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Overview of ablation test-cases

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Introduction

- Motivation
  - Why did we start this? -> pure curiosity
  - How do codes compare? – if same model.
  - How do models compare? – if different physics implemented.
- Goal
  - propose problems of increasing complexity until it is agreed that the most-elaborated well-defined problem is formulated
- Method to design a test case
  - census on problems of interest
  - census on code capabilities
  - draft a proposition of test case (necessarily a compromise)
  - iterate with the community until the test-case definition is clear and complete
- We try our best to propose **SOFT** test-cases
  - Simple, Open, Focused, Trouble-free

Previous Test-cases

- 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. Mostly a simple heat transfer problem chosen for it's simplicity
- 2nd test-case series (2012) – progress: convective boundary condition & recession
  - 2.1 - bridge between 1st and 2.2 (non-physical but useful for code developers)
  - 2.2 - 1D state-of-the art design level – low heat-flux
  - 2.3 - 1D state-of-the art design level – high heat-flux
  - 2.4 - Comparison of methods to compute recession rates (e.g. B' tables)
- 3rd test-case series:
  - Initial version (2012): 5th Ablation Workshop, Lexington, KY
  - First complete version (2013): Gordon Research Conference, Ventura, CA

Phenomenology

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Macroscopic phenomenology

Long distance effects
- Radiation

Material/flow coupling
- Boundary layer transfers (heat and mass)
- Recombination/catalicity
- Ablation (oxidation, sublimation, spallation)

Interface phenomena: Heat and mass balance (1),
Subsurface phenomena
- In-depth ablation (3)
- Penetration of radiation (3)
- Gas flow entering into the material (3)

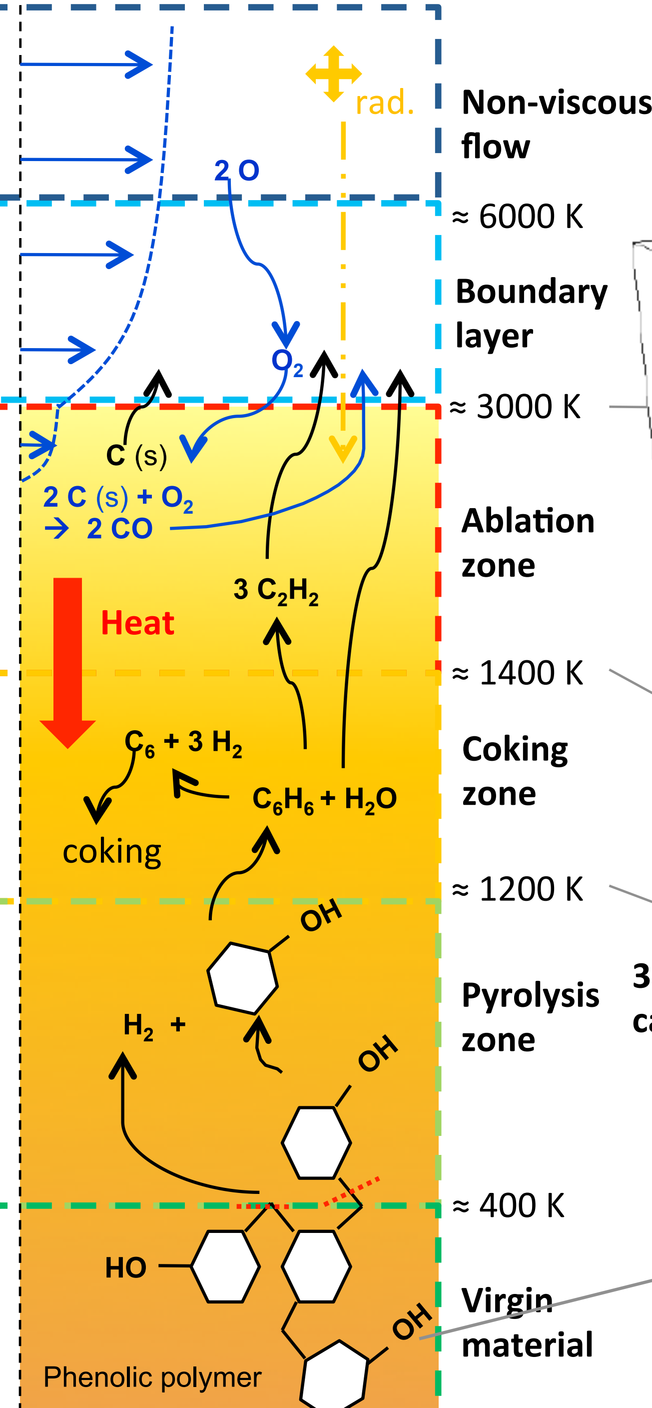
- Conduction heat transfer (1)
- Radiation heat transfer (empirical: 1, modeled: 3)
- Finite-rate chemistry of the pyrolysis gases (3)
- Coking (3)

