MSC.Marc-ATAS: Advanced thermal analysis software for modeling of rocket motors and other thermal protection systems.

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Abstract

Design of solid rocket motors requires an extensive knowledge of the thermal behavior for reliability and optimization of the payload. Within a solid rocket motor, a complex thermo-chemical-aerodynamic process occurs. During the launch, the combustion of the solid propellant generates intense heat, often reaching 3600 K. This results in a thermal decomposition of the combustion chamber housing and the nozzle due to pyrolysis, and the ablation/erosion of these latter due to thermal, chemical, and mechanical processes. Additionally, within the engine, radiation occurs which is dependent upon the current geometry, and the amount of combustion that has occurred. MSC.Marc, the chosen simulation software for the thermal aspects of the problem is being extended to model these phenomena. This paper discusses the numerical simulation of the pyrolysis, surface energy inputs and thermal contact.

Introduction

Snecma Moteurs, Rocket Motors Division, through its subsidiaries Europropulsion and G2P, is the prime contractor for developing the solid propellant rocket motors of Ariane 5 launchers and of the French deterrence force. It is also involved in the development of nozzle exit cones for liquid rocket motors such as the PW RL-10 motor equipping the Boeing Delta 3 launcher. Also, Snecma Moteurs develops thermal protection systems for reentry vehicles and bodies, and spatial probes.

What these products have in common is that some parts are subject to very high thermal fluxes (both convective and radiative), thermochemical oxidation by reactive chemical species, sometimes large mechanical and thermomechanical loads, and mechanical and chemical interactions with impacting liquid and solid particles. These loads have their origin in the high temperature, highly reactive and often particle laden surrounding flow generated either by the combustion of the fuel or by the speed of the vehicle. For instance, the nozzle and the internal thermal protection liners of a solid rocket motor can undergo fluxes up to 10 MW.m\(^{-2}\) and alumina particles impacts, during one or two minutes, from the flow produced by the combustion of the solid propellant. Thermal fluxes up to 100 MW.m\(^{-2}\) are encountered by some bodies on re-entry.

To sustain such conditions, these motors and vehicles use advanced composite materials, such as carbon/carbon composites, carbon/phenolic composites,
silica/phenolic composites, ceramic matrix composites, and reinforced rubber-like materials as shown above. Among these materials, some are thermodegradable and undergo a chemical transformation known as pyrolysis producing decomposition gases and possibly brittle solid residue. Also, those materials and others which are not thermodegradable can undergo surface recession, due to heterogeneous chemical reactions with the oxidizing chemical species of the surrounding flow, in which case we speak of thermochemical ablation or due to mechanical erosion by different mechanical loads. Also, thermochemical ablation and mechanical erosion can occur due to particle impacts.

The parts under discussion play a fundamental role for the thermal and mechanical integrity of the motor/vehicle for its safety, reliability, and performance. Hence, the temperature through the material, the thermo-poro-mechanical behavior induced, and the modifications of the geometry due to thermochemical ablation/mechanical ablation must be perfectly mastered.

In the past, the convenient design and sizing was obtained by a large sequence of destructive full-scale motor tests. Now, the need for cost and design cycle reduction for solid rocket motors, due to severe concurrence on the market, leads to the requirement for more comprehensive and precise numerical models. This allows for the design of the motor with fewer tests, minimal material, and, perhaps, more cost effective material.

During the last 40 years, many people have dealt with the modeling of the behavior of the above-mentioned materials in such environments. Numerous references can be found on this topic. This work has lead to more or less comprehensive models, and numerous in-house developed software programs often dedicated to a single material modeling. The modeling of the behavior of a whole motor, with its nozzle and its combustion chamber coated by thermal protection during and after the combustion of the grain, often implies the use of four or five different simple software programs, each focused on a peculiar aspect of the problem. Often, this software is limited to one-dimensional or two-dimensional conditions. The cooperative use and maintenance of several aging software programs cost time and manpower.

