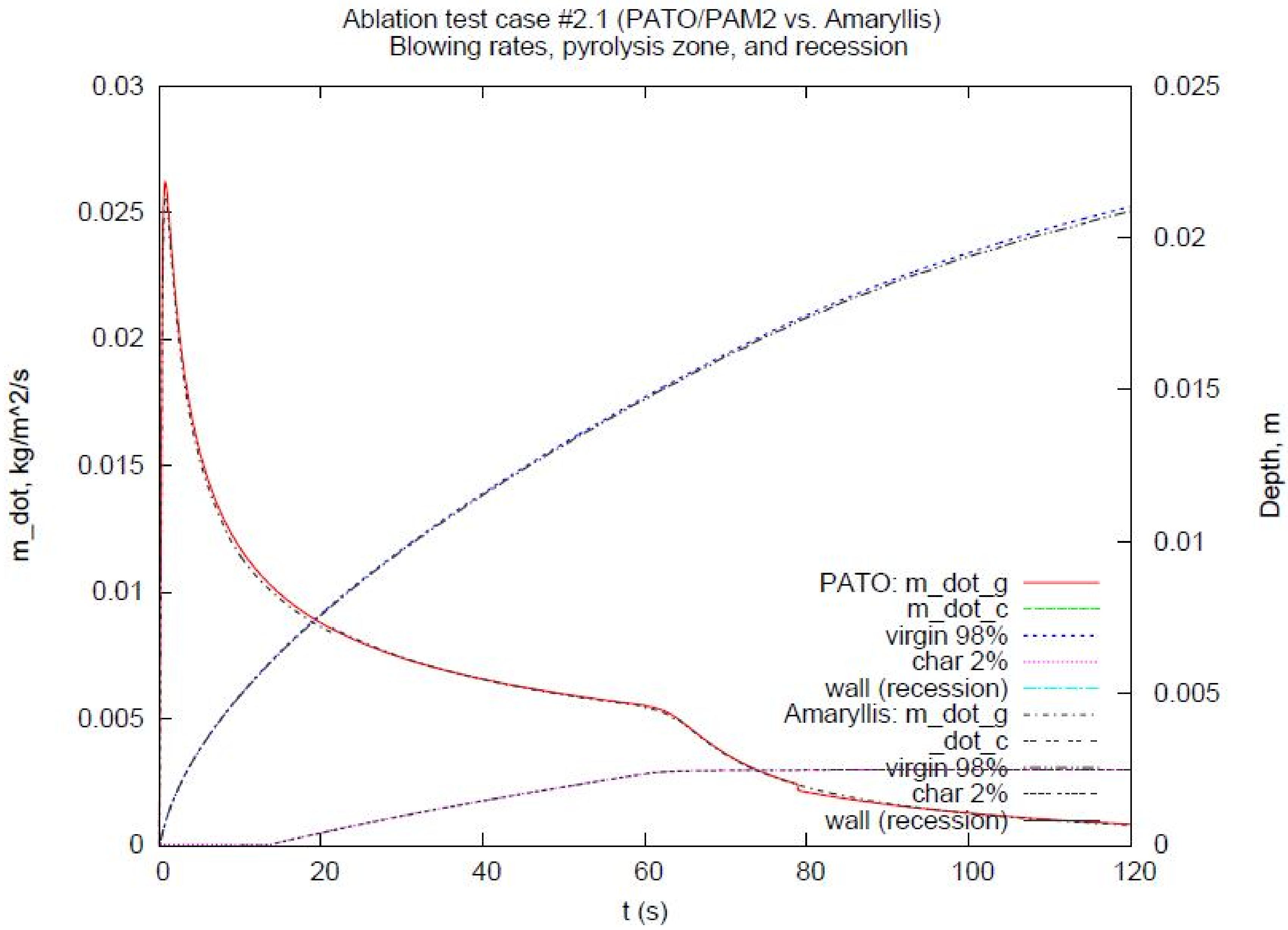
. 2nd series: required output for comparison (1/2): Energy

