A SHORT REVIEW OF ABLATIVE-MATERIAL RESPONSE MODELS AND SIMULATION TOOLS

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ABSTRACT

A review of the governing equations and boundary conditions used to model the response of ablative materials submitted to a high-enthalpy flow is proposed. The heritage of model-development efforts undertaken in the 1960s is extremely clear: the bases of the models used in the community are mathematically equivalent. Most of the material-response codes implement a single model in which the equation parameters may be modified to model different materials or conditions. The level of fidelity of the models implemented in design tools only slightly varies. Research and development codes are generally more advanced but often not as robust. The capabilities of each of these codes are summarized in a color-coded table along with research and development efforts currently in progress.

Key words: Ablative material; modeling; design tool.

NOMENCLATURE

Latin

\begin{itemize}
  \item $F_i$ Diffusion flux of the $i^{th}$ species, $kg \cdot m^{-2} \cdot s^{-1}$
  \item $\dot{m}$ Mass flow rate, $kg \cdot m^{-2} \cdot s^{-1}$
  \item $A_i$ Gaseous species $i$
  \item $A_t$ Arrhenius law pre-exponential factor, $SI$
  \item $C_H$ Stanton number for heat transfer
  \item $C_M$ Stanton number for mass transfer
  \item $c_p$ Specific heat, $J \cdot kg^{-1} \cdot K^{-1}$
  \item $\epsilon$ Specific energy, $J \cdot kg^{-1}$
  \item $E_i$ Arrhenius law activation energy, $J \cdot kg^{-1}$
  \item $F_j$ Fraction of mass lost through pyrolysis reaction $j$
  \item $h$ Specific enthalpy, $J \cdot kg^{-1}$
  \item $j$ Diffusive flux, $mol \cdot m^{-2} \cdot s^{-1}$
  \item $K_{ij}$ Chemical equilibrium constant for reaction $i$
  \item $l$ Thickness or length, $m$
  \item $m_i$ Arrhenius law parameter
  \item $M_k$ Molar mass of species $k$, $kg \cdot mol^{-1}$
\end{itemize}

Greek

\begin{itemize}
  \item $\beta$ Klinkenberg coefficient, $Pa$
  \item $\epsilon$ Volume fraction
  \item $\gamma_{ji}$ Stoichiometric coefficient, reaction $j$ species $i$
  \item $\mu$ Viscosity, $Pa \cdot s$
  \item $\omega$ Reaction rate, $mol \cdot m^{-3} \cdot s^{-1}$
  \item $\omega_s$ Solid reaction rate, $mol \cdot m^{-3} \cdot s^{-1}$
  \item $\Pi$ Pyrolysis gas production rate, $kg \cdot m^{-3} \cdot s^{-1}$
  \item $\rho$ Density, $kg \cdot m^{-3}$
  \item $\tau$ Characteristic time, $s$
  \item $\xi_j$ Advancement of pyrolysis reaction $j$
\end{itemize}

Subscripts

\begin{itemize}
  \item $g$ Number of gaseous species
  \item $n_i$ Arrhenius law parameter
  \item $N_p$ Number of pyrolysis reactions
  \item $q$ Heat flux, $J \cdot m^{-2} \cdot s^{-1}$
  \item $R$ Perfect gas constant, $J \cdot kg^{-1} \cdot K^{-1}$
  \item $v$ Convection velocity, $m \cdot s^{-1}$
  \item $y$ Mass fraction
  \item $F_0$ Forchheimer number
  \item $K$ Permeability
  \item $p$ Pressure, $Pa$
\end{itemize}

Conventions

\begin{itemize}
  \item $\partial_{x}$ Divergence
  \item $\partial_{t}$ Time derivative
  \item $\mathbf{T}$ Second order tensor
  \item $\mathbf{u}$ Vector
1. INTRODUCTION

During re-entry, a fraction of the heat is transferred to the thermal protection system (TPS) leading to a gradual temperature increase of the material (figure 1). With the temperature increase, the virgin material is successively transformed and removed by two phenomena. The first transformation phenomenon is called pyrolysis. During pyrolysis, the pyrolyzing phase of the material (often a polymer matrix) progressively carbonizes and loses mass producing pyrolysis gases. The pyrolysis gases are transported out of the material by diffusion and convection through the pore network. During this transfer, their chemical composition evolves as their temperature increases. The second transformation phenomenon is the ablation of the char that is composed of the residual carbonized matrix and of the non-pyrolyzing phase (often a carbon or silicon-carbide fibrous preform). Depending on reentry conditions, ablation may be due to heterogeneous chemical reactions (oxidation, nitridation), phase change (sublimation), and/or mechanical erosion (spallation). Material response models should predict accurately the ablation rate and the peak temperature of the bondline at the interface of the TPS and the substructure. The first open literature publication providing a very detailed and comprehensive analysis of ablative material response in high enthalpy environments is the Aerotherm report from 1968 describing their suite of design tools [16]. CMA and ACE, Aerotherm’s in-depth material response and surface ablation codes respectively, are cited as a reference in most publications in the field. The models implemented in current design-capable tools are mostly replicas (or parallel developments) of the Aerotherm model with slight variations. Interestingly, the modifications to the Aerotherm model have mainly involved simplifications, with some of the Aerotherm capabilities currently no longer maintained in most of the major tools. Recent interest in manned-rated and challenging design missions (e.g. high mass, very high velocity, porous materials) has raised the need for high-fidelity models capable of providing optimized design and comprehensive uncertainty quantifications. All the capabilities of the Aerotherm’s suite of tools and the rich academic work on pyrolysis and ablation are being revisited and progressively introduced (or re-introduced) both in research codes and in design tools. In a complementary effort, several academic, government, and industrial teams are working on the development, the implementation, and the validation of original physics-based models that will enable anchoring of CMA/ACE-based design tools, accurate uncertainty analysis, and maybe become the future base models for design-rated codes. This paper first presents the pyrolysis-ablation problem through the governing equations (mass, momentum, and energy conservation) and boundary conditions. Different levels of modeling fidelity are presented and discussed. An effort was made to gather information on the simulation tools that are actively used either for design or for research and development. The capabilities of each of these codes are summed up in figure 4.

