CHALEUR - MODIFICATIONS AND SAMPLE RESULTS

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Chaleur Capabilities

- One-dimensional heat transfer calculations.
  - Multiple materials with user defined properties, including radiation gap elements.
  - Constant or user defined source terms.
- Planar, cylindrical, or spherical geometry.
  - For cylindrical and spherical geometries, initial ablating boundary can be set as either the inner or outer radius (such as for a rocket nozzle or reentry body, respectively).
- Thermochemical ablation for non-decomposing materials (such as carbon-carbon).
- Thermochemical ablation for decomposing materials (such as carbon-phenolic).
  - Capable of modeling Darcy flow of pyrolysis gases due to pressure gradients within the solid.
- Equilibrium properties at the gas-solid interface can be obtained either from a user-supplied subroutine or from thermochemistry tables.

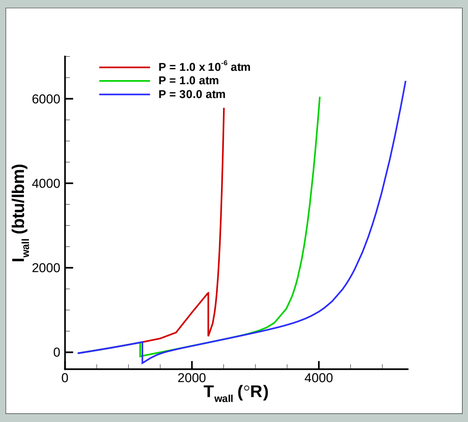
Thermochemistry Tables

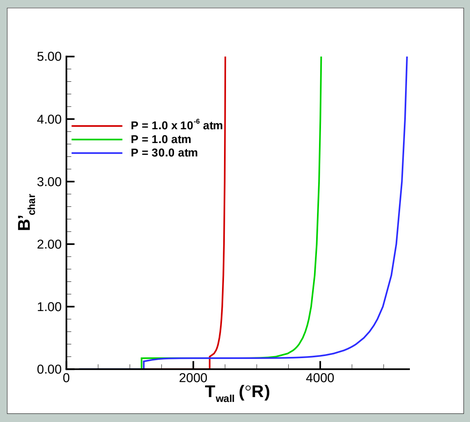
Thermochemistry tables provide information about the properties at the gas-solid interface. Their format changes somewhat depending on the problem being simulated.

- Non-ablating problems: The tables provide the surface enthalpy (I_{wall}), which is simply the enthalpy of equilibrium air at the wall pressure and temperature (P_{wall} and T_{wall}).
- Ablating problems, where the diffusion coefficients of the various chemical species are assumed equal:
  - For non-decomposing materials, the tables provide the enthalpy of the gas mixture at the surface (I_{wall}) and the nondimensional ablation rate (B'_{char}) as a function of P_{wall} and T_{wall}.
  - For decomposing materials, the tables provide I_{wall} and B'_{char} as a function of P_{wall}, T_{wall}, and the nondimensional pyrolysis gas mass flux (B'_{gas}).
- Ablating problems, where the diffusion coefficients of the various chemical species are not assumed equal:
  - For non-decomposing materials, the tables provide the chemical and sensible enthalpies ($I_{wall-chemical}$ and $I_{wall-sensible}$) of the gas mixture at the surface and B'_{char} as a function of P_{wall} and T_{wall}.
  - For decomposing materials, the tables provide $I_{wall-chemical}$, $I_{wall-sensible}$, and B'_{char} as a function of P_{wall}, T_{wall}, and B'_{gas}.
  - In addition, for either case, a seperate set of tables provides the chemical and sensible enthalpies of the edge gas ($I_{edge-chemical}$ and $I_{edge-sensible}$) as a function of P_{wall} and T_{wall}.

Thermochemistry Table Data

It is often useful to plot portions of the thermochemistry tables, in order to examine the physics and check for any obvious problems. The plots below are for carbon-carbon with air as the edge gas. The image on the left shows I_{wall} as a function of T_{wall} at several values of P_{wall}. Note the sharp discontinuity at the temperature for which ablation first begins to occur. Also note that this temperature varies with P_{wall}. The image on the right shows B'_{char} as a function of T_{wall} for those same values of pressures.