Test-case 2.1 – low heating, no recession



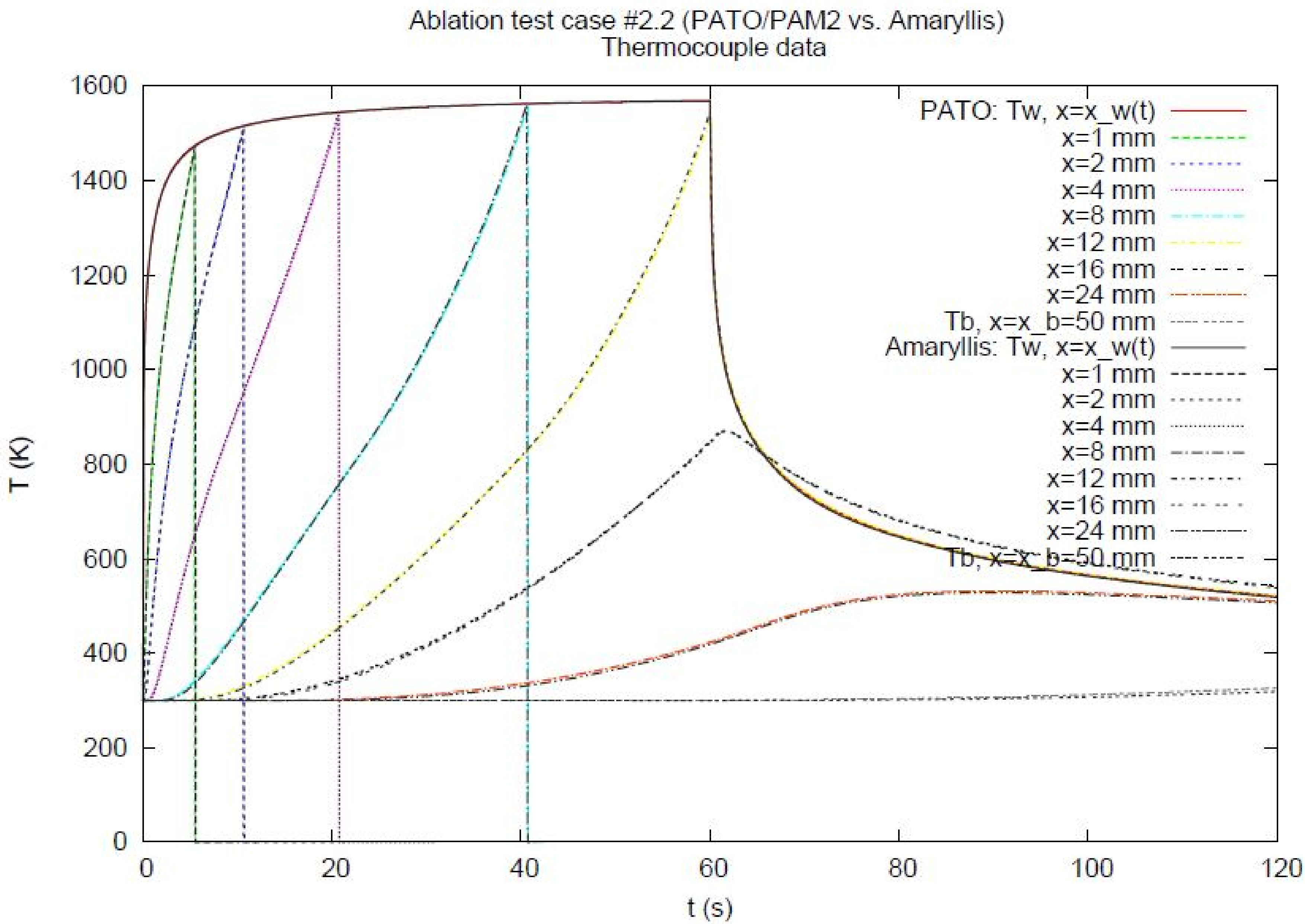
. 2nd series: required output for comparison (2/2): Mass