2. CONSTITUTIVE MODELS

2.1. Mass conservation

The gaseous mass-conservation equation includes a production term (right-hand side) to account for the pyrolysis gas production, noted $\Pi$, and reads

$$\partial_t (\rho_g v_g) + \nabla \cdot (\rho_g v_g v_g) = \Pi$$

In several codes, the time derivative is omitted and the gas flow problem is treated as a succession of steady state problems (see section 4). This simplification is correct when the variation of the intensive variables (temperature, pressure) are slow compared to the characteristic time of the flow in the porous medium. The characteristic time of the pyrolysis gas flow, $\tau_{pg}$ may be defined as the ratio of the thickness of the char layer - $l_c$ - to the velocity of the gas. In typical re-entry applications, $\tau_{pg} = l_c/v_g \approx 0.01/1 = 0.01s$. Therefore, the omission of the time derivative is an acceptable practice for situations for which the variations of the intensive variables are negligible over time steps of $\tau_{pg} \ll \tau_{step} = 1s$. The determination of the direction of the gas velocity, $v_g$, is necessary to solve the average mass-conservation equation. In several one-dimensional codes, this equation is numerically integrated with the assumption that the gas flow is perpendicular to the surface and directed towards the surface. This is exact in one-dimensional steady-state problems with an impermeable back face. In other conditions and in multi-dimensional problems, the direction of the flow has to be determined by resolution of the momentum-conservation equation.

The pyrolysis gas production is obtained by fitting thermogravimetry analysis of the resin decomposition using
one or several Arrhenius laws. For example, for phenolic polymers, it has been shown that the pyrolysis degradation process follows four steps [36], that may be described by four heterogeneous decomposition reactions [37]. A convenient notation for \( j \in [1, N_p] \) pyrolysis reactions is

\[
P M_j \rightarrow \sum_{i=1}^{N_g} \gamma_{ij} A_i
\]  

(2)

where \( P M_j \) is a fictive solid species of the pyrolysing polymer matrix (PM). The pyrolysing matrix density is then given by

\[
\epsilon_m \rho_m = \epsilon_m \rho_{m0} \sum_{j=1}^{N_p} F_j (1 - \xi_j)
\]  

(3)

where

\[
\frac{\partial_t \xi_j}{(1 - \xi_j)^{m_j}} = T^{m_j} A_j \exp \left( \frac{-\xi_j}{RT} \right)
\]  

(4)

The pyrolysis-gas production is given by

\[
\Pi = -\partial_t (\epsilon_m \rho_m) = \epsilon_m \rho_{m0} \sum_{j=1}^{N_p} F_j \partial_t (\xi_j)
\]  

(5)

In the literature, the equations used to describe pyrolysis models vary but they are mathematically equivalent.

It is important to mention that state-of-the-art design codes do not track the species production. Only the average mass production \(-\Pi\) is computed from the Arrhenius laws. A constant elemental fraction of the pyrolysis gas is assumed. The gas chemical composition and derived quantities (gas enthalpy, viscosity, mean molar mass) are then computed using the chemical equilibrium assumption or heuristic methods.

The pyrolysis gas production rate for each species \( i \) could readily be obtained using

\[
\langle \pi_i \rangle g = \epsilon_m \rho_{m0} \sum_{j=1}^{N_p} [\partial_t \xi_j] F_j \bar{\gamma}_{ji}
\]  

(6)

where

\[
\bar{\gamma}_{ji} = \frac{\gamma_{ji}}{\sum_{k=1}^{N_g} \gamma_{jk} M_k}
\]  

(7)

This requires the experimental determination of the stoichiometric factors \( \gamma_{ji} \), which are not directly available in the literature but may be derived from experimental studies [34, 36, 37]. The overall pyrolysis gas production may still by obtained from: \( \Pi = \sum_{i=1}^{N_p} \pi_i M_i \).