Recently, Snecma Moteurs recognized that the general behavior of the different materials listed above could be described by a single theory defined by five levels of complexity depending on the phenomena included or not included in each level. This offers the opportunity to implement some of these modeling levels in a single, general, multi-material software capable of 3-D analysis, capable of replacing all the former in-house developed software programs, and capable of more comprehensive, precise, and user-friendly modeling.

Because of possible further extension to fully coupled poro-thermal/thermo-poro-mechanical models, Snecma Moteurs chose to develop this new software on the basis of the general thermal/mechanical finite element analysis code MSC.Marc in close cooperation with MSC Software and its subcontractor CS-SI. The developments deal with four major issues: thermochemical ablation/mechanical erosion, pyrolysis and poro-thermal heat transfer, advanced thermal couplings capabilities, and advanced radiative heat transfer modeling.

This paper presents the status of this software development. It is planned to couple this new software with two other software programs dealing with the modeling of thermal, mechanical, and chemical loads, namely an advanced CFD software, and an advanced radiative heat transfer for anisotherm particle-laden semi-transparent media. However, these issues are not discussed here, neither the numerous couplings between the flow and the response of the material influencing the magnitude of the thermal flux.

1. Poro-thermal and ablative behavior of thermodegradable material
This paragraph focuses on the thermal aspects of the problem, and very little will be written on the associated poro-thermo-mechanical aspects. Nevertheless, the reader may keep in mind that the discussed pore pressure and thermal degradation of the material have tremendous effects on these aspects.

Let us consider, for instance, the case of a carbon/phenolic material used as a thermal protection liner in solid rocket motors. When such a material is exposed to a high thermal flux and chemically reactive environment, thermal degradation occurs and its structure changes as shown.

Starting from the rear side of the material opposite to the heated face, we find first, a nondegraded low temperature zone, with original low porosity and permeability, where thermal evaporation of trapped chemical species as water occurs [1-2]. This produces a high internal pore pressure.

At higher temperature range (300°C – 600°C) for solid propulsion heating rate conditions, the primary pyrolysis chemical reactions occur, turning the long polymer chains constituting the resin matrix into high molecular weight gaseous chemical species, and a carbonaceous solid residue [3-5]. In this zone, a pore pressure also develops although the porosity and the permeability of the material are increasing rapidly due to the loss of solid mass. The solid density decreases.

This pore pressure induces a flow of the rather cool gaseous products through the residue toward the heated surface upstream the heat flux, producing a cooling internal convection effect.

As higher temperatures are encountered (1000°C-1400°C), the thermal cracking of the gaseous phase continues further, generating less molecular weight chemical species. Depending on the local conditions, the gas can be in a state of chemical equilibrium or disequilibrium [6-7]. Besides these gas/gas reactions at still higher temperatures, some other reactions and transformations may occur. For instance, a graphitization of the residue can sometimes be observed. Another important phenomenon is the so-called coking [8]. The flowing gaseous products are introducing too much carbon than the chemical equilibrium allows at these temperatures. Hence, a solid carbon deposit in the residue is observed, which can reduce the porosity and the permeability, and again increase the local density left by the...
primary pyrolysis. This latter effect increases the resistance of the material to the thermochemical ablation discussed below.

Just below the heated surface, where the temperature can reach the range of 2500°C-2800°C, the thermodynamic conditions and the chemical species available in the internal gas flow change the direction of heterogeneous gas/solid reactions. There, instead of a carbon being deposited by coking, the carbon of the residue is now turned into gaseous species. At the surface itself, the external flow around the part contains similar gaseous chemical species, such as water vapor and carbon dioxide. Globally, the heterogeneous chemical reactions between these species at the solid surface and just below lead to a mass loss. This is known as thermochemical ablation and results in a recession of the surface. Numerous papers and books are devoted to this phenomenon, for instance [3,9-15]. The process can be controlled either by chemical kinetics or by the rate of diffusion of the chemical species through the boundary layer of the external flow, depending on the local temperature and flow conditions.