Test-case 2.1 – low heating, no recession



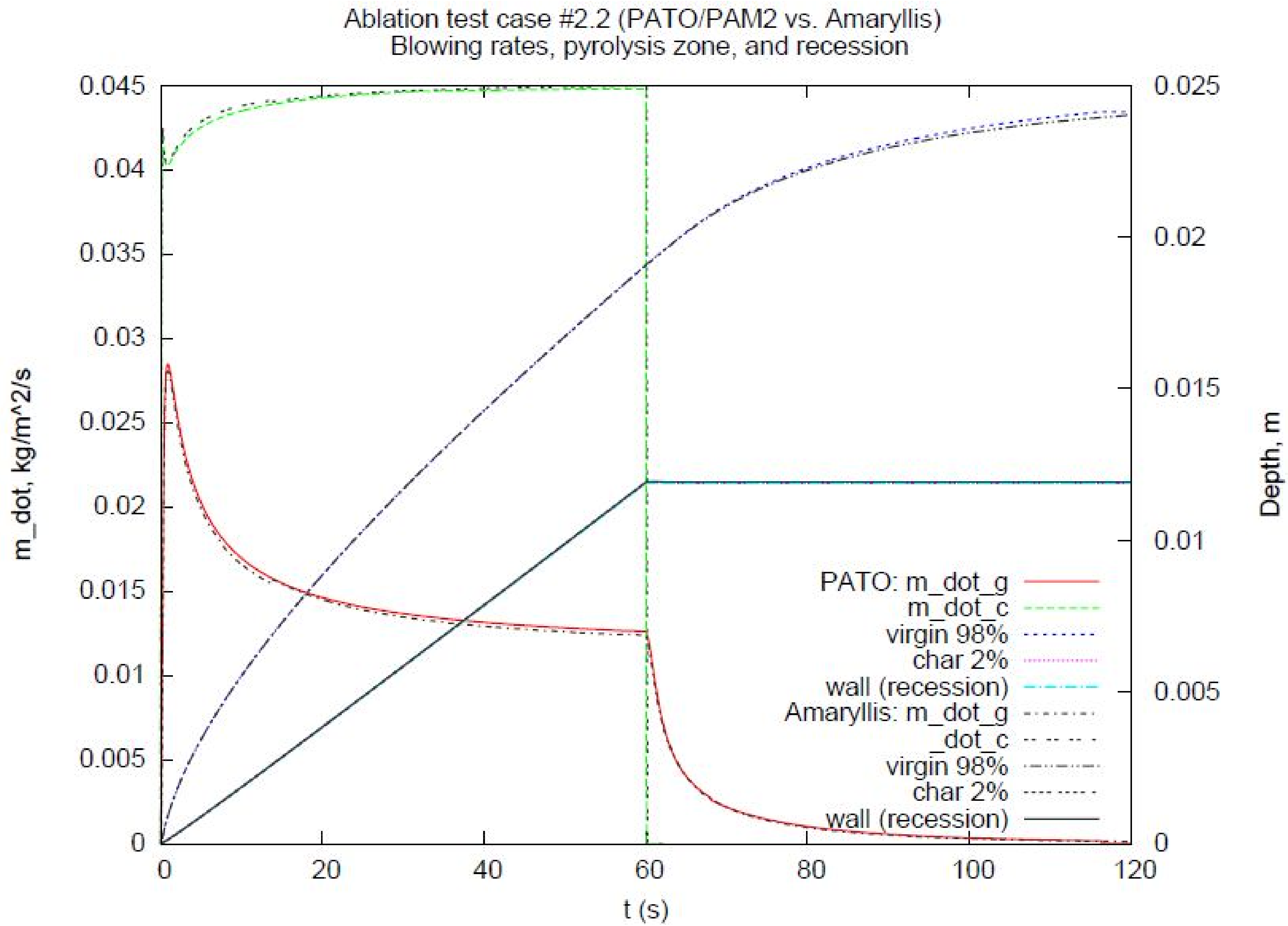
. 2nd series: required output for comparison (1/2): Energy