Higher fidelity models are being developed and implemented. They account for species production, transport, and chemical reactions (finite-rate chemistry) within porous media. The species conservation equation may be written in mass fraction \( y_i \) as

\[
\partial_t (\epsilon_g \rho_g y_i) + \partial_x (\epsilon_g \rho_g y_i v_g) + \partial_x F_i = \pi M_i + \epsilon_g \omega_i M_i
\]  

(8)

Both pyrolysis species production \( \pi_i \) and chemical species production \( \omega_i \) are needed. For the computation of \( \omega_i \), the finite-rate chemistry model developed by Pike and April in the late 1960s [28, 2] is used for preliminary analyses. This model was developed using chemical data and experimental techniques available at this time. Efforts are being undertaken in several teams to develop up-to-date finite-rate chemistry models and modern experimental set-ups for their validation [20]. \( F_i \) is the diffusion flux of the \( j^\text{th} \) species. At low pressures, mass transfer (diffusion) in porous media is not negligible compared to advection [18]. Mass transfer in porous media is a complex problem. The effective diffusion coefficient is smaller than the bulk diffusion coefficient due to the porosity and the tortuosity of the material [18]. Several models are available. A popular extension of the Stefan-Maxwell model [12] to porous media is the dusty gas model [25]. To our knowledge no fully capable ablation material-response code has such a capability yet. High-fidelity models including in-depth finite-rate chemistry will need to account for diffusion.

The solid-phase mass conservation is also integrated to compute the effective density of the solid. The volume-averaged density change of the matrix (due to pyrolysis \(-\Pi\)) is currently modeled using forms equivalent to

\[
\partial_t (\epsilon_m \rho_m) = \Pi
\]  

(9)

which is easily derived from equation 5. The current assumption is that there is no ablation or coking in-depth. Coking is neglected and ablation is modeled as a surface phenomenon only. Therefore, ablation is accounted for using a prescribed recession velocity at the wall, handled as a boundary condition (rather than as an in-depth constitutive equation) as described in section 3.

Current research efforts aim at developing models for in-depth coking and ablation. For this application, the solid mass-conservation equation may be generalized to account for heterogeneous reactions

\[
\partial_t (\epsilon_s \rho_s) = \partial_t (\epsilon_m \rho_m + \epsilon_f \rho_f) = -\Pi - \sum_{i \in s} \epsilon_g \omega_i^M M_i
\]  

(10)
However, the determination of the heterogeneous reaction rates \( \omega_{r}^{+} \) is not an easy task and is still being investigated.

### 2.2. Momentum conservation in porous media

The average gas velocity is obtained by resolution of the momentum-conservation equation. In porous media, the volume-averaged momentum conservation may be written as

\[
v_{g} = -\frac{1}{\epsilon_{g}\mu} \frac{1 + \beta/p}{1 + F_{O}K_{c}} \cdot \partial_{p} p
\]

(11)

Most of the materials are anisotropic, therefore, the permeability \(- K_{c}\) is a second order tensor. For example, Fiberform, the carbon preform of PICA [35], has orthotropic permeability properties [23]. For creeping (Stokes) flows in the continuum regime (in the pores of the material), the volume-average momentum conservation degenerates into Darcy’s law \((\beta = 0, F_{O} = 0)\). The term \(1 + \beta/p\) is the Klinkenberg correction to account for slip effects (at the pore scale) when the Knudsen number (ratio of the mean free path to the mean pore diameter) is not small. The term \(1 + F_{O}K_{c}\) is the Forchheimer correction to account for high velocity effects at the pore scale (flow separation in the continuum regime). Typically, Forchheimer effects are expected to occur for pyrolysis gas velocities higher than \(50\) \(m/s\) (that is, in high-density ablative materials submitted to very high heat fluxes). It is not advised to use both corrections simultaneously as they address different regimes.

### 2.3. Energy conservation

According to Puiroux [29], solid and gas phases are in thermal equilibrium as long as the Péclet number for diffusion of heat within the pores is small \((Pe = \epsilon_{g}\rho_{g}h_{p}v_{g}/k_{g})\). In most of the applications of interest for space agencies, the small pore size \(< 100\) \(\mu m\) and the slow pyrolysis gas flow \((v_{g} \sim 1\) \(m/s\)) insure a small Péclet number: the gas temperature accommodates to the solid temperature within the pores. Under the thermal equilibrium assumption, the energy conservation may be written as

\[
\partial_{t} \rho_{a} e_{a} + \partial_{x} (\epsilon_{g}\rho_{g}h_{g}v_{g} e_{g}) + \partial_{x} \sum_{i=1}^{N_{a}} (h_{i} J_{i}) = \partial_{x} (K_{c} \cdot \partial_{x} T) + \mu c_{p} (K_{c}^{-1} \cdot \nabla) \cdot \nabla
\]

(12)

where the total (storage) energy of the ablative material is the sum of the energy of its components

\[
\rho_{a} e_{a} = \epsilon_{g}\rho_{g} e_{g} + \epsilon_{m}\rho_{m} h_{m} + \epsilon_{f}\rho_{f} h_{f}
\]

(13)

The second and third terms of the left-hand side are the energy convected (advection) and the energy transferred (diffusion) by the pyrolysis gases, respectively. Heat transfer is conveniently modeled as an effective diffusive transfer (Fourier’s law). The effective conductivity \(- K_{c}\) is a second order tensor accounting for conduction in the solid, conduction in the gas, and effective radiative heat transfer. The validity of this volume-averaged approach is questionable. The main issue is the validity of the linearization of the radiative heat transfer. A theoretical study has shown that radiative heat transfer may be linearized for two-dimensional carbon-fiber pre-forms [40, 41]. The applicability to other materials is not straightforward and needs to be investigated. The second term on the right-hand side is the energy dissipated by viscous effects in Darcian regime [10]. It is small compared to the heat transfer term and often neglected.