- Multi-component diffusion (3)
- Convective transport (Darcy: 2, Klinkenberg: 3)
- Charring process (evolution of the density: 1, porosity: 2, tortuosity: 3, permeability: 2, effective conductivity: 1, effective surface area: 3)

- Phenolic-decomposition product (3)
- Phenolic-decomposition rate (1)

1 : in all material response models (type 1)
2 : in SOA material response models (type 2)
3 : in future material response models (type 3)

Macroscopic illustration

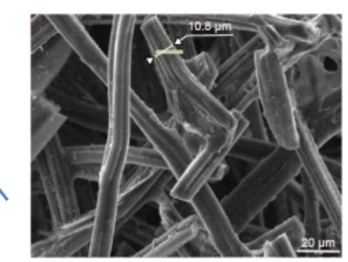


Chemistry mechanisms (simplified illustration)

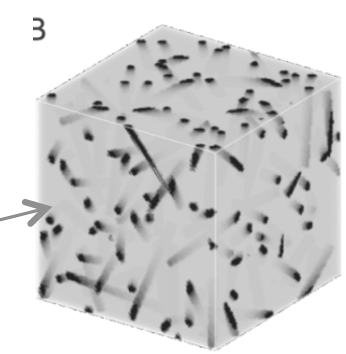
Microscopic illustration

Gas/surface Interactions in porous fibrous media (3):
- in-depth ablation
- erosion
- in-depth recombination
- convective heat trans
- radiative heat trans

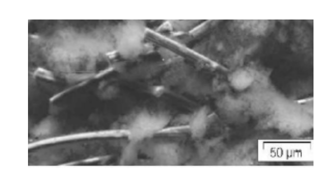
3D simulation of the ablation of a carbon/phenolic composite [Lachaud, 2010]



Scanning Electron Microscopy (SEM) : Carbon preform



3D reconstitution of a carbon/phenolic composite



SEM: carbon/phenolic (virgin) [Stackpoole, 2008]

Basic equations 1D

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Gas species mass conservation

$$\partial_t(\epsilon_g \rho_g y_i) + \partial_{\mathbf{x}} \cdot (\epsilon_g \rho_g y_i \mathbf{v_g}) + \partial_{\mathbf{x}} \cdot \mathcal{F}_i = \pi_i M_i + \epsilon_g \omega_i M_i$$

gas content — convective flux — diffusive flux — heterogeneous reaction source — homogeneous reaction source

Solid species mass conservation

$$\partial_t(\epsilon_s \rho_s) = \partial_t(\epsilon_m \rho_m + \epsilon_f \rho_f) = -\Pi + \sum_{i \in s} \epsilon_g \omega_i M_i + \sum_{i \in s} \tau_i M_i$$

solid content — resin — fibers — heterogeneous reaction source — coking — fiber erosion

Momentum conservation

$$\mathbf{v_g} = -\frac{1}{\epsilon_g \mu} \frac{1 + \beta/p}{1 + Fo} \underline{\underline{\mathbf{K}}} \cdot \partial_{\mathbf{x}} p$$