Ablation absorbs a great quantity of energy, as the water evaporation and pyrolysis reactions do. Another influence on the heat transfer reduction is due to the blowing of the boundary layer of the external flow by the gaseous products of thermal decomposition and ablation. With the above-mentioned internal convection cooling effect, these phenomena explain why these materials exhibit excellent thermal insulation properties.

Besides these chemical processes, if the residue is brittle, mechanical or dynamical loads can erode it [12-13]. Mechanical erosion is important for instance in the case of rubber-like materials used as internal thermal protection for the combustion chamber of the solid rocket motor [16].

As the combustion of solid propellant produces liquid or solid alumina particles, these latter can impact the walls of the motor and cause additional thermochemical ablation or mechanical erosion depending on the impact conditions. Impacts are also encountered in other applications of these materials [13].

In the case of a silica/phenolic composite, the process can be more complex, with additional phenomena such as reactions between the silica constituting the reinforcement and the carbon produced by the pyrolysis, fusion of the silica reinforcement, re-oxidation at the surface of some gaseous silicon oxide into liquid products [7,17-19]. On the contrary, with nonthermodegradable and tuff materials such as carbon/carbon composites, only the surface thermochemical ablation is relevant [11].

2. Short description of several modeling levels

Letting apart the surface phenomena such thermochemical ablation and mechanical erosion, at least five levels of complexity for the description of the internal behavior of the thermodegradable materials can be defined.

The level-1 simple model consists of ignoring the chemical processes and using effective thermal properties for an equivalent homogeneous material. The heat absorbed by the pyrolysis is integrated into a modification of the thermal heat capacity, similar to latent heat effects in phase change problems. There is, nevertheless, a discrepancy with the case of conventional materials. The modification in the properties accounting for the pyrolysis should be used only once during the initial heating phase, and not later during cooling or reheating phases. So, one must keep track of the history of the local heating in order to use the correct effective properties. The only variable calculated is the temperature.

The level-2 model includes the phenomena of primary concern, which are the mass loss due to pyrolysis, the associated energy absorption, and the internal convection cooling effect. The most drastic assumption made here is that the gas generated inside the material is not stored and flows instantaneously towards the heated surface. It means that the pore pressure is
not calculated; neither is the velocity of the pore pressure driven flow. Fundamentally, this model is one-dimensional, which allows one to group the density and the velocity of the gaseous phase in a single scalar variable: the mass flow rate of the gas. Then, the calculated variables are the local density of the solid phase, the temperature, and the mass flow rate. The set of coupled scalar equations for the mass balance, the energy balance, and the kinetic description of the pyrolysis are sufficient to calculate the latter. Also, constitutive laws for the properties of the partially degraded material must be introduced. To the knowledge of the authors, Moyer and Rindal [3] first proposed this model inspired by earlier studies on coal and wood combustion. This model was further enhanced and used by many authors, see [12-14,20]. It is simple, includes the essential physics, is adaptable to many different materials and situations, and does not require too much material characterization. That explains its very large popularity. It can be extended to include some second-order effects such as water evaporation and coking [8]. Nevertheless, its one-dimensional nature is a severe limitation for using it in many situations of rocket motors and TPS modeling. In the two-dimensional or three-dimensional case, the difficulty is that the mass flow rate is no longer a scalar but a vector, and missing in the model are two scalar equations for two of the three components of this vector. The missing 'physical' equations must be replaced by geometric conditions. The simple method is to imagine that the gas flows along some assumed streamlines towards the heated surface. The condition of a null scalar product of two components of the mass flow rates with the tangent vector of the streamlines give the missing equations. Some authors extended the model to the two-dimensional case by using a regular mesh and applying the model in each column of the mesh without allowing the gas to flow from a column to its neighbor. It is basically the geometric condition mentioned above. But it is not yet general enough to deal with some applications and complex geometry. In the framework of this study, the model has been extended to the three-dimensional case with fewer restrictions on the mesh. The concept of geometrical streamlines was introduced into the finite element method in order to obtain a general implementation of this level-2 model. This is discussed in more detail below.