### 3. BOUNDARY CONDITIONS

At the bondline, conservative boundary conditions are generally used (adiabatic and impermeable). At the wall and in ablative conditions, surface energy balance and surface mass balance are used as boundary conditions. [Of course, simple wall boundary conditions may always be used for simple analyses, e.g. fixed temperature.]

#### 3.1. Surface energy balance

![Figure 2. Energy balance at the wall](image)

The surface energy balance at the wall depicted in figure 2 reads

\[
q_{\text{conv}} = (\rho V)h_{w} + q_{\text{rad,in}} - q_{\text{rad,out}} - q_{\text{cond}} + \dot{m}_{pg} h_{pg} + \dot{m}_{ca} h_{ca} = 0
\]

(14)

where the convective heat flux \(- q_{\text{conv}} = \rho_{w} u_{w} C_{H}^{r} (h_{w} - h_{w})\) - and the radiative heat flux are extracted from CFD simulations. The Stanton number \(C_{H}\) is corrected to account for the blockage induced by the pyrolysis-ablation gas-blowing; that is, the heat transfer coefficient is corrected. For example, the following correction is widely used \(C_{H}^{r} = C_{H} \ln(1 + 2B^{*})/\ln(2B^{*})\), where \(B^{*} = (\dot{m}_{pg} + \dot{m}_{ca})/(\rho_{w} u_{w} C_{M})\) is a dimensionless mass flow rate and \(\lambda\) is a scaling factor usually taken equal to 0.5 [6].
3.2. Surface mass balance and recession rate

The pyrolysis-gas flow rate - \( \dot{m}_{pg} \) - is directly obtained in the material-response code by integration of the pyrolysis, transport, and mass equations, as explained previously. However, the ablation rate - \( \dot{m}_{ca} \) - is a function of both the mass transfer in the boundary layer and the thermo-chemical properties at the wall (pyrolysis-gas blowing rate and composition, temperature, pressure, boundary-layer gas composition). A common practice is to assume thermo-chemical equilibrium at the wall to compute the ablation rate. The model still in use in the community was developed in the sixties [27]. It is based on element conservation in steady-state in a control volume close to the wall as sketched in figure 3. The underlying hypothesis is that over a time increment \( \Delta t \), the equilibrium chemistry problem in the control volume is quasi-steady (decoupling of the material response and of the boundary-layer problem). This increment \( \Delta t \) should be at least as long as the time increment of the heat transfer simulation (material response code) but short enough so that \( p, T, \dot{m}_{pg} \), and \( y_{pg} \) variations may be neglected. This is verified in typical applications. For this presentation, we shall assume equal diffusion coefficients of the elements. Failure modes (spallation, mechanical erosion) are not included and the char is assumed to be composed of a single element (for example, carbon).

\[ \rho V = m_{pg} + m_{ca} \]

\[ \dot{m}_{pg} y_{pg} \]

\[ \dot{m}_{ca} y_{ca} \]

Pyrolysis gas (pg) flux
Char ablation (ca) flux

**Figure 3. Element mass-fraction conservation at the wall**

The inputs and outputs to this problem are:

- **Inputs**: \( \dot{m}_{pg}, y_{pg}, y_{ca} = 1, y_{ke}, p, T \).
- **Outputs**: \( \dot{m}_{ca}, y_{ke} \).

The conservation of the mass-fraction of element \( k \) in the control volume close the the wall reads:

\[ j_{k, w} + (\rho V) y_{k, w} = \dot{m}_{pg} y_{pg} + \dot{m}_{ca} y_{ca} \]  

(15)

where pg= pyrolysis gases, ca = char ablation products, w= wall (or control volume). Notes:

- Since \( p, T \) are fixed, the element mass-fraction conservation in the control volume is equivalent to the mass conservation.

Under the hypotheses that \( Prandtl = Lewis = 1 \) and that the diffusion coefficients are equal for the elements, equation 15 may be rewritten as

\[ \rho e u e C_H (y_{k, w} - y_{ke}) + \rho V y_{k, w} = \dot{m}_{pg} y_{pg} + \dot{m}_{ca} y_{ca} \]  

(16)

where, \( C_H \) is the Stanton number and \( \rho V = \dot{m}_{pg} + \dot{m}_{ca} \).

