

Research Topic for the ParisTech/CSC PhD Program

1. ***Field (cf. List of fields below):**

Chemistry, Physical Chemistry and Chemical Engineering

Energy, Processes

Subfield: Applied Physics and Chemistry

Title: Study of carbon particles nucleation and growth in methane plasma cracking

ParisTech School: MINES ParisTech

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(Lab, website):

PERSEE, Center for Processes, Renewable Energies and Energy Systems

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Short description of possible research topics for a PhD: (10-15 lines in English + optional figure)

In the prospect of a large scale deployment of Renewable Energy for electricity production, plasma will definitively be a major option to get tunable high temperature enthalpy source without direct CO₂ emission. In this frame, plasma cracking of methane for the simultaneous synthesis of hydrogen and high value-added carbon black is particularly interesting for both energy and materials industries.

The PhD work will consist in making a global model of carbon particles nucleation and growth from a gas phase in the methane plasma cracking. First, an exhaustive review of physicochemical phenomena occurring in gas phase during the carbon particles formation process will be done, mainly based on the works in the field of combustion. Then, as a continuation of a modeling work already started in our group for few years (Maxime Gautier's PhD), the candidate will have the objective to improve the existing model based on a discretized Smoluchowski's approach by developing/implementing: (i) the reaction mechanisms taking place in the nucleation step, (ii) the physical phenomena allowing the growth of the carbon particles, particularly the transition from a coalescent coagulation (giving the elementary particles) to a non-coalescent one (giving the agglomerates). This last step is one of the most difficult steps to model because of the influence of multiple driving factors. At the end, the model will be able to give the distribution of particles at the outlet of a typical plasma cracking reactor from the process parameters.

Required background of the student: (Which should be the main field of study of the applicant before applying)

The candidate must have a strong background in physics and chemistry and must be familiar with numerical modeling, particularly by Finite-Volume technic. Knowledge of following softwares will be greatly appreciated: Fluent, Chemkin, Matlab. From a more global point view, the candidate should have a passion for physical and chemical sciences.

A list of 5(max.) representative publications of the group: (Related to the research topic)

Gautier M., Rohani V., Fulcheri L., Direct decarbonization of methane by thermal plasma for co-production of carbon black and hydrogen, *Int. Journal of Hydrogen Energy*, 42 (2017) 28140-28156

Gautier M., Trelles J. P., Rohani V., Fulcheri L., Influence of Temperature and Pressure on Carbon Black Size Distribution during Allothermal Cracking of Methane, *Aerosol Science and Technology*, 50, 1 (2016)

Gautier Maxime, PhD thesis: Etude de la formation de nanoparticules de carbone au cours de la décomposition thermique d'hydrocarbures : application au craquage thermique du méthane, Mines ParisTech, 2016