MODELING OF HETEROGENEOUS CATALYSIS FOR HYPERSONIC FLOWS

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A vehicle entering the atmosphere of a planet faces extreme conditions in terms of heat load, which are due to large temperature gradients and furthermore due to chemical interactions of the gas with the vehicle surface. The von Karman Institute is involved in the experimental determination of the physico-chemical surface properties of Thermal Protection Materials in severe environmental conditions employing inductively coupled plasma generators. It appears that the principles, which govern these properties are not sufficiently known.

The purpose of this thesis is to investigate the gas-surface interaction and to develop a mechanism based catalysis model for carbon dioxide and air in contact with metallic and silica based materials. This approach shall justify properly an extrapolation of a model, developed in a laboratory, to flight conditions.
The new models shall then be applied and tested in a representative environment in ground and flight experiments.

The study has been started with a numerical and theoretical approach. The understanding of the mechanism of the gas-surface interaction must be established by interpreting literature data and using tools that simulate on a microscopic level the behavior of gas particles on a surface. In Figure 1 is shown how the catalytic behavior of a material can depend on the gas properties leading to a low catalytic surface for extreme conditions and a high catalycity for intermediate ones,

The findings shall later be applied to a real hypersonic re-entry flight situation. For this aim, a flight experiment has been set up in the context of the ESA EXPERT mission. Thus, the Thermal Protection System of the re-entry vehicle shall be instrumented with thermocouples. Special attention will be drawn to the catalytic effect taking place when the flow passes first a low catalytic surface and then a higher catalytic one. Due to the availability of atoms for a recombination process at the latter surface, which can release their dissociation energy, a high heat flux is expected.

This yields a severe engineering problem: the assumption of having a fully catalytic wall at the nose is not conservative at the junction point.

The goal of the PhD project is to predict the impact of the overheating due to a catalytic jump applying the newly developed catalysis model and compare it to the measured heating rate of the flight experiment.

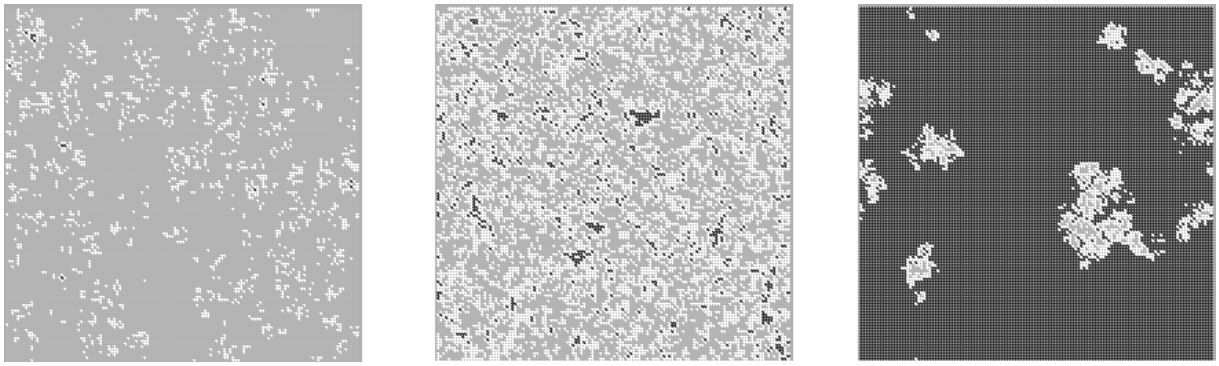

Figure 1: Results of a kinetic Monte Carlo Simulation: shown is adsorbed CO (red), O (green) and free surface sites (white). For a low partial pressure of CO in gasphase the surface is covered mainly with O(left). Only few reaction occur. For a high partial pressure of CO the surface is mainly covered with CO (right). Only few reactions occur. For a suitable partial pressure the surface is highly catalytic (middle)