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Numerical Investigations of Chemical Kinetics for Methane Catalysis and Pyrolysis

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Primary Technical Area: Theoretical Modeling and Numerical Simulation Techniques for Chemical Propulsion Topics
Secondary Technical Area: Environmentally-Friendly "Green" Propellants

Extended Abstracts

In the framework of the active and regenerative cooling of hypersonic and space structures, a kinetic mechanism should be proposed to investigate numerically the fuel pyrolysis and the coke formation with a possible surface effect (catalytic reactions). This chemical mechanism should be suitable for Computational Fluid Dynamics approach (limited number of species and reaction). The objective of this study is to obtain a mechanism which permits to compute methane pyrolysis considering both heterogeneous reactions and the coke production.
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For this purpose, this work presents some homogeneous and heterogeneous calculations of methane chemistry with metallic catalysts in order to test a kinetic mechanism with the integration of surface reactions. Three catalysts are considered: platinum, nickel and rhodium. A mechanism has been selected. Then, its size (i.e. number of reactions and of species) has been reduced. A parametric study is achieved and several reactors natures are tested.
Small differences are noted between the three catalysts for a low value of site density while a strong one appears for a higher one.

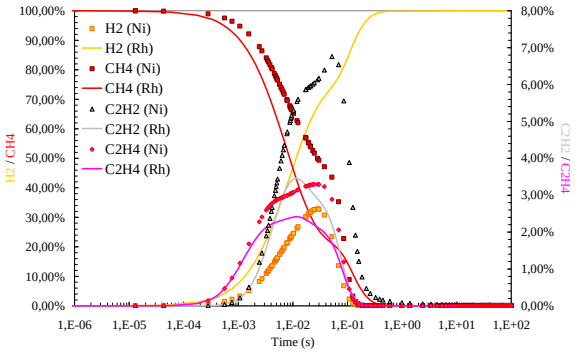

Figure 1. Effect of catalyst nature on light specie production (mol.%).

Both the product distribution and the dynamic are affected. The reactor type used for the computations has been also tested. The differences are limited considering nickel or platinum catalyst while some important discrepancies are observed for the rhodium.
These simulations have highlighted some differences and demonstrated the importance of the site density value on the results.