The formation reaction of species \( A_i \) may be written:

\[ A_i \rightleftharpoons \sum_{k \in Elements} \nu_{i,k} A_k \]  

(17)

The \( i \) chemical equilibriums read:

\[ \sum_{k \in Elements} \nu_{i,k} \ln(x_k) - \ln(x_i) - \ln(K_i) = 0 \]  

(18)

with \( x_i = 1 \) if \( A_i \) is a solid species. Species mole fractions sum to one:

\[ \sum_{i \in Species} x_i = 1 \]  

(19)

To sum up, the set of equations solved is:

\[ \rho e u e C_H (y_{k, w} - y_{ke}) + \rho V y_{k, w} = \dot{m}_{pg} y_{pg} + \dot{m}_{ca} y_{ca} \]  

\[ \sum_{k \in Elements} \nu_{i,k} \ln(x_k) - \ln(x_i) - \ln(K_i) = 0 \]  

(20)

(21)

with \( x_i = 1 \) if \( A_i \) is a solid species.

\[ \sum_{i \in Species} x_i = 1 \]  

(22)

The base model may be extended when needed to account for multicomponent mass transfer, non-equal diffusion coefficients, failure (spallation, melting), a solid phase made of more than one element (example: \( SiO_2 \)), corrections to account for heterogenous finite-rate chemistry. Current development efforts aim at fully modeling the boundary layer and coupling it to material codes, with the recession directly computed in the flow solver.

The surface pressure is an input to the material code (obtained from CFD simulations). It is the boundary condition required for the averaged momentum equation.

4. SIMULATION TOOLS

More than twenty ablative-material response tools are currently in use or in development for hypersonic re-entry
applications. The name of the codes and useful information are provided in table 1. The contact listed is either the code developer or a current active user. For each code, one open-literature reference is provided (for most of them, many are however available). Our understanding of the current code capabilities and/or development strategies based on open-literature publications are summarized in figure 4.

5. CONCLUSION

A review of the governing equations and boundary conditions used to model the response of ablative materials submitted to a high-enthalpy flow has been proposed. The heritage of model-development efforts undertaken in the 1960s is extremely clear: the bases of the models used in the community are mathematically equivalent. Most of the design-rated material-response codes implement a single model in which the equation parameters may be modified to model different materials or conditions. The level of fidelity of the models implemented in design tools only slightly varies. Research and development codes developed for analysis - at least in a first stage - are generally more advanced but often not fully capable. To sum-up, more than twenty codes are currently in use or in development, with an active community both maintaining state-of-the-art capability and seeking to increase the fidelity of the state-of-the-art model.

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REFERENCES

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<td>Fluid Gr. Eng.</td>
<td>Design</td>
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<td>T. Modares Univ., Iran</td>
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<td>G. Candler</td>
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<td>UM</td>
<td>Analysis</td>
<td>[13]</td>
</tr>
</tbody>
</table>

Table 1. List of currently available simulation tools

- **References**: The references for the tools are as follows:


### Code capabilities

<table>
<thead>
<tr>
<th>Green: verified</th>
<th>Yellow: under verification/to be released</th>
<th>Red: in development</th>
</tr>
</thead>
<tbody>
<tr>
<td>AMARYLLIS</td>
<td>CAMAC</td>
<td>CATHAP</td>
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<td>FADATAL</td>
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### Summary

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<tr>
<th>Model fidelity (1-3)</th>
<th>2 1 3 2 1 2 2 1 2 1 2 1 2 1 2 2 2 3 3 1 1 1 1 1</th>
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<td>Code dimensionality (nD= 1-3)</td>
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<td>Code maturity level (1-3)</td>
<td>3 1 2 2 2 3 3 2 2 3 2 2 3 1 1 2 1 1 2 2 3 3 3 2 1</td>
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</table>

### Gas-phase Mass Conservation

#### In-depth: Eq. 1
- Storage (δt, ...)
- Divergence (δx, ...)
- Pyrolysis production (Π)

### Pyrolysis model

#### In-depth: Eq. 2-7
- SoA Arrhenius laws (-> Π)
- Species production (-> πi)

### Gas-species Conservation

#### In-depth: Eq. 8
- Storage (δt, ...)
- Divergence (δx, ...)
- Multi-component diffusion (δxF)
- Finite-rate chemistry (πi, ωi)

### Solid-phase mass conservation

#### In-depth: Eq. 9-10
- Pyrolyzing matrix mass loss
- In-depth ablation/coking

### Momentum conservation

#### In-depth: Eq. 11
- Darcy’s law
- Klinkenberg/Forchheimer

### Energy conservation

#### In-depth: Eq. 12-13
- Storage (δt, ...)
- Divergence (δx, ...)
- Effective conduction
- Viscous dissipation

### Boundary conditions

#### At the wall: Eq. 14-22
- Surface energy balance
- Wall chemistry from B’ table
- Internal wall chemistry solver

### Other utilities

- Equilibrium chemistry solver
- Integrated boundary layer code
- Script - coupling to CFD code
- Integrated libraries

---

Figure 4. Simulation-tool list and capabilities. [The authors wish to apologize in advance for any missing or incorrect information contained in this figure. Corrections and addenda will be greatly appreciated.]
A short review of ablative-material response models & simulation tools

Jean Lachaud*, Thierry E. Magin’, Ioana Cozmutax, and Nagi N. Mansour+

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  ′von Karman Institute, magin@vki.ac.be
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*Sponsored by NASA’s Fundamental Aeronautics Program - Hypersonics Project

7th Aerothermodynamics Symposium (European Space Agency)
9 - 12 May 2011, Site Oud Sint-Jan, Brugge, Belgium
Session : Thermal Protection Systems

