

PhD position at IFP Energies nouvelles (IFPEN) In Chemical Engineering and Chemical Kinetics

Predicting Combustion Behaviors of the Emitted Gas during Thermal Runaway of Lithium-Ion Batteries

Electric vehicle is a promising solution to de-carbonization and massive deployment is foreseen. However, the safety concerns are obstructing their large-scale applications. One of the main safety concerns is the thermal runaway (TR) of batteries, which has caused many accidents around the globe. These accidents often lead to combustion and explosion, presenting dangers to human lives. The risk of thermal runaway is becoming even higher because the thermal stability of battery materials is found to decrease as battery technologies are evolving towards higher energy density.

During the process of battery thermal runaway, various gaseous components are formed by both exothermic decomposition reactions between battery materials and the evaporation of liquid electrolyte. These emitted gases, usually flammable and toxic, are responsible for the drastic events such as battery cell rupture, venting, combustion, explosion, and flames. During different phases of TR, the risk and severity of combustion may vary, depending on the composition of the gas mixture and the gas-phase reactions under the corresponding temperature and pressure. However, currently the relation between the gas-phase combustion and the thermal runaway in condensed phases are still unclear. Therefore, this PhD topic aims to understand such relations and develop a multi-physics kinetic model with validation based on experiments to predict the entire process of emitted gas combustion, from their formation in the solid/liquid phase to their combustion behaviors in the gas phase. The thesis will be able to address many scientific questions around combustion during thermal runaway, e.g., when, where, and how combustion initiates, propagates, and affects the progress of thermal runaway. The PhD candidate will gain a solid experience in lithium-ion battery, combustion, and chemical kinetics through the multi-physics modeling activities.

Keywords: Thermal Runaway, Lithium-Ion Battery, Kinetic Modeling, Combustion, Auto-Ignition, Flame

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Doctoral School	ED626 – IP Paris / École Doctorale de l'Institut Polytechnique de Paris, https://www.ip-paris.fr/en/education/phd-programs/ip-paris-doctoral-school
IFPEN supervisor	Dr. XU Boyang, Research Engineer, Division of Mobility and System, boyang.xu@ifpen.fr
PhD location	IFP Energies nouvelles, Rueil-Malmaison, France
Duration and start date	3 years, starting time flexible throughout year 2024
Employer	SAFT, Bordeaux, France Coordinator: Guillaume Gimenez, guillaume.gimenez@saft.com
Academic requirements	University Master degree in chemical engineering, physical chemistry, electrochemistry, or materials engineering
Language requirements	Fluency in English, willingness to learn French
Other requirements	Modeling. Programming (Python). Knowledge in chemical kinetics is a plus.

To apply, please send your cover letter and CV to the IFPEN supervisor (boyang.xu@ifpen.fr).

About SAFT CIFRE Bursary and IFP Energies Nouvelles

This thesis is funded through CIFRE bursary provided by SAFT. SAFT is a leading battery company that specializes in designing and manufacturing advanced batteries for various industries including aerospace, defense, and transportation. For more information, see [SAFT official WEB site](#). The PhD candidate is employed by SAFT but will work at IFPEN. Part of the thesis work will be confidential and owned by SAFT. IFP Energies Nouvelles is a French public-sector research, innovation and training center. Its mission is to develop efficient, economical, clean and sustainable technologies in the fields of energy, transport and the environment. For more information, see [our WEB site](#). IFPEN offers a stimulating research environment, with access to first in class laboratory infrastructures and computing facilities. All PhD students have access to dedicated seminars and training sessions. For more information, please see our [dedicated WEB pages](#).