



**Thesis Title:**

Influence of Boundary Layers on the Measurement of Auto-Ignition Delays in High-Pressure Shock Tubes – Application to the Kinetics of Biomass-Derived Fuels – Simulation and Experimentation

**Host Laboratory:**

Laboratoire DRIVE  
49 rue Mademoiselle Bourgeois  
58000 Nevers – France

**Specialization of the Doctorate :** Energetics

**Keywords:** Shock tube, auto-ignition delay, biomass, boundary layers, CFD, kinetics

**Detailed Description of the Thesis:**

The depletion of fossil fuels and climate change, partly caused by emissions from their combustion, represent major societal challenges. Alternative fuels derived from bioresources (biofuels, hydrogen, ammonia) appear as promising solutions to overcome these challenges, particularly in the transportation sector, especially for heavy-duty vehicles and energy processes. Although the combustion of certain alternative fuels at high temperatures and low pressures has been extensively studied in the literature using fundamental reactors such as laminar flames and perfectly stirred reactors [12], research is limited under high temperature and high pressure conditions similar to those operating in thermal reactors such as internal combustion engines, gas turbines, and turbojets (400-2000K, 1-100Bar) [3]. The shock tube is one of the fundamental reactors that allows the study of the combustion of alternative fuels under such conditions by measuring auto-ignition delays [4], profiling intermediate species [5], and validating kinetic models to understand the degradation of these fuels [6]. One of our recent studies [7] showed that the auto-ignition delay measured in the shock tube can be affected by boundary layers [8] under certain conditions and impact the prediction of kinetic models.

From this observation, the thesis objective will be to characterize the impact of boundary layers on the auto-ignition delay measurements in the DRIVE laboratory's shock tube. This characterization will then allow to more precisely investigate the combustion kinetics of biomass-derived compounds under high pressure condition. The work will be carried out in four stages:

1. A comprehensive literature review will be conducted, relying on databases such as Web of Sciences, to examine previous work on laboratory experiments and both CFD (Computational Fluid Dynamics) and kinetic modeling.
2. CFD modeling will be performed using Ansys Fluent software to evaluate the impact of boundary layers on the auto-ignition delay in the DRIVE shock tube.

3. A series of experiments will be conducted at the DRIVE laboratory to measure the auto-ignition delay of a bio-fuel/O<sub>2</sub>/Ar mixture in a shock tube at high pressure (20-40Bar) and high temperature (900-1600K).

4. Based on the data obtained, kinetic modeling will be carried out using Ansys Chemkin-Pro, integrating the results of CFD modeling to deepen the understanding of the oxidation kinetics of biofuel.

#### **Bibliographic References**

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[7] H.-Q. Do, B. Lefort, Z. Serinyel, L. LeMoyne, G. Dayma, Comparative study of the high-temperature auto-ignition of cyclopentane and tetrahydrofuran, *International Journal of Chemical Kinetics* 56 (2024) 199–209.

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#### **Requested Profile:**

- Engineer/Master's in process engineering or fluid mechanics/energy with possible knowledge in chemical kinetics.
- Fluent in English, ability to work in a team
- Send CV, cover letter, letters of recommendation from supervisors, transcripts from the first and second year of Master's degree or last two years of engineering degree to the supervisors and thesis director.

#### **Funding: MESRI Establishment**

Application to be sent before **May 25, 2024** (Interview at the end of May, beginning of June)

Start of contract: October 1, 2024

Gross monthly salary: €1975

#### **Thesis Direction:**

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