The level-3 model considers explicitly a model for the pore pressure driven flow. New variables are introduced, such as the local density of the flow and its velocity, the pore pressure, the porosity, the permeability. To provide additional equations for closure, we consider the momentum balance for the gas in the approximate form of Darcy's law, a state equation for the gaseous phase, and evolution models for the porosity and the permeability. The concept of geometrical streamlines is no longer useful here. The principal restriction in this model is that no consideration is given to the details of the chemical reactions inside the gaseous phase, the details of the chemical reactions of the gas with the solid phase, or reactions in the solid phase such as carbon/silica reactions. Some assumptions upon the chemical composition and its thermodynamical state have to be made. As for the level-2 model, such phenomena as stored water evaporation and coking may be included but some precaution has to be taken regarding the assumptions on gas behavior. Different variants of level-3 model have been published, some as a part of higher-level models, for instance [1-2,7,21-23]. In the framework of this project, the resulting set of coupled partial differential equations is solved by the finite element method.

The level-4 model is the same as level-3, accepted that the details and the kinetics of the gas/gas, gas/solid, and solid/solid chemical reactions listed above are taken into account. An example of such a model is presented in the reference [7]. To the knowledge of the authors, this level is still restricted to one-dimensional situations because of the huge amount of chemical computations required. As there is a lack of data on these reactions, this model level is not considered in the current project.
Up to the level-4 model, the poro-thermal problem described here is only a one-way coupled with the corresponding level of modeling for the associated thermo-poro-mechanical problem, in the sense that the latter uses the results of the former such as the temperature, the pore pressure, the extent of pyrolysis, etc., but there is no retroaction of the latter on the former. The level-5 model introduces the full coupling between the two problems. For instance, the influence of the state of deformation upon the permeability, and, hence, upon the pore pressure, is taken into account. There is not a widely well-established accepted formulation for this modeling level. Some propositions can be found for instance in the references [21-22]. Once again, this kind of model requires a very large amount of material characterization as well as a large amount of computational time. So, the level-5 model is not included in the current project. Nevertheless, the way in which the level-3 model is implemented and the general structure of the MSC.Marc program should allow such a development in the future.

All the model levels described above assume thermal equilibrium between the gaseous phase and the different constituents of the solid phase, hence; there is only one temperature variable locally. In some cases, there could be such rapid transients that this assumption becomes false. The gaseous phase and the solid phase (even the matrix and the reinforcement inside the solid phase) may be in thermal disequilibrium. A different temperature must be assigned to each phase and components, and thermal exchanges between them modeled which leads to 'multiple-temperature' versions of the models described above. For instance, a two-temperature level-3 model with thermal disequilibrium between the solid phase and the gaseous phase is proposed in the reference [23]. Such developments are not considered in the current project.

3. Physical models, numerical methods, and results for ablation and pyrolysis

3.1 Physical models

Many different models with increasing complexity can be considered concerning the surface energy balance under thermochemical ablation and mechanical erosion conditions. For instance, the ablation rate and the surface temperature may be imposed by the user from test results, the popular concept of heat of ablation may be used, or a full energy balance such as proposed by Kendall, Rindal and Bartlett [9]. Some different models will be available in MSC.Marc-ATAS, but only the latter is discussed here.

The full surface energy balance (SEB) is required to determine the conductive flux entering the material, the surface temperature, and the surface recession velocity during an ablation/erosion process, from the external flow configuration. Besides the conductive flux, the SEB takes into account convective heat flux with a possible blowing effect due to mass injection, a radiative balance, an enthalpy flux due to molecular diffusion of the chemical species in the boundary layer, three enthalpy fluxes associated with the mass transfer due to thermochemical ablation by gases and thermal internal decomposition, two enthalpy fluxes associated with thermochemical ablation, and a mechanical erosion by liquid or solid particles impacts, and possible removal of liquid phases formed at the surface.

