Notes on Pyrolysis Material Study

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Introduction 1

These notes intend to progressively introduce the reader to the physics commonly adopted to describe ablative materials for Thermal Protection Systems (TPSs) in the literature. Commonly used for very high speed reentry in aerospace industry, they are highly studied as the sizing of the TPSs is currently one of the bottleneck for increasing the payload for space exploration.

This class of material have to be distinguished from passive materials, that only store incoming energy and are used as heat sink, but can be re-used several times, and actively cooled materials, which benefits from local heat dissipation to mitigate the incoming heat flux. On the other hand, pyrolising TPS are employed for their high potential in limiting the transport of energy in depth of the space vehicle, at the expanse of selfdegradation due to surface and in-depth heterogeneous reactions under high temperature, preventing their employ for future mission. This degradation process leads to an expel of energy due to out-gassing of hot products resulting from material ablation out of the vehicle. Eventually, the underlying surface blowing is increasing the thickness of the boundary layer, mitigating further convective heating in complex multi-physics processes. This will not be considered in these notes.

All the presented models derived thereafter are already implemented in the open source software PATO, and all the presented examples have been obtained using it. Starting from a simple heat transfer problem, the specificity of pyrolysing materials will be progressively introduced, and examples will provide an overview of the sensitivity of the results regarding the multiple physical processes at play within TPSs during atmospheric reentry. Finally, a note on ablation process and its effects on in-depths energy transport will close this note. The main literature sources used to write these notes are the following: [1], [2] and [3]. For porous material literature, the results presented in this note are demonstrated in general books such as [4].

$\mathbf{2}$ TPS Physical Modelling

In this section, the physics of ablative materials is described step by step by starting from a simple heat conduction problem that will serve as a reference as it is the behaviour of passive TPS. As the problem may be seen by some as artificial, the readers already familiar with the topic are encouraged to look directly at the main references used for these notes. Finally, for readers more interested by surface and mass balance between the TPS and the boundary layer, the topic is addressed in section 3.

A Simple Conduction Problem 2.1

Let's start by considering a material submitted to a time independent imposed temperature on one end, whereas the other is considered adiabatic (see Figure 1). The imposed temperature is chosen to be representative of temperature usually encountered over TPS surface such as it is expected it will trigger pyrolysis in the future.

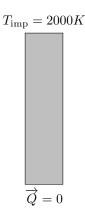


Figure 1: Schematic of the configuration studied in the next section.

If the material is assumed to be non porous such as passive materials, the description of energy transport is generally assumes to follow the Fourier law [5] which reads as:

$$\frac{\partial}{\partial t} \left(\rho^s c_p^s T^s \right) - \nabla \left(\lambda^s \nabla T^s \right) = 0 \tag{1}$$

$$\frac{\partial}{\partial t} \left(\rho^s \right) = 0 \tag{2}$$

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The upper script s denotes solid phase related properties. In the future, for porous material, the upper script ^g will be used for gas phase related variables. Additionally, it is assumed for now that the solid material is homogeneous, *i.e.* made of only one pure phase such as steel or carbon graphite. However, the reader should keep in mind that in the next parts, the composite nature of the TPS will be introduced, and the different solid phases will be indexed as $s_1, s_2, ..., s_n$ following the notation in [2]. In equation (1), the assumption of solid material energy $e^s = c_v^s T^s$ has been made. For an incompressible solid, $c_v^s = c_p^s$, [5], and most often the literature is using the notation in equation (1) to describe the energy distribution in time [1]. Equation (2) translates the fact that for a non porous and incompressible material, there is no variation of material density a priori. Any phase change or heterogeneous chemical reactions are happening at the boundary (the material being **non porous**, no volumetric chemistry

is considered) and only surface ablation can be considered in such configuration (see section 3).

An example of simulation with this kind of material is shown on Figure 2. In this example, for the sake of simplicity, the material properties c_p^s and λ^s has been chosen constant and are reported on Table 1. In that configuration, an analytical solution exists [5] (TO DO: FIND IT!).

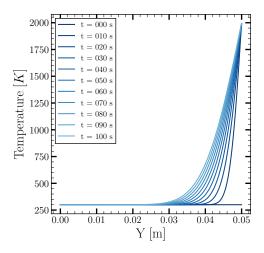


Figure 2: Solution of the pure conduction model (1)-(2) in time.

$\rho^s \left[\mathrm{kg/m^3} \right]$	1600
$c_p^s [\mathrm{J/kg/K}]$	732.7
λ^s [W/m/K]	0.3975

Table 1: Parameters for pure the conduction problem (1)-(2).