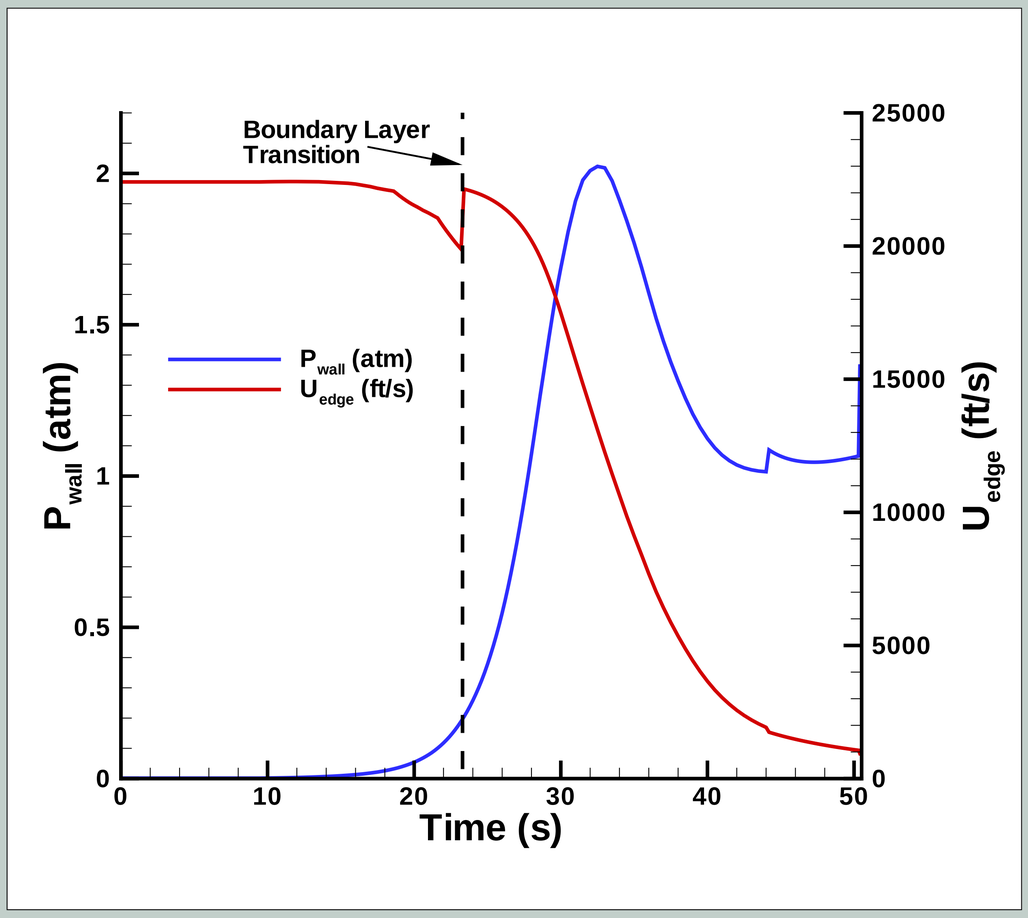
Thermochemistry Subroutine

A user-supplied subroutine can also be used in place of the thermochemistry tables. A significant part of my work at Sandia this summer involved modifying Chaleur to improve this functionality. In the past, a few material specific subroutines were included with Chaleur, but they were only valid for those materials and only for specific problem types. I modified Chaleur to allow for the use of a user-supplied subroutine for any desired problem type. Of course, the user still must supply a subroutine for the specific ablation material and edge gas. In theory, this would also allow for the use of finite rate chemistry as opposed to equilibrium chemistry, although this has not yet been tested. The subroutine must accept the same input and return the same output as would be obtained from the tables. For my work this summer, I modified a subroutine version of ACE, which is the code that was used to generate the thermochemistry tables in the first place. The current version of the ACE subroutine only works for non-decomposing materials, but since the main ACE program works for decomposing materials as well, enabling this functionality in the subroutine should be fairly straightforward. In the future, other programs could be modified to serve as thermochemistry subroutines, including possibly CEA (NASA-Glenn) or Cantera (open source).

Gas-surface Interface Conditions			Input to Thermochemistry Subroutine	Output from Thermochemistry Subroutine
No Ablation			P_{wall}, T_{wall}	I_{wall}
Ablation	Non-Decomposing Material	Equal Diffusion Coefficients	P_{wall}, T_{wall}	I_{wall}, B'_{char}
		Unequal Diffusion Coefficients	P_{wall}, T_{wall}	$I_{wall-sensible}$, $I_{wall-chemical}$, $I_{edge-gas-sensible}$, $I_{edge-gas-chemical}$, B'_{char}
	Decomposing Material	Equal Diffusion Coefficients	P_{wall}, T_{wall}, B'_{gas}	I_{wall}, B'_{char}
		Unequal Diffusion Coefficients	P_{wall}, T_{wall}, B'_{gas}	$I_{wall-sensible}$, $I_{wall-chemical}$, $I_{edge-gas-sensible}$, $I_{edge-gas-chemical}$, B'_{char}

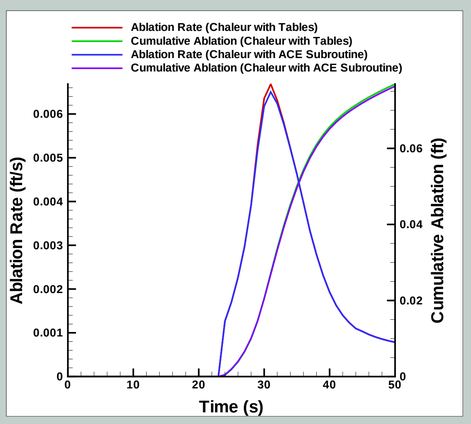
Sample Trajectory Data

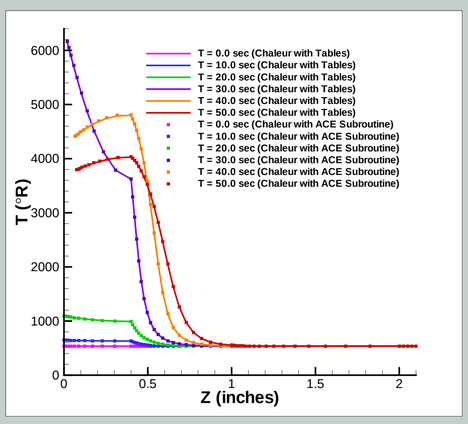
The plot below shows the values of P_{wall} and U_{edge} as functions of time for the specific trajectory analyzed here.



Non-Decomposing Material (carbon-carbon) Results

These two plots show results from Chaleur using the thermochemistry tables compared to results from Chaleur with the ACE subroutine incorporated. The results match up very well. The discrepancy is due to the fact that the subroutine version, while slower to run, is slightly more accurate because it does not require interpolation between table entries.





Decomposing Material (carbon-phenolic) Results

Due to the fact that the ACE subroutine does not yet support decomposing materials, only results from Chaleur using the thermochemistry tables are shown here.