Test-case 2.2 – low heating, recession



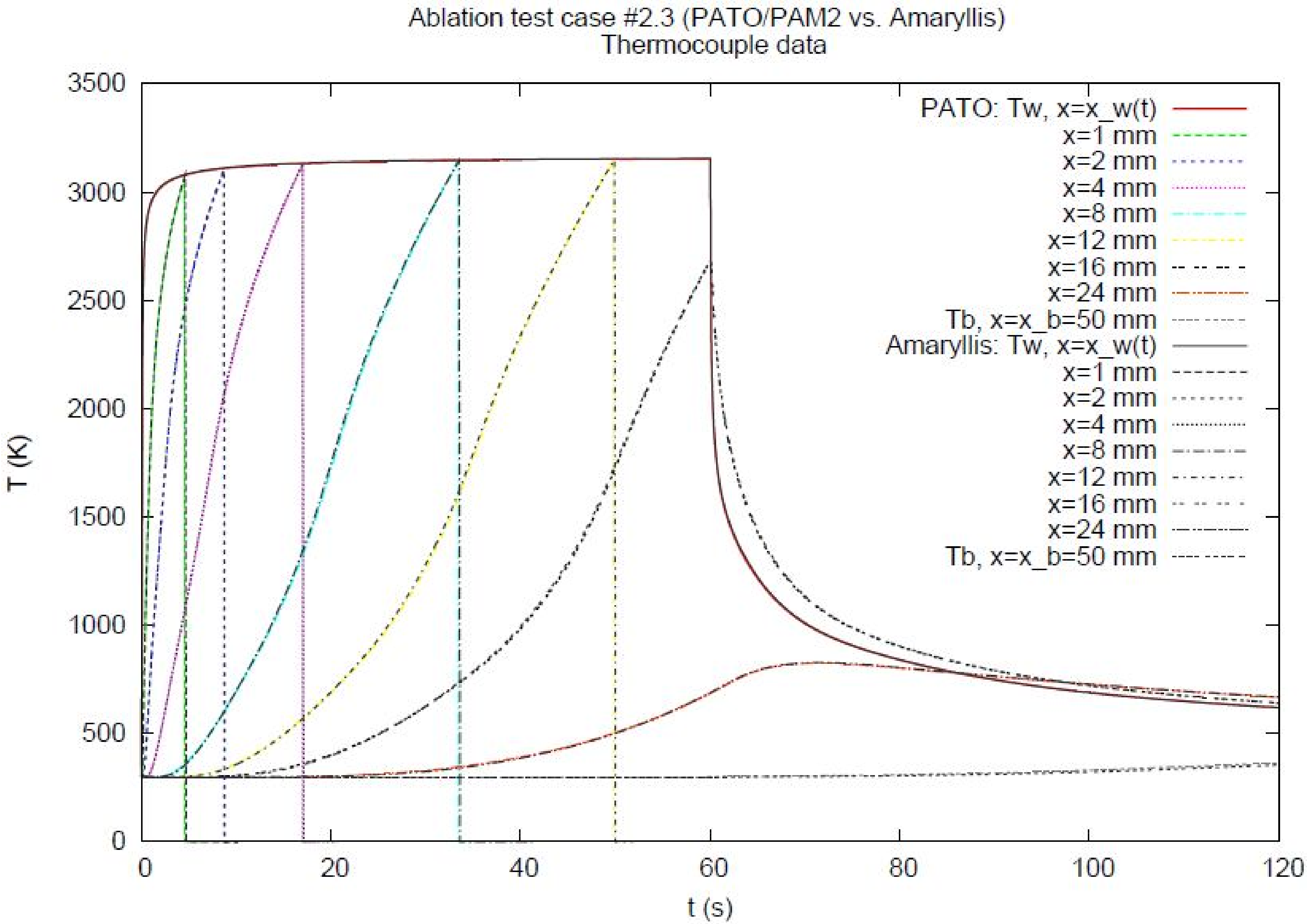
. 2nd series: required output for comparison (2/2): Mass