It can be noted that as previously said, this example is artificial in the sense that there are currently no dissipative processes occurring on the top boundary of the numerical domain. Consequently, surface temperature keeps increasing to the prescribed temperature whereas in reality:

- Radiative cooling would **bound** the surface temperature, preventing it from reaching such a high value. This cooling is the most efficient one (as it scales with the fourth power of surface temperature, see section 3), but additional local dissipation processes would also intervene in reality (melting, sublimation...)
- The surface heat flux is directly provided by the thermal state of the boundary layer. The use of a **constant** Dirichlet boundary condition is physically irrelevant, as the effect of convective heating over the material is reduced as surface temperature rises (let's consider for example a simple

Newton's approximation for boundary layer heat flux of the form $\overrightarrow{Q} = \alpha \left(T_e^g - T_s^s\right)$ with T_e^g the gas phase boundary layer edge temperature and T_s^s the material surface temperature. Ultimately, as material surface temperature becomes hotter than the boundary layer, the heat flux sign would reverse, and the fluid would cool down the surface.

2.2 Heat Transfer in a porous material

Let now assume that the material is not completely solid, but has **connected** holes inside which are making it **porous** (*c.f.* Figure 3). The pores are filled with gas, and the molecules composing this air are subjected to the same processes that are affecting the gas phase in the hypersonic region. Nevertheless, the tempera-

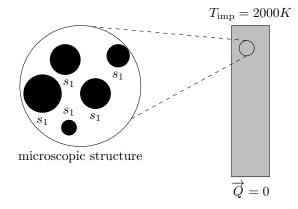


Figure 3: Despite their multiphase intrinsic characteristics at a **microscopic** level of description, transfer in TPS are described at the **macroscopic** level of description.

ture of the material is often lower that the post-shock region, which allows for several simplifying hypothesis.

- It is usually assumed that heat transfer within individual solid and gas phase is much faster than the transfer of energy within the material (*i.e.* the microscopic Peclet number is far lower than macroscopic Peclet number). This allow to consider that at each location of the material, the gas phase and the solid phase are at the same temperature.
- Depending of the material porosity ϕ^s , it is usually assumed that flow of gas phase within the pore are slow enough such as the gas phase is assumed to be in chemical equilibrium at any time. This permits to discard a priori any finite rate consideration when computing gas phase composition and transport properties.

Lets consider a material of porosity ϕ^s which corresponds to the microscopic ratio of the solid phase s over the total Representative Elementary Volume (REV)[4] characterizing the material:

$$\phi^s = \frac{1}{V} \iiint \mathcal{H}_s(x) \, dV \tag{3}$$

$$\mathcal{H}_s(x) = \begin{cases} 1 & \text{if } x \in s \\ 0 & \text{if } x \notin s \end{cases} \tag{4}$$

When several materials will be considered, a function \mathcal{H}_{s_i} would be consider of each solid phase i present in the REV, such as equation (3) naturally apply for each material component. In the same spirit, the gas phase volume fraction can be computed by equation (3) and is noted ϕ^g . The equation of mass conservation of the gas phase reads [4]:

$$\frac{\partial}{\partial t} \left(\phi^g \rho^g \right) + \nabla \cdot \left(\phi^g \rho^g \mathbf{v}^g \right) = 0 \tag{5}$$

In equation (5), the right hand side is purposely set to 0 to meet the hypothesis previously stated that the gas phase is mostly in an chemical equilibrium state while flowing within the material. For this reason, no source terms are considered for mass exchange between gaseous species.

Although it is not mandatory, the software PATO is solving a different equation than (5) to compute the transport of gas phase in the material. As the gas is in equilibrium, the calorific perfect gas assumption permits to write:

$$p^g = \frac{\rho^g RT}{M^g} \tag{6}$$

We not that phase temperature is not phase-distinct in equation (6) correspondingly with the first hypothesis on the material, which states that locally $T^g = T^s = T$. Furthermore, the gas phase velocity in a porous media can be described using Darcy law [4]:

$$\mathbf{v}^g = -\frac{1}{\phi^g \mu^g} \underline{\mathbf{K}} \nabla p^g \tag{7}$$

With $\underline{\mathbf{K}}$ the permeability tensor and μ^g the gas phase viscosity. Using equation (6) and (7) in equation (5) yields the PATO gas phase non-linear transport equation [1]:

$$\frac{\partial}{\partial t} \left(\phi^g \frac{p^g M^g}{RT} \right) + \nabla \cdot \left(-\frac{p^g M^g}{RT \mu^g} \underline{\mathbf{K}} \nabla p^g \right) = 0 \qquad (8)$$

Such as the material internal gas phase pressure p^g can be computed for each time with equation (8). It now remains to model the transport of energy through the gas phase.

3 Surface Balance for TPS

Now that the physics at play inside ablative material have been (more or less) uncovered, the attention of the reader is drawn on the surface specific processes whose consequences results in the self-degradation of ablative material as discussed in the previous section 2.

Bibliography

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