. Introduction

Physics and Chemistry in Ablative Materials

Type 1 model

Three types of material-response models have been identified & defined [during the 4th AFOSR/SNL/NASA Ablation Workshop. March 1-3, 2011, Albuquerque, NM]:

- **Type 1**: Heat transfer, pyrolysis, simplified transport of the pyrolysis gases, equilibrium chemistry, surface ablation (current state-of-the-art)
- **Type 2**: **Type 1** + averaged momentum equation for the transport of the pyrolysis gases (e.g. Darcy’s law)
- **Type 3**: High-fidelity model (**Type 2** + finite-rate chemistry, multi-component diffusion, in-depth ablation/coking, explicit radiative transfer model, …)

Motivation: Pure curiosity, review currently available codes and models

1 – In-depth modeling
   1.1 – Mass conservation
   1.2 – Mass transport
   1.3 – Energy conservation

2 – Boundary conditions
   2.1 – Surface energy balance
   2.2 – Surface mass balance and recession rate

3 – Summary
   3.1 – Table 1: List of codes, contacts, and references
   3.2 – Table 2: Codes capabilities
1.1. Mass conservation (gas/solid system)

Candid illustration of the chemistry of Pyrolysis & Ablation: incomplete mechanism!

**Shock**

**Boundary layer**

**Ablation zone**

**Char**

Not ablated

~ 1200°C

**Pyrolysis zone**

~ 200°C

**Virgin**

Phenolic formaldehyde resin

Chemistry of the pyrolysis gases

Pyrolysis & Pyrolysis-gas production

Ablation (leads to surface recession)
1.1. Mass conservation (gas/solid system)

Models: Type 1 / Type 2 / Type 3  
- In green: Experiments -

**Type 1** codes - hypothesis: instantaneous transfer (no storage)

\[ \partial_x \cdot (n_g) = \Pi \]

Pyrolysis gas flux

Pyrolysis laws (Arrhenius) = f(Temperature)
- Thermogravimetry analysis (TGA)

**Type 2 & Type 3**

\[ \partial_t (\varepsilon_g \rho_g) + \partial_x \cdot (\varepsilon_g \rho_g v_g) = \Pi \]

Open porosity  
- Pycnometry

\[ \rho_g = \frac{pM}{RT} \]

Mean molar mass: \( M = \sum_i x_i M_i \)

- Equilibrium chemistry  
  + elemental composition

- Finite-rate chemistry  
  + species conservation

Need to determine Gas Composition  
(in mole fractions of the species)
1.1. Species conservation (gas/solid system)

Models: Type 1 / Type 2 / Type 3 - In green: Experiments -

• **Gaseous Species Conservation**

\[
\frac{\partial}{\partial t} \left( \varepsilon_g \rho_g y_i \right) + \frac{\partial}{\partial x} \left( \varepsilon_g \rho_g y_i v_i \right) = \pi_i M_i + \varepsilon_g \omega_i M_i
\]

- Mass fraction of species \( i \)
- See mass transport
- Pyrolysis production rate for each species
- Thermogravimetry analysis (TGA) + mass spectroscopy / chromatography
- Finite-rate chemistry mechanism
  - Flow reactor + spectro/chromato

• **Solid-phase volume-fraction conservation** (in-depth ablation/coking)

Porosity increase/decrease due to heterogeneous reactions
- Hypotheses: no swelling, constant intrinsic solid densities

- Fibers: \( \dot{\varepsilon}_f = -\Omega_f \sum \varepsilon \omega_i \)
- Carbonized matrix: \( \dot{\varepsilon}_m = -\Omega_m \sum \varepsilon \omega_i \)

- Molar volume

Quantification of porosity change/heterogeneous chemistry
- Scanning Electron Spectroscopy (SEM) / Tomography before and after testing.
1.1. Species conservation (gas/solid system)

Pyrolysis-gas SPECIES-production modeling

Measured by Sykes for phenolic in 1967 - gas chromatography -

<table>
<thead>
<tr>
<th>j</th>
<th>Pyrolysis balance equations</th>
<th>Peak</th>
<th>$F_j$</th>
<th>$A_j$</th>
<th>$E_j$</th>
<th>$m_j$</th>
<th>$n_j$</th>
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<td>Inferred from Sykes 1967 [19]</td>
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<td>[19, 21]</td>
<td>[19]</td>
<td>Trick [21]</td>
<td>[21]</td>
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<td>2</td>
<td>$PFR_1 \rightarrow H_2O$ (physiosorbed)</td>
<td>100°C</td>
<td>0.02*</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>$PFR_2 \rightarrow 0.69 H_2O + 0.01 C_6 H_6$</td>
<td>500°C</td>
<td>0.73</td>
<td>$1.9 \cdot 10^3$</td>
<td>$9.8 \cdot 10^4$</td>
<td>1</td>
<td>1</td>
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<tr>
<td>2</td>
<td>$+ 0.01 C_7 H_8 + 0.23 C_6 H_6 O + 0.06 C_7 H_8 O$</td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>3</td>
<td>$PFR_3 \rightarrow 0.09 CO_2 + 0.33 CO + 0.58 CH_4$</td>
<td>600°C</td>
<td>0.21</td>
<td>11</td>
<td>$7.7 \cdot 10^4$</td>
<td>1</td>
<td>1</td>
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<tr>
<td>4</td>
<td>$PFR_4 \rightarrow H_2$</td>
<td>800°C</td>
<td>0.06</td>
<td>$6.6 \cdot 10^6$</td>
<td>$2.0 \cdot 10^5$</td>
<td>1</td>
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</table>
1.1. Species conservation (gas/solid system)