Test-case 2.2 – low heating, recession



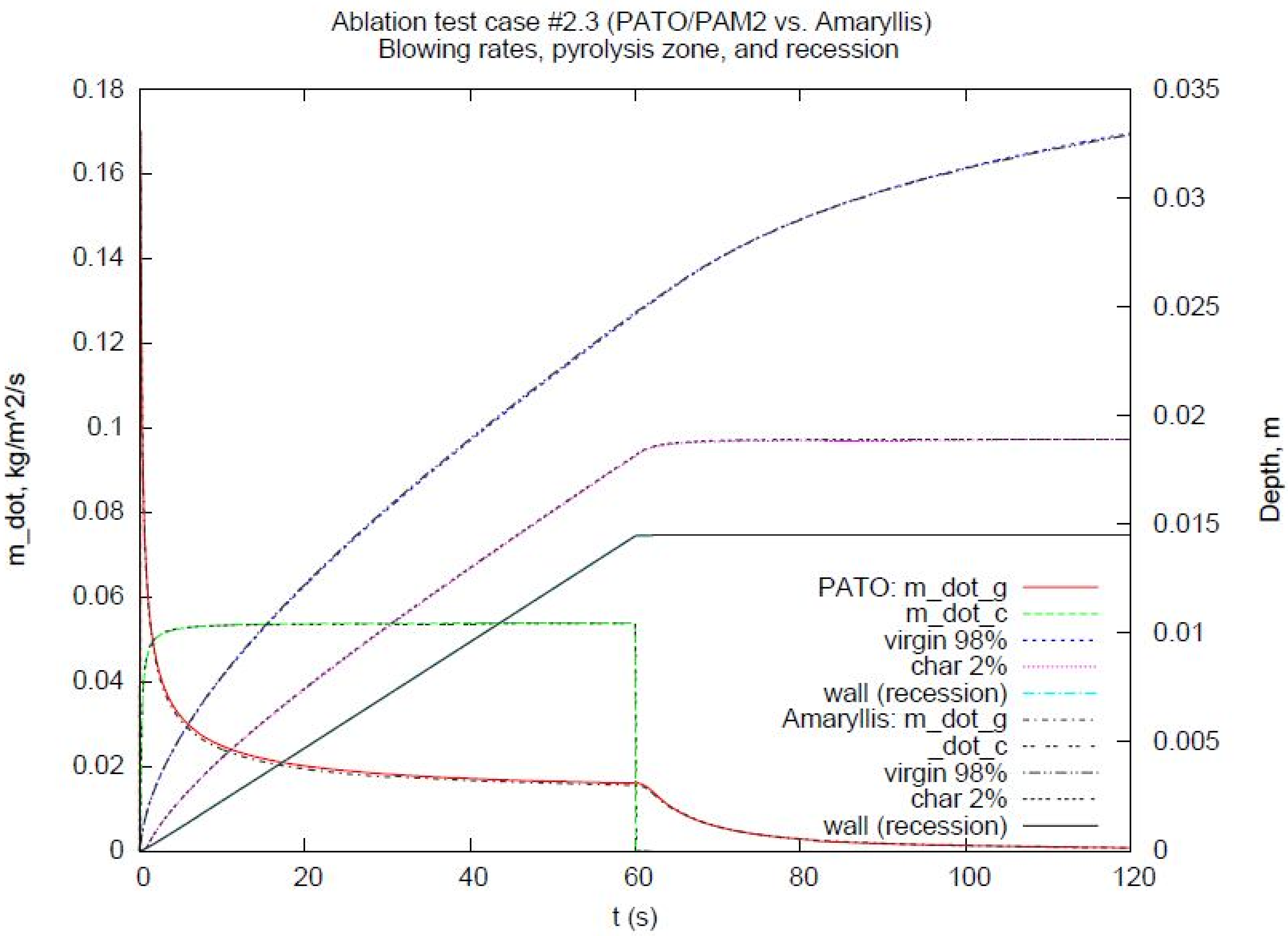
. 2nd series: required output for comparison (1/2): Energy