The surface energy balance (SEB) allows one to obtain the recession due to thermochemical ablation by gases or particles. The other part of the surface recession, due to the mechanical erosion, is calculated by other means. Both contributions are summed to obtain the total surface recession.

The SEB is coupled with the heat transfer into the material by the conductive heat flux, and with the mass flow rate towards the surface due to thermal decomposition gases generated inside the material.
The following figure illustrates the in-coming and out-going flux in a control volume at the surface.

The adopted expression for the SEB is:

$$
\lambda, \frac{\partial T}{\partial n}_{\text{surface}} = \alpha_M \left( H_{\text{rec}} - H_{\text{g}}^T \right) - (\rho v)_w H_w + \alpha_M \sum_i \left( Z_{\text{er}} - Z_{\text{is}}^* \right) H_i^T + \dot{m}_{s,\text{th,g}} H_s + \dot{m}_g H_g
$$

$$
+ f_{\text{th,p}} \sum_j G_{\text{th,p},j} \dot{m}_{p,j} \Delta H_{r,p,j} - \sum_l \dot{m}_l H_l + \Phi_{\text{rad,absorbed}} - \Phi_{\text{rad,emis}}
$$

The reader should refer to classical papers and books on ablation for further insight in the SEB [9,14-15]. A set of so-called classical G-Law model is used for modeling thermochemical ablation by impacts of several different families of particles.

Both gases and impacting particles contribute to a chemical ablation that can be expressed by:

$$
\dot{s}_h = (\dot{m}_{s,\text{th,g}} + \dot{m}_{s,\text{th,p}}) / \rho_s,
$$

with

$$
\dot{m}_{s,\text{th,g}} = f_{\text{th,g}} \sum_j G_{\text{th,p},j} \dot{m}_{p,j}
$$

where $\dot{s}_h$ is the recession velocity due to chemical reactions and $\rho_s$ the solid density.

Besides this thermochemical ablation, mechanical erosion can occur:

$$
\dot{s} = \dot{s}_h + \dot{s}_{\text{mech}}
$$

Until now, the development has dealt with level-1 and level-2 models discussed above, for the modeling of internal behavior. This paper focuses on the latter in a simplified form, and nothing is written on water evaporation and coking.

In the level-2 model, the decomposition of the material is represented by two equations: the mass balance gives as a result the mass flow rate of the pyrolysis gas and the solid density, and the energy balance, which takes into account the contribution of the pyrolysis one, through which one obtains the temperature. Moreover, the concept of geometrical streamlines explained above is used.

The expression for the mass balance is:

$$
\nabla \dot{m}_g = - \frac{\partial \rho_{s,p^*}}{\partial t}
$$
where \( \frac{\partial \hat{\rho}_{s,p}}{\partial t} \) is the rate of decomposition of the solid material, and \( \dot{m}_g \) the mass flow rate of pyrolysis gas.

As the material can be composed by several components, the rate of decomposition is a sum of Arrhenius laws.

\[
\frac{\partial \hat{\rho}_{s,p}}{\partial t} = \sum_{j=1}^{n} \Gamma_j \frac{\partial}{\partial T} \exp\left( -\frac{T}{T_j} \right) \hat{\phi}_{svj} \left( \frac{\hat{\rho}_{svj} - \hat{\rho}_{sj}}{\hat{\rho}_{svj}} \right)
\]

where \( \hat{\rho}_{svj} \) is the density of the virgin material, and \( \hat{\rho}_{spc} \) is the density of the charred material, and \( \hat{\rho}_{sj} \) is the current density of the \( j \)th component of the solid.

