

PhD position in chemical reaction engineering (Kinetic modeling & thermal runaway)



Duration: 3 years (Starting from October-November 2026)

Salary: ~2300 € gross/month

Supervisors: Sébastien Leveneur (sebastien.leveneur@ircelyon.univ-lyon1.fr)
& co-supervisor: Carine Michel (carine.michel@ens-lyon.fr)

Location: IRCELYON & LCH

Keywords: Kinetic modeling, calorimetry, thermal runaway, biomass valorization

At the lab scale, when we think about chemical production, the focus is on optimizing yield, distribution, or conversion by testing different operating conditions (pressure, concentration, temperature, etc.) and at isothermal conditions. Then, we develop kinetic models, but these models are reliable only for operating conditions quite close to the optimum production conditions and in isothermal conditions.

By working at isothermal conditions, one aspect could be overlooked: heat transfer and the risk of thermal runaway. Thermal runaway remains a significant safety risk in the chemical industry, accounting for nearly 25% of accidents [1].

The [QUANTASTIC project \(ANR-25-CE51-7405\)](#) aims to develop innovative methodologies for early detection and mitigation of thermal runaway by combining:

- Multifactorial kinetic modelling
- Calorimetry
- Quantum chemistry (DFT)
- Artificial intelligence

This thesis will evolve in the framework of [QUANTASTIC project \(ANR-25-CE51-7405\)](#).

Our previous research showed that biomass valorization involves exothermic reactions that could lead to thermal runaway scenarios [2-4].

The [QUANTASTIC's consortium](#) fiercely believes in combining chemical reaction engineering and DFT calculation for a better understanding of thermal runaway reactions.



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The recruited **QUANTASTIC PhD** student will:

- Contribute to the development of an experimental setup,
- Develop and evaluate different kinetic models, including runaway scenarios,
- Work in close collaboration with **DFT QUANTASTIC researchers** to increase model accuracy and with **Automatic QUANTASTIC researchers** to improve detection.

References:

1. A. Dakkoune, L. Vernières-Hassimi, S. Leveueur, D. Lefebvre, L. Estel, Analysis of thermal runaway events in French chemical industry, *Journal of Loss Prevention in the Process Industries*, 62 (2019) 103938. <https://doi.org/10.1016/j.jlp.2019.103938>
2. Y. Wang, L. Vernières-Hassimi, V. Casson-Moreno, J.-P. Hébert, S. Leveueur, Thermal risk assessment of levulinic acid hydrogenation to γ -valerolactone, *Organic Process Research & Development*, 22(9) (2018) 1092-1100. <https://doi.org/10.1021/acs.oprd.8b00122>
3. W. Y. Pérez-Sena, T. Salmi, L. Estel, S. Leveueur, Thermal risk assessment for the epoxidation of linseed oil by classical Prileschajew epoxidation and by direct epoxidation by H₂O₂ on alumina, *Journal of Thermal Analysis and Calorimetry*, 140 (2020) 673–684. <https://doi.org/10.1007/s10973-019-08894-2>
4. Yanjun Wang, Igor Plazl, Lamiae Vernières-Hassimi, Sébastien Leveueur, From calorimetry to thermal risk assessment: γ -valerolactone production from the hydrogenation of alkyl levulinates, *Process Safety and Environmental Protection*, 144 (2020) 32-41 <https://doi.org/10.1016/j.psep.2020.07.017>

What you will gain

- Strong expertise in advanced kinetic modeling
- Hands-on experience with calorimetric instrumentation
- Exposure to DFT and AI methodologies
- Publications in high-impact journals
- Participation in international conferences
- Interdisciplinary training environment
- Based in Lyon — widely regarded as the gastronomic capital of France — the position offers both scientific excellence and a vibrant lifestyle.

Requirements:

- Master's thesis in chemical engineering (or provisional certificate) **OR** master's thesis in chemistry but with good knowledge in chemical reaction engineering (or provisional certificate);
- Experience in experimental work and solid background in analysis;
- Experience in catalyst preparation and characterization will be appreciated.
- The candidate should have good knowledge in kinetic modeling;
- Fluent in English;
- This thesis will be embedded in the **QUANTASTIC project**. Thus, the Ph.D. student must also be open to other scientific activities, such as automatic and DFT methods.

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How to apply and get further information :

The candidates should send a detailed curriculum vitae, a motivation letter, a transcript of record (Bachelor and Master), and other valuable documents (recommendation letters, language and degree certificates, awards, etc.). **These documents must be sent via the following website [Portail Emploi CNRS - Job offer - PhD position in chemical reaction engineering M/F](https://emploi.cnrs.fr/Offres/Doctorant/UMR5256-SEBLEV-001/Default.aspx?lang=EN)** (<https://emploi.cnrs.fr/Offres/Doctorant/UMR5256-SEBLEV-001/Default.aspx?lang=EN>)

The screenshot shows the CNRS job portal interface. At the top, there is a navigation bar with 'Portail Emploi', 'Our job offers', 'Candidate help', 'Your Career', and a 'Sign in' button. Below this, the breadcrumb trail reads 'Home > Portail Emploi CNRS - Job offer - PhD position in chemical reaction engineering M/F'. The main content area features a 'NEW' badge and the title 'PhD position in chemical reaction engineering M/F'. The employer is identified as 'Institut de Recherches sur la Catalyse et l'Environnement de Lyon, VILLEURBANNE • Rhône'. The offer details include 'FTC PhD student / Offer for thesis', '36 month', and 'BAC+5'. There are two informational boxes: 'This offer is available in English version' and 'This offer is open to people with a document recognizing their status as a disabled worker.' A dark blue box titled 'Offer at a glance' provides key details:

The Unit Institut de Recherches sur la Catalyse et l'Environnement de Lyon	Workplace 69100 VILLEURBANNE
Contract Type FTC PhD student / Offer for thesis	Contract Duration 36 month
Working hHours Full Time	Date of Hire 05/09/2026
	Remuneration 2300 € gross monthly

 At the bottom of this box is an 'Apply' button and an 'Application Deadline : 26 March 2026 23:59' warning. A red arrow points from the 'Sign in' button to a list of steps: '1. Create an account' and '2. Apply'. A blue arrow points from the 'Apply' button to the same list.

Assessment

The candidate assessment is a two-step evaluation. The candidates will be evaluated by a jury of three researchers (including Sébastien Leveneur and Carine Michel).

In the first step, the jury will evaluate the different applications based on the provided documents. The selection of the candidates for the second step (i.e., interview in English) will be done based on the quality of their chemical engineering and chemistry education (courses and marks), their abroad experience in research or other activity, their language skills (mainly English), the relationship between their master thesis and this doctoral thesis, their scientific publication (article and/or communication on congresses), their recommendation letters and the quality of their resume and motivation letter.

In the second step, the selected candidates (from the first step) will pass an interview. This interview can be done online by video conference calls. The interview procedure will last ca. 15 minutes per candidate, and the candidate will present themselves and describe their research activities. The evaluation will be done based on their presentation, quality of their responses, and motivation to do this thesis.

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