Finite-rate chemistry of the pyrolysis gases

<table>
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<th>Reaction Number</th>
<th>Reaction</th>
<th>Rate Law</th>
<th>Activation Energy E (Kcal/gm-mole)</th>
<th>Frequency Factor</th>
<th>s</th>
<th>References</th>
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<tbody>
<tr>
<td>(6-1)</td>
<td>$\text{CH}_4 = 1/2 \text{H}_2 + 1/2 \text{C}_2\text{H}_6$</td>
<td>$k_{fA}$</td>
<td>95.0</td>
<td>$7.6 \times 10^{14}$</td>
<td>0</td>
<td>14, 15, 16, 17, 18, 19</td>
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<td>(6-2)</td>
<td>$\text{C}_2\text{H}_6 = \text{C}_2\text{H}_4 + \text{H}_2$</td>
<td>$k_{fA}$</td>
<td>100.0</td>
<td>$6 \times 10^{14}$</td>
<td>0</td>
<td>14, 20, 16, 17, 18, 21</td>
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<tr>
<td>(6-3)</td>
<td>$\text{C}_2\text{H}_4 = \text{C}_2\text{H}_2 + \text{H}_2$</td>
<td>$k_{fA}$</td>
<td>10.0</td>
<td>$2.1 \times 10^{10}$</td>
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<td>(6-4)</td>
<td>$\text{C}_2\text{H}_2 = 2\text{C} + \text{H}_2$</td>
<td>$k_{fAB}$</td>
<td>17.0</td>
<td>$2.0 \times 10^{9}$</td>
<td>0</td>
<td>30, 31, 23, 24, 25, 26, 32</td>
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<td>(6-5)</td>
<td>$\text{C} + 2\text{H}_2 = \text{CH}_4$</td>
<td>$k_{fA}$</td>
<td>17.0</td>
<td>$2.0 \times 10^{13}$</td>
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<td>49</td>
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<td>(6-6)</td>
<td>$\text{C}_6\text{H}_6\text{O} + \text{H}_2 = \text{H}_2\text{O} + \text{C}_6\text{H}_6$</td>
<td>$k_{fA}$</td>
<td>45.0</td>
<td>$2.0 \times 10^{13}$</td>
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<tr>
<td>(6-7)</td>
<td>$\text{C}_9\text{H}_6 = 3 \text{C}_2\text{H}_2$</td>
<td>$k_{fA}$</td>
<td>35.0</td>
<td>$1.4 \times 10^{9}$</td>
<td>0</td>
<td>33</td>
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<tr>
<td>(6-8)</td>
<td>$\text{C} + \text{H}_2\text{O} = \text{CO} + \text{H}_2$</td>
<td>$k_{fAB}$</td>
<td>82.0</td>
<td>$1.2 \times 10^{12}$</td>
<td>-1</td>
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<tr>
<td>(6-9)</td>
<td>$\text{CO} + \text{H}_2\text{O} = \text{H}_2 + \text{CO}_2$</td>
<td>$k_{fAB}$</td>
<td>30.0</td>
<td>$1.0 \times 10^{12}$</td>
<td>0</td>
<td>41, 35, 36, 38, 39, 40, 43, 44</td>
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<tr>
<td>(6-10)</td>
<td>$\text{C} + \text{CO}_2 = 2 \text{CO}$</td>
<td>$k_{fA} - k_{fR}^2$</td>
<td>50.0</td>
<td>$1.6 \times 10^{6}$</td>
<td>-1</td>
<td>45, 46, 35, 36</td>
</tr>
</tbody>
</table>

* 1st Order (sec⁻¹)  ** 2nd Order (cm³/gm-mole·sec)  *** 0th Order (gm-mole/cm³·sec)

1.1. Mass conservation (gas/solid system)

Illustration: oxidation of a carbon preform.

\[ p = 0.12 \text{ atm} ; T = 898 \text{ K} \Rightarrow \text{Recession: } 0.7 \text{ cm in 1 hour.} \]

Two principal observations:
- reduction of fiber diameter eventually leading to recession
- sharp ablation front (about 0.2 mm) [i.e. oxygen is quickly consumed, reaction >> transport]

Validation of a volume-averaged fiber-scale model for the oxidation of a carbon-fiber preform.

