Radiative heating attenuation through heat-shield doping: a multi-scale approach from *ab initio* to CFD

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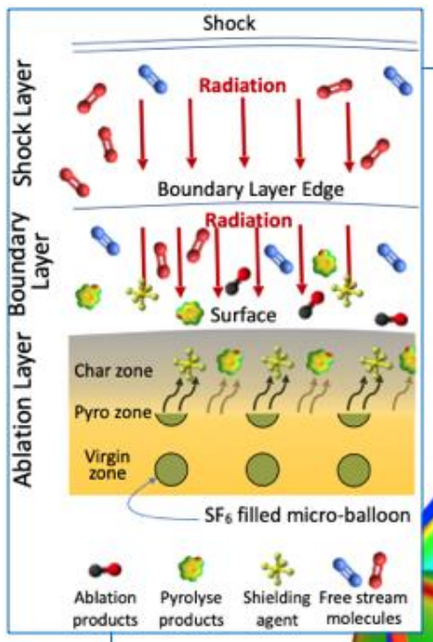
Topic 4 – Modeling of Shock Layer Radiation and Chemical Kinetics for Planetary Entry.



Research Objectives

- *Construct a first principles based model for the thermodynamic, optical* and *kinetic properties* of the most important ablation species in boundary layers and wakes.
- Material response modeling of the *entire heat-shield, coupled to the flow field simulation.*
- *Active control* of the "optical properties" of the gas by doping the TPS with a shielding agent (e.g., SF6) to absorb oncoming radiation.
- Integration of the model in the NASA codes (US3D / LAURA).

- The first principle calculation of the thermodynamic and kinetic properties corresponds to TRL 2. The application to CFD and the feasibility study of a new TPS concept with SF_6 doping corresponds to TRL 2.

Approach

- Uncertainty Quantification to guide the model development.
- *Ab initio* quantum mechanical calculations to compute thermodynamic and kinetic properties of the gas.
- Model reduction by means of the ME-QCT method and integration into CFD.
- Tightly coupled simulation of radiation, material response and flow physics.
- NASA solvers will be used for the flow and radiation, while KATS-MR will be used for the modeling of the material response.
- Embedded SF_6 micro balloons modeling for radiative heating mitigation in the KATS-MR code.

Potential Impact

This project has the potential to impact all the upcoming NASA missions, by enhancing the fidelity and predictability of heat flux computations over the entire surface of entry vehicles via an accurate description of the thermodynamics, radiation and kinetic properties. Examples include:

- Hyperbolic entry into Earth
- Missions to Titan
- Mars entry (MSR/Mars 2020)

- Reconstruction of the in-flight data requires modeling. While conservative margin policy can solve the problem of the TPS sizing, the rebuilding of the aero thermal environment using in flight data requires accurate modeling.
- **Novel approach of TPS doping could revolutionize the field!**