The mass balance is integrated along the geometrical streamlines:

\[
\int \int \int \int \frac{\partial \dot{m}_g}{\partial x} \, dx \, ds = \int \int \frac{\partial \hat{\rho}_{s,p}}{\partial t} \, dx \, ds.
\]

This leads to the following numerical scheme to calculate the mass flow rate of the pyrolysis gas:

\[
s(x_i) \dot{m}_g(x_i, t^{n+1}) = s(x_i) \dot{m}_g(x_i, t^{n+1}) - 0.5 \sum_{n=2}^{k} (x_i - x_{i-1}) \left( \frac{\partial \hat{\rho}_{s,p}(x_i)}{\partial t} + \frac{\partial \hat{\rho}_{s,p}(x_{i-1})}{\partial t} \right) s(x_i)
\]

The rate of decomposition is evaluated with the temperature of the previous time step.

As quoted above, the solid and the gas are assumed to be in thermal equilibrium leading to a one-temperature model. The energy balance includes a convective term due to the motion of the pyrolysis gas in the porous media and an enthalpic term \[3\]. It is written as:

\[
\hat{\rho}_s c_p \frac{\partial T}{\partial t} + c_{pg} \dot{m}_g \nabla T = \nabla \cdot (\lambda^* \nabla T) + \frac{\partial \phi_{s,p}}{\partial t} \left( H_{g,p} - H_{s,p,c} \right)
\]

where enthalpies are absolute enthalpies, defined by \( H = \Delta H^0 + h = \Delta H^0 + \int_{T_0}^T c_p dT \) and where \(( H_{g,p} - H_{s,p,c} )\) represents some kind of 'heat of pyrolysis', with

\[
H_{s,p,c} = \frac{\rho_{s,p,c} - \rho_{s,p,c}}{\lambda_{s,p,c}} \text{ being an effective enthalpy for the degrading solid.}
\]

The energy equation is solved in the standard fashion by finite elements in MSC.Marc.

3.2 Material behavior

During the pyrolysis, the material undergoes a phase transformation from the outside surface to the interior region as shown below. It is assumed that coking takes place in completely pyrolysed material. The effective material properties are defined as:

\[
\lambda^* = (1 - \xi_p) \lambda_v + \xi_p (1 - \xi_c) \lambda_c + \xi_c \xi_p \lambda_{cd}
\]

which relates the effective conductivity \( \lambda^* \) to the virgin \( \lambda_v \), charred \( \lambda_c \) and coked conductivity \( \lambda_{cd} \) using the rate of pyrolysis \( \xi_p \) and the rate of coking \( \xi_c \). Hence, the user need to define the material properties in three states, all of which may be anisotropic and temperature dependent. To facilitate this, a new THERM-PORE option has been introduced to allow these properties along with their respective enthalpy of formation. A new option has also been introduced to
allow the user to associate a table (MSC.Patran Field) to any material property. These tables may have up to four independent variables to permit general spatial variation without the need of user subroutines. This capability has been generalized to support all of the material properties, boundary conditions, and contact data in MSC.Marc.

3.3. Numerical methods

Ablation analysis

As previously discussed an important aspect of modeling thermal protection systems is examining the consequences of surface recession by ablation. Building on the pioneering work in MSC.SuperForm (formerly MSC.AutoForge) automatic remeshing procedures have been developed. In conventional heat transfer analysis, mechanical displacements are not considered. In these analyses, a zero displacement has been introduced, except at the surface nodes where recession is allowed. The surface recession rate may be due to one of the sources discussed above or may be a simple user-defined function. The recession model and the relevant surface are defined in a new RECEIVING SURFACE option. This recession rate is evaluated at the surface integration points and a consistent nodal displacement is obtained. The next step is to determine when remeshing is required. For manufacturing analysis, the common criteria are based upon mesh distortion as the finite element mesh degenerates with distortion. In these ablation problems, where, initially, very thin elements are used, these distortion criteria were determined to be inadequate. Rather, a criteria based upon the percentage reduction in element thickness in the direction of the streamline was developed. Furthermore, the time step is adaptively controlled among other restraints so that the surface recession distance per time step must be less than a critical dimension. It should be noted that while the element aspect ratio often is greater than 50:1, this does not lead to computational difficulties for heat transfer analysis.