1.2. Mass transport in porous media

Models: Type 1 / Type 2 / Type 3

- In green: Experiments -

\[ \mathbf{v}_i = \mathbf{v}_g + \mathbf{V}_i \]

Species velocity

Average gas velocity

Momentum Conservation in porous media

\[ \mathbf{v}_g = -\frac{1}{\varepsilon_g \mu} \left( K \frac{1 + \beta/p}{1 + F_o} \right) \partial_x p \]

Generalization of Darcy’s law

- K: permeability
- \( \beta \): Klinkenberg coefficient (low density, slip effect) – typically \( p < 0.1 \) atm
- \( F_o \): Forchheimer number (high velocity, separation) – typically \( v_g > 50 \) m/s
- \( \mu \): viscosity, computed from the gas composition, cf options for \( M \)

Diffusion velocity

Multicomponent mass transfer in porous media

(e.g. Dusty Gas Model: Stefan-Maxwell + Bosanquet)

In porous media, the effective diffusion coefficient is reduced (because wall collisions decrease the effective mean free path)

\[ D_{eff} = \frac{\varepsilon_g}{\eta} D_{ref} \]

Tortuosity

- Diffusivity apparatus
- Tomography + DNS

Permeameter
- Tomography + DNS
1.3. Energy conservation

Thermal equilibrium between the phases studied by N. Puiroux [AIAA 2002-3336]. His conclusion is that the thermal equilibrium assumption is valid.

One temperature model

\[
\partial_t (\rho_a e_a) + \partial_x (\varepsilon_g \rho_g h_g v_g) = \partial_x (k \cdot \partial_x T) + \partial_x \sum_{i \in S} \varepsilon_g \rho_g y_i h_i V_i + \mu \varepsilon^2 K^{-1} \cdot \nu \cdot \nu
\]

Computed or neglected
Solid enthalpies
- Differential Scanning Calorimetry (DSC)

Effective conductivity (conduction + radiative transfer)
- Guarded Hot Plate
- Flash diffusivity
- Arc Jet calibration
Outline

Motivation: Pure curiosity, review currently available codes and models

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   3.2 – Table 2: Codes capabilities
2.1. Surface Energy Balance

At the wall

\[ q_{\text{conv}} - (\rho V) h_w + q_{\text{rad},\text{in}} - q_{\text{rad},\text{out}} - q_{\text{cond}} + m_{pg} h_{pg} + m_{ca} h_{ca} = 0 \]

From CFD

**Unknown**: mass loss rate (kg/m\(^2\)/s)

\(-\) Will provide the recession rate

\[ v_{\text{ablation}} = \frac{m_{ca}}{\rho_{\text{char}}} \]
2.2. Surface mass balance and recession rate

At the wall (simplified description: equilibrium chemistry, no spallation)

1- Conservation of element mass fraction in the control volume \( (y_{k,w}) \)

\[
j_{k,w} + (\rho V) y_{k,w} = \dot{m}_{pg} y_{k,pg} + \dot{m}_{ca} y_{k,ca}
\]

2- Equilibrium chemistry

Provides both the ablation rate \( \dot{m}_{ca} \) and the gas composition \( y_{k,w} \) in the control volume (and derived quantities, like wall enthalpy)

The dimensionless tabulation of \( \dot{m}_{ca} = f(m_{pg}, T, p) \) is called a B’ table.
. Outline

Motivation: Pure curiosity, review currently available codes and models

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3.1. Table 1: List of codes, contacts, and references

We found 25 codes actively used and with open-literature references…

<table>
<thead>
<tr>
<th>Name</th>
<th>Contact</th>
<th>Owner</th>
<th>Users</th>
<th>Applications</th>
<th>References</th>
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<td>G. Candler</td>
<td>Univ. of Minn., USA</td>
<td>UM</td>
<td>Analysis</td>
<td>[40]</td>
</tr>
</tbody>
</table>

… please help us extending the list!
Table 2: Codes capabilities

Please accept our apologies for any error.
Corrections and suggestions of improvement will be greatly appreciated!

**Conclusion**
- **25+ codes** actively used
- **same base model** (from the 1960s)
- **design-rated tools**: simple and robust
- **analysis and research tools**: generally more advanced but often not fully capable for design
- **very active and diverse community**
APPENDICES
1.3. Energy conservation

Radiative heat transfer in fibrous preforms. 2D DNS & volume averaging

- Collision based ray-tracing algorithm to compute the form factors
- Finite-element code SAMCEF

Question: is it correct to linearize the radiative heat transfer in fibrous media?

Method: DNS using geometrical optics
[Refraction and diffraction negligible for T > 700K (i.e. when radiation not negligible)]

Expression of the effective conductivity

\[ \sigma_{\text{eff}} T^3 \Delta x \]

(following linearization of the radiative transport)

Objective: compute the extinction coefficient and verify the accuracy of the effective model

Numerical Validation of an Effective Radiation Heat Transfer Model for Fiber Preforms.
14 participants: we are still working on the analysis of the results, but a few remarks
- 13 codes (type 1 and/or type 2) gave results in agreement with FIAT (cf. PAM_1, PAM_2, CAT). Some differences attributed to: numerical errors (+/- 1%) and misinterpretation of the data for 2 codes (+/-6%).
- 1 code out-of-range (difference > 200%)
- Type 3 (with finite-rate chemistry) predicts lower temperatures (PAM_3).
2.3. Sensitivity analysis


Profile at t= 60s
Pyrolysis gas composition with finite-rate chemistry

(3) Transport & finite-rate chemistry
(2) Transport with frozen chemistry (low temperature)
(1) Production of the pyrolysis gases

surface (x=0)