- •Darcy's Law
- •Forchheimer correction
- •Klinkenberg correction

Energy conservation

$$\partial_t \rho_a e_a + \partial_{\mathbf{x}} \cdot (\epsilon_g \rho_g h_g \mathbf{v_g}) + \partial_{\mathbf{x}} \cdot \sum_{i=1}^{N_g} (h_i \mathcal{F}_i) = \partial_{\mathbf{x}} \cdot (\underline{\underline{\mathbf{k}}} \cdot \partial_{\mathbf{x}} T) + \mu \epsilon_g^2 (\underline{\underline{\mathbf{K}}}^{-1} \cdot \mathbf{v}) \cdot \mathbf{v}$$

energy content — convective flux — diffusive flux — conductive flux — viscous flux

$$\rho_a e_a = \epsilon_g \rho_g e_g + \epsilon_m \rho_m h_m + \epsilon_f \rho_f h_f$$

Current Codes

Name	Contact	Owner	Users	Applications
Amaryllis	T. van Eekelen	LMS Samtech, Belgium	EADS Astrium, ESA	Design
CAMAC	W.-S. Lin	CSIST, Taiwan	Taiwan Ins. of Sci. Tech.	Unknown
CAT	N. N. Mansour	NASA ARC, USA	NASA ARC	Analysis
CHALEUR	B. Blackwell	SNL, USA	SNL	Design
CHAP	P. Keller	Boeing, USA	Boeing	Design
CHAR	A. Amar	NASA JSC, USA	NASA	Analysis
CMA	R. Beck	Aerotherm, USA	NASA, SNL	Design
CMA/SCMA	C. Park	Tokyo Univ., Japan	JAXA	Design
CMA/KCMA	P. Reygnier	ISA, France	ISA/ESA	Analysis
FEAR	J. Dec	NASA LaRC, USA	NASA LaRC	Analysis
FABL	J. Merrifield	Fluid Grav. Eng. Ltd., UK	ISA/ESA/FGE	Analysis
FIAT	Y.-K. Chen	NASA ARC, USA	NASA, SpaceX	Design
3DFIAT	Y.-K. Chen	NASA ARC, USA	NASA ARC	Analysis
HERO	M. E. Ewing	ATK, USA	ATK	Analysis
ITARC	M. E. Ewing	ATK, USA	ATK	Design
libAblation	R. R. Upadhyay	Univ. of Tex. Aust., USA	UTA	Analysis
MIG	S. Roy	Univ. of Flo., USA	Univ. of Florida	Analysis
MOPAR	A. Martin	Univ. of Mich., USA	UKY/Univ. of Michigan	Analysis
NEQAP	J. B. Scoggins	N. Carol. St. Univ., USA	NCSU	Analysis
NIDA	G. C. Cheng	Univ. Alab. Birm., USA	UAB	Analysis
PATO	J. Lachaud	NASA ARC, USA	Univ. Calif. Santa Cruz	Analysis
STAB	B. Remark	NASA JSC, USA	NASA, FGE	Design
TITAN	F. S. Milos	NASA ARC, USA	NASA	Analysis
TMU	A. R. Bahramian	T. Modares Univ., Iran	TMU	Analysis
US3D	G. Candler	Univ. of Minn., USA	UM	Analysis