Initially it was felt that mesh generators, such as the advancing front or Delauney, could be applied to remesh the region after ablation occurred. But, based upon the requirements imposed due to the streamline integration technique and for the mesh requirements to accurately capture high thermal gradients, these methods proved fruitless. Rather, two methods of remeshing have been implemented: mesh relaxing and mesh shaving. In the first technique, the number of elements remains the same and the nodal coordinates are perturbed in the direction of the normal. This results in equal spacing through the thickness. In the second technique, the outside element is stripped off when it becomes arbitrarily thin. The other elements are left undisturbed. Depending on whether the recession is uniform over the surface, an element will be either fully removed or degenerated to a triangle, followed by subsequent removal. Either method may be advantageous based upon the geometric configuration and the magnitude of the thermal gradient through the thickness. In either case, after the mesh is modified, the elemental data is mapped (rezoned) to the new integration points. A similar process is performed for streamline data. When using such techniques, care must be exercised when viewing conventional results for the history of a nodal quantity is dubious, as the node does not represent a constant material particle. For this reason, special tracking options have been developed.

Because the shaver mesher changes the element and node numbers that are on the exterior surface, a new geometry based boundary capability was added to MSC.Marc. Using this procedure, all boundary conditions (prescribed temperatures, fluxes, convection) may be applied to a point, curve (2-D), or surface (3-D). The conventional finite element entities (nodes, element-faces) are attached to the geometric entities. As the finite element model changes, the new mesh is automatically associated with the geometry, and boundary conditions are correctly applied. This treatment of boundary conditions also facilitates
improved connectivity to CAD in the future. The new boundary condition procedure works in conjunction with tables to allow maximum flexibility.

**Streamline Definition for level-2 model**

In the numerical procedure outlined above, the flow rate is integrated along geometrical streamlines to represent simplified one-dimensional fluid flow. The program, based upon the assumption that a regular but not necessarily uniform mesh is provided for regular two- or three-dimensional analysis, automatically calculates the streamlines. Certain quantities are evaluated at the stream integration points (SIP), shown in the figure below. Unfortunately, finite elements impose the requirements that these quantities are at the conventional integration points to evaluate the material properties, and other source terms. Hence, first a weighted nodal average of the extrapolated quantities are obtained followed by interpolating to the conventional integration points. Because of the large number of elements through the thickness, this procedure did not show any loss in accuracy.

### 3.4 Results

An example of ablation calculation is given below, comparing MSC.Marc-ATAS results with a previously developed Snecma Moteurs in-house software program. Using the same boundary conditions, the surface recession and the temperature inside the material are similar for both programs.

Temperature field in the material for different times while ablation.

Below is another example of calculation with pyrolysis but no ablation. A comparison is made with another older in-house developed Snecma Moteurs software program. The temperature fields inside the material are in good correlation.
During the process, the material is pyrolysed, and we can see the pyrolysis progressing and the density decreasing inside the material.

The thermal decomposition produces gases that are assumed to flow out instantaneously. The gas quantity created is summed along the streamlines, and we obtain the following curve that shows the mass flow rate of the gas arriving at the surface during the process. This quantity is used in the SEB.
These examples are based on one-dimensional configurations and used for the validation of MSC.Marc-ATAS. Nevertheless, as quoted above, this latter allows the program to deal with general multi-dimensional configuration not possible for the older level-2 software, and includes the level-3 model for which no software is currently available.

As an example of two-dimensional behavior the thermal solution of a simplified reduction area was obtained. This model complex surface energy input is dependent upon the distance along the flow, and the current area relative to the throat area. The analysis was performed twice, to evaluate the two remeshing techniques required due to ablation. Comparable results were obtained. The red line indicates the original surface location.