Test-case 2.3 – high heating, recession



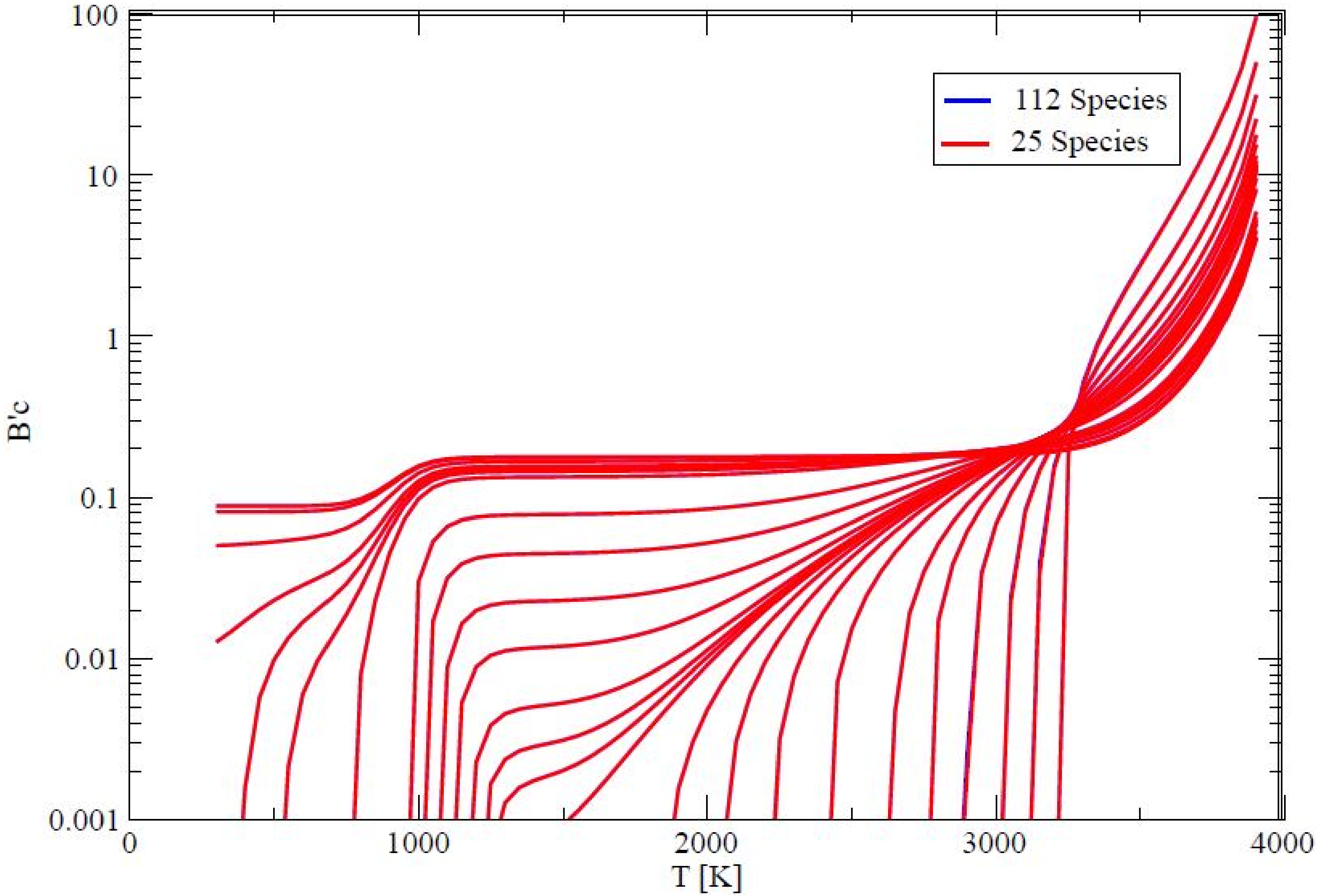
. 2nd series: required output for comparison (2/2): Mass

Test-case 2.3 – high heating, recession



. 2^{nd} series: required output for comparison: B'-table format

Test-case 2.4 : illustration of 2.4.1 (25 species) vs a proposition of 2.4.2 (112 species)



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.
B' table provided in the TACOT_2.2.xls spreadsheet.

. Conclusion and perspectives

Feedback on 0, 1, 2 – Suggestions on 3, 4 – will we need a 5?

Enriched for each test case (e.g. B', non-isotropy)

0 – TACOT: Theoretical Ablative Composite for Open Testing created from literature data. It is a low-density carbon/phenolic.

Closed but new results are welcome

1st test-case (2011) : 15 participants / 25 codes in the open literature

In-depth analysis only: fixed surface temperature, no recession, 1D.

Last update after the workshop

2nd test-case series (2012) – progress: convective boundary condition & recession

2.1 - 1D numerical test – low heat-flux but recession forced to be zero (non-physical but useful for code developers)

2.2 - 1D state-of-the art design level – low heat-flux (0.45 MW/m²)

2.3 - 1D state-of-the art design level – higher heat-flux (7.7 MW/m²)

2.4 - Comparison of methods to compute recession rates (e.g. B' tables)

Preliminary version presented today

3rd test-case series (2013) – progress: 2D & 3D, see presentation by Tom van Eekelen

3.1 - Pseudo-IsoQ axi-symmetric - 2D axi

3.2 - Pseudo-IsoQ with orthotropic material properties (conductivity, permeability, etc) – full 3D

3.3 - Sprite

Analyses and discussions in progress

4th test-case series (2014) – progress: coupling & flight tests

Coupled ground-test problem: IsoQ in ArcJet; Sprite in ArcJet

Coupled or uncoupled flight: tbd.