Numerical methods

Name	Numerical method	Spatial accuracy	Temporal accuracy
Amaryllis[22]	Finite-Element	First-order	First order
CAMAC[23]	Unknown	Unknown	Unknown
CAT[24]	Implicit Finite Volume	Second-order	Second-order
CHALEUR[25]	Control Volume Finite-Element	Second-order	First-order
CHAP[26]	Implicit Finite-Difference	First-order	Second-order
CHAR[27]	Galerkin Finite Element	Second-order	Second-order
CMA[28]	Implicit Finite-Difference	First-order [2]	First-order
CMA/SCMA[29]	Implicit Finite-Difference	Second-order	First-order
CMA/KCMA[30]	Implicit Finite-Difference	Second-order	First-order
FABL[32]			
FIAT[20]	Implicit Finite-Volume	First-order	First-order
3DFIAT[33]	Implicit Finite-Volume	First-order	First-order
FEAR[31]	Galerkin Finite Element	Second-order[1]	Second-order[1]
HERO[34]	Finite-Element	Second order	First order [3]
ITARC[34]	Control Volume	Up to 3rd-order [1]	First order
libAblation[35]	Newton on analy. eq.	First-order in space	No time integration
MIG[36]	Discrete Galerkin	Up to 4th-order	3rd-order
MOPAR[37]	Control Volume Finite-Element	Second-order	First-order
NEQAP[38]	Implicit Finite-Difference	Second order	Second order
NIDA[39]	Finite-Difference	Second order	Unknown
PATO [40]	Implicit Finite-Volume	First-order[1]	First-order[1]
STAB[41]	Implicit Finite-Difference	Second-order	First-order
TITAN[42]	Implicit Finite-Volume	First-order	First-order
TMU[43]	Explicit Finite-Difference	First-order	Unknown
US3D[44]	Implicit Finite-Volume	Second-order	First-order

Codes Capabilities

Code capabilities Green : verified and available (G) Yellow : under verification, not in the official version/ release (Y) Red : in development (R)	AMARYLLIS	CAMAC	CAT	CHALEUR	CHAP	CMA	CMA S	CMA K	CODE-JSC	CODE-LaRC	FABL	FIAT	3DFIAT	HERO	ITRAC	LIBABLAT	MIG	MOPAR	NEQAP	NIDA	PATO	STAB	TITAN	TMU	US3D MOD
Summary																									
Model fidelity (1-3)	2	1	3	2	1	1	2	1	2	1	2	1	1	2	2	1	2	2	2	3	3	1	1	1	1
Code dimensionality (nD= 1-3)	3	1	1	1	1	1	1	1	3	1	1	1	3	3	1	1	1	1	1	1	3	1	2	1	1
Code maturity level (1-3)	3	1	2	3	3	3	3	2	2	2	2	3	2	2	3	1	1	2	1	1	2	3	2	2	1
Gas-phase Mass Conservation	**In-depth : Eq. 1**																								
Storage (∂_t …)	R		G	G					G			Y	Y				G	G	G	G	G			G	G
Divergence (∂_x…)	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G
Pyrolysis production (Π)	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G
Pyrolysis model	**In-depth: Eq. 2-7**																								
SoA Arrhenius laws (-> Π)	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G		G	G	G	G	G	G
Species production (-> πi)			G																	Y	Y				
Gas-species Conservation	**In-depth: Eq. 8**																								
Storage (∂t …)			G																G	G	G				
Divergence (∂x…)			G																G	G	G				
Multi-component diffusion (∂xF)			R																		R				
Finite-rate chemistry (πi , ω_i)			Y																G	G	G				
Solid-phase mass conservation	**In-depth: Eq. 9-10**																								
Pyrolyzing matrix mass loss	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G
In-depth ablation/coking			R																		Y				
Momentum conservation	**In-depth: Eq. 11**																								
Darcy's law	G		G	G		Y	G		G			Y	Y	G	G	G	Y	G	G	G	G	G			G
Klinkenberg			R						G				Y								Y				
Forchheimer			R	G					G				Y					G							
Energy conservation	**In-depth: Eq. 12-13**																								
Storage (∂t …)	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G
Divergence (∂x…)	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G
Effective conduction	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G
Viscous dissipation			Y	G													G	G		Y	Y				
Boundary conditions	**At the wall: Eq. 14-22**																								
Surface energy balance	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	R	G	G	G	Y	G	G	G	G	G
Wall chemistry from B' table	G			G	G	G	G	G	G	G	G	G	G	G	G	R	R	G		Y	G	G	G		Y
Internal wall chemistry solver			Y									Y	Y								Y		Y		
Other utilities	**Integrated libraries**																								
Equilibrium chemistry solver			Y						G								Y			Y	Y				Y
Integrated boundary layer code			R																		R				
Script-coupling to CFD code			R									Y	R					G			R		Y		