4. Thermal Contact

A solid rocket motor is built from many different parts, constituted by several materials having very different thermal properties, and, by design, there are some gaps allowing the thermomechanical expansion to occur without failure. So, it can be very boring to mesh the whole body continuously with an adaptation of the mesh density to the local material properties and to introduce manually thermal exchanges in the gaps.

To simplify the model of these discrete parts, a new thermal contact option has been added to MSC.Marc. This option may also be successfully be used to model assemblies of noncongruent meshes. The thermal contact behavior option behaves in a similar manner to the contact option in thermal-mechanically coupled analyses, but with several enhancements. The flux across a surface is based upon three potential states:

No contact – distance from nodes to another surface $dX > d_{\text{near}}$

$$q = h_{\text{cv}}^* (T_{1} - T_{\text{env}})$$

Near contact – distance from node to another surface $d_{\text{contact}} < dX < d_{\text{near}}$

$$q = h_{\text{cv}}^* (T_{2} - T_{1}) + h_{\text{nt}}^* (T_{2} - T_{1}) + s^* e^* (T_{2}^4 - T_{1}^4) + (h_{\text{ct}} - (h_{\text{ct}} - h_{\text{bl}}))^* dX^* (T_{2} - T_{1})/d_{\text{near}}$$

True contact – distance from node to another surface $dX < d_{\text{contact}}$

$$q = h_{\text{ct}}^* (T_{2} - T_{1})$$
Where $h_v$ is the convective coefficient, $h_n$ is the natural coefficient, $h_b$ is the convective coefficient at the boundary layer, and $h_t$ is the contact coefficient. All coefficients may be spatially and temporally dependent. $T_1$ and $T_2$ are the temperatures at surface 1 and 2, respectively, while $T_{env}$ is the temperature of the environment. For near contact, a simplified radiation model is available. The assumption is that the radiation is between the two closest surfaces, with no shadowing or other geometric effects. This capability is available for both two- and three-dimensional models.

5. Radiation

Currently MSC.Marc provides a general radiation capability for transparent media where the geometric view factors are calculated using the Monte Carlo method. As part of this project, two additional simplified radiation models have been developed: one for the radiation between two bodies as discussed in the thermal contact section and a radiation to space model. At a later stage of this project, more sophisticated radiation models will be investigated. Changing shapes, both due to ablation and nozzle pitch, complicates radiation modeling within the rocket engine. Analysis programs such as MSC.Nastran or MSC.Marc calculate the geometric view factors once. The plan is to embed the view factor calculation within the transient heat transfer analysis. The view factors will be recalculated periodically, based upon the change in shape to achieve accurate results at a reasonable cost. The computations are further complicated because the media changes almost instantaneously from being optically thin to optically thick and, then, relatively slowly back to optically thin. During the burning of the grain, metal particles may be discharged that lead to complex absorption and scattering. This requires a frequency dependent approach to radiation though a diffusion approximation may be more cost effective. This will be investigated over the next year.

6. Other applications

The study of pyrolysis and ablation, while critical for the rocket and reentry vehicle industry, has important value to other industries as well. The key common denominator is the presence of high fluxes and potential thermal-chemical degradation of the material. We observe these phenomena every morning when we make toast. The same technology is applicable to furnaces and other fire retardant insulation. Aspect of ablation are applicable in disk brakes, tire wear, gears, and potentially machining applications. Laser cutting exhibits many of the same physical phenomena that may be modeled using this technology.

Conclusions

The status of the development of the ATAS capabilities in MSC.Marc has been discussed. Excellent correlation has been found with previously developed simple modeling tool. The formulation incorporated in MSC.Marc will have far greater generality, allowing simulation of phenomena that was previously intractable. This will lead to reducing the time associated with design and in building and testing costly prototypes. Also, the use and maintenance of a single thermal software program with user-friendly inputs, plus being capable of coupled thermal/thermomechanical coupled analyses, will save time and money compared to the use of several older purely thermal software programs.

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