

PhD thesis offer at PC2A, Lille, France:

## Experimental study and kinetic modelling for the combustion chemistry of biomass's tar surrogates

### Context:

This PhD thesis is part of the ambitious program “*Support innovation to develop new largely carbon-free industrial processes*” supported by the French Government in the framework of the decarbonization of the industry to achieve carbon neutrality by 2050.

The decarbonation of the industry partly relies on the development and intensification of processes for CO<sub>2</sub> capture. This PhD thesis is offered as part of the OXY3C project aiming at improving knowledge and skills in oxycombustion for the optimization of eco-efficient processes. The consortium working on this project gathers seven French academic laboratories and IFPEN.

### Objectives of the thesis:

This study aims at investigating chemical kinetics of soot precursors and measuring soot particles from biomass's tar surrogates in the framework of a close collaboration between PC2A, LRGP, and IFPEN. Experiments and simulations will be performed under CO<sub>2</sub> and H<sub>2</sub>O vapor atmosphere at a wide range of temperatures covering the temperature range in the Chemical Looping Combustion application. This work comprises two main parts.

*The first part* is establishing a reliable experimental database that includes mole/volume fraction profiles of reactants, products, intermediates and soot particles in the pyrolysis and combustion of a biomass's tar surrogate. These data will be measured in a burner system at PC2A and in a jet-stirred reactor or a tubular reactor at LRGP. Chemical species will be measured using gas chromatography and mass spectrometry. Soot volume fraction profiles in flames will be measured in situ by extinction or cavity ring-down extinction. Selected soot samples thermophoretically collected in the above flames will be analyzed at IFPEN for characterizing soot morphology using microscopy (STEM + possibly TEM or HRTEM).

*The second part* is developing a detailed kinetic model for soot precursor formation from the pyrolysis and combustion of this biomass's tar surrogate. The model will include a base model containing common species, a sub-model for the pyrolysis and combustion of a biomass's tar surrogate, a sub-model of aromatics. The model will be tested against the experimental database under CO<sub>2</sub> and H<sub>2</sub>O atmosphere that will be obtained in the above experimental part. The model will be transferred to IFPEN for soot modeling.

### Requirements:

Candidates must have a master degree, in chemistry-physics or process engineering or automobile propulsion or equivalent. Modeling and experimental skills, experiences in the field of combustion and chemical kinetics will be appreciated. Fluent English and ability to work in a team are expected.

### Scientific leaders:

Dr. Luc-Sy TRAN, CNRS Research Scientist at PC2A UMR 8522, CNRS, University of Lille, luc-sy.tran@univ-lille.fr, <https://pro.univ-lille.fr/luc-sy-tran/>

Dr. Pascale DESGROUX, CNRS Research Director at PC2A UMR 8522, CNRS, University of Lille, pascale.desgroux@univ-lille.fr

**Remuneration:** 2100 € gross income per month

**Duration and start date of the thesis:** 3 years with a start in October 2023 after recruitment

**Practical information:** The thesis will take place mainly at PC2A (<https://pc2a.univ-lille.fr/>) in Lille, France. A stay of 6 months at LRGP (<https://lrgp-nancy.cnrs.fr/>) in Nancy, France is planned.

**How to apply:** Email to the scientific leaders mentioned above:

- your CV
- a cover letter
- References