

# Acquisition and Physico-Chemical Data Analysis of Oxygenated Compounds from Biomass Using Microfluidics.

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Global warming-related climate change demands prompt actions to reduce greenhouse gas (GHG) emissions, particularly carbon dioxide. To reduce GHGs, biomass-based biofuels containing oxygenated compounds represent a promising alternative of energy source. To convert biomass into energy, a variety of conversion processes performed at high pressure and high temperature conditions are required, and the design of such processes need as support, thermophysical property data, particularly thermal conductivity. The conventional methods to measure thermal conductivity are often time consuming and/or requires important quantities of products. Microfluidics has been proven as an appropriate support to overcome these issues thanks to its low reagent consumption, fast screening, low operating time, improvement of heat and mass transfers etc. It allows the automated manipulation, performing high throughput experimentation. In addition, over the last 10 years, a new field of investigation called "high pressure and high temperature (HP-HT) microfluidics" [1] has gained increasing interest, in particular for the determination of the thermo-physical properties of fluids systems[2] [3]. Currently, available methods for measuring thermal conductivity in microfluidics are not adapted to HP-HT conditions. Also, thermal conductivity data of oxygenated compounds are scarce in literature or not available in extreme conditions. Therefore, the use of alternative methods such as models, combined with microfluidics, are essential to complement experimental data. Machine learning (ML) provides powerful predictive tools with the ability to learn from available data. The aim of this thesis is to develop a microfluidic device capable of measuring thermal conductivity of oxygenated compounds, operating at HP-HT (up to 100 bars and 100 °C), complementing it with modeling as a view to "high throughput" production of experimental data. In this study, two types of sensor devices are implemented within a microfluidic device, allowing the measurement of thermal conductivity using different methodologies. In parallel, a data compilation resulting in a database has been established for the development of a ML based predictive model to estimate thermal conductivity of oxygