



# PhD in CHIMICA INDUSTRIALE E INGEGNERIA CHIMICA / INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING - 40th cycle

**THEMATIC Research Field: PYROLYSIS AND GASIFICATION CHEMISTRY FOR PLASTICS**

**Monthly net income of PhDscholarship (max 36 months)**

**€ 1400.0**

In case of a change of the welfare rates during the three-year period, the amount could be modified.

## **Context of the research activity**

**Motivation and objectives of the research in this field**

Our society is currently facing a dual problem: depletion of resources and accumulation of waste. Despite its huge potential, plastic waste recycling is still strongly limited by technical difficulties and lack of knowledge. Most types of plastic can only be mechanically recycled a limited number of times before becoming degraded (?downcycling?). In this context, chemical recycling and, in particular, thermal processes such as pyrolysis and gasification of plastic waste can play a key role. In a circular economy, the plastic waste should be recycled to produce the small building blocks needed by the chemical industry, making it a feedstock for sustainable chemical processes.

The development of comprehensive chemical kinetic models plays a vital role in understanding plastic waste pyrolysis, but also gasification and combustion. This complexity arises from the multicomponent, multiphase, and multiscale nature of thermochemical conversion of solid fuels. Indeed, it involves various stages, starting from the accurate characterization of the feedstock, followed by the description of volatiles release at the particle level, and culminating in understanding the impact of secondary gas-phase reactions at the reactor scale. All these aspects significantly influence plastic waste thermovalorization processes and have a direct influence on valuable product distribution and on the formation of pollutants.



	<p>The objective of this doctoral program is to improve the model by undertaking the following activities:</p> <ol style="list-style-type: none"> <li>1. Characterize the composition of plastic waste.</li> <li>2. Develop a unified decomposition model for plastics, describing the pyrolysis and gasification chemistry of plastic feeds in both gas and liquid phases.</li> <li>3. Validate this predictive model estimating the production of olefins, dienes, naphthenes, (poly)aromatics upon pyrolysis, and syngas, CO<sub>2</sub>, hydrocarbons, tars, and char upon gasification.</li> <li>4. Develop a reduced and optimized kinetic model for reactor modeling purposes and/or CFD simulations of plastic waste pyrolysis.</li> <li>5. The research will focus on maximizing desirable outputs and predicting how residence time and reaction temperature influence the composition of the obtained product streams.</li> </ol>
<p><b>Methods and techniques that will be developed and used to carry out the research</b></p>	<p>The expertise available at the Creck Modeling Lab will enable the doctoral candidate to develop cross-cutting skills in kinetics and of plastic waste utilization. The candidate will investigate the chemistry of waste thermal degradation (pyrolysis) including the role of the secondary gas-phase reactions. The project includes chemical reaction model development to describe the pyrolysis and subsequent (O<sub>2</sub> and steam) gasification chemistry of plastic feeds in both gas and liquid phases. The kinetic model will aim at estimating the production of olefins, dienes, naphthenes, (poly)aromatics upon pyrolysis and syngas, CO<sub>2</sub>, hydrocarbons, tars and char upon gasification. The model will start with polyethylene (PE), polypropylene (PP), and polystyrene (PS), but other polymers could be investigated.</p> <p>The goal is to understand the decomposition products from both pyrolysis and gasification chemistries to maximize desirable outputs and attempt to predict how residence time and reaction temperature will change the gas composition.</p> <p>In particular, the problem will be analyzed with a multi-scale approach, starting from elementary reaction pathways, up to the macroscale (i.e., reactor), where</p>



	<p>mixing and turbulence strongly interact with chemical kinetics aspects.</p> <p>Furthermore, the candidate will include the data and kinetic models for plastic pyrolysis and gasification inside Sciexpem, a data ecosystem for experimental data and predictive models. <a href="https://sciexpem.polimi.it/">https://sciexpem.polimi.it/</a></p> <p>The research activity will be mostly carried out at Politecnico di Milano, Italy.</p>
<b>Educational objectives</b>	<p>The PhD activity will develop a unified decomposition model for plastics via pyrolysis and gasification. The candidate will be involved in cutting-edge research and contribute to advancing sustainable chemical recycling technologies for circular processes. This PhD program is funded by Dow Benelux BV and will be carried out in collaboration with the company.</p>
<b>Job opportunities</b>	<p>Job opportunities include R&amp;D areas in the most varied industrial sectors, in particular those requiring advanced modeling skills. Straightforward areas include technology development (e.g. in energy and process industries), as well as opportunities in data science and process optimization fields. This PhD program is carried out in collaboration with a large company belonging to the chemical sector.</p>
<b>Composition of the research group</b>	<p>2 Full Professors 3 Associated Professors 2 Assistant Professors 10 PhD Students</p>
<b>Name of the research directors</b>	<p>Prof. Tiziano Faravelli</p>

**Contacts**

Telephone: 02-2399-3282  
 Email: [Tiziano.farevalli@polimi.it](mailto:Tiziano.farevalli@polimi.it)  
 Web-pages of the research group: <https://creckmodeling.chem.polimi.it/>

**Additional support - Financial aid per PhD student per year (gross amount)**

<b>Housing - Foreign Students</b>	--
<b>Housing - Out-of-town residents (more than 80Km out of Milano)</b>	--



Scholarship Increase for a period abroad	
Amount monthly	700.0 €
By number of months	6

**Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information**

**Confidentiality:** since this is a thematic scholarship, the management of Confidential Information, Results and their publication is subordinate to the restrictions agreed upon with the funding company.

Upon acceptance of the scholarship, the beneficiary must sign a specific commitment.

**Individual budget for research** (about 5.700 euro):

1st year: 1.900 euro;

2nd year: 1.900 euro;

3rd year: 1.900 euro

**Teaching assistantship** (availability of funding in recognition of supporting teaching activities by the PhD student): there are various forms of financial for activities of support to the teaching practice. The PhD student is encouraged to take part in these activities within the limits allowed by the regulation.

**Computer availability, desk availability, any other information** The PhD student will have a dedicated pc and desk, and access to the Creck lab's proprietary Linux High Performance Computing Cluster with ~700 processors located at POLIMI. Availability of in-house and commercial codes for CFD and combustion kinetic calculation (ideal reactors, kinetic mechanism reduction, flames, droplet combustion, solid particle pyrolysis-gasification-combustion, data management and analysis etc.)