Coach	Supervisor	Funding
Kevin Van Geem	Laura Pires	-

# Unlocking the Secrets of Contamination in Pyrolysis Oil: A Predictive Modeling Framework

#### Aim

This research aims to investigate the presence and potential impact of contaminants in plastic waste, with a focus on their origin, function, and fate during pyrolysis. Specifically, the study will:

- Additives database development: construction and validation of an additive database with information on polymer matrices, functional role, mass fraction and physicochemical properties.
- **Predictive modelling:** investigate the fate of identified contaminants during the pyrolysis process, determining whether they are retained in the solid char, volatilized into the gas phase, or partitioned into the liquid pyrolysis oil based on the physicochemical properties or possible reactions.
- **Step-wise pyrolysis evaluation:** assess the effectiveness of step-wise pyrolysis as a pretreatment method to remove or reduce the concentration of specific contaminants, thereby improving the quality of the resulting pyrolysis oil.
- Evaluation of other purification methodologies: assess if washing, adsorbents or chemicals (e.g., metal oxides), hot filtration, or other strategies can help to reduce contamination in plastic pyrolysis oil.

## Justification

Pyrolysis offers a promising solution for converting plastic waste into valuable fuels and chemicals. However, the quality of the resulting pyrolysis oil, particularly its contaminant profile, can significantly influence its suitability for further processing and utilization.

While extensive research has been conducted on pyrolysis oil purification techniques, a fundamental understanding of the origin and nature of contaminants remains elusive. This lack of knowledge hinders the development of efficient and targeted purification strategies. By identifying and characterizing the specific contaminants present in pyrolysis oil and correlating them with the composition of the input plastic waste, we can gain valuable insights into the factors influencing oil quality.

## Program

## 1. Literature Review and Database Construction

• Comprehensive literature review to identify common additives in plastic waste.



• Construction of a detailed database containing information on additive types, functions, physicochemical properties, and potential impact on pyrolysis oil.

#### 2. Data-analysis and predictive modelling

- Consideration of factors such as vapor pressure, boiling point, thermal stability, and reactivity.
- Prioritization of additives related with polyolefins, PS and PET

#### 3. Experimental Validation

- **Thermal analysis:** Employ techniques like thermogravimetric analysis (TGA) to assess the thermal behaviour of pure additives and dopped polymers.
- **Pyrolysis experiments:** Conduct pyrolysis experiments on model compounds to validate the predictions and investigate the formation of contaminants in the pyrolysis oil.
- Characterization of pyrolysis products: Analyse the resulting pyrolysis oil, char, and gas products using techniques such as 2D gas chromatography-mass spectrometry (2D GC-MS) and Inductively Coupled Plasma (ICP).



Figure 1. Degradation temperature or boiling point of 8 chemical elements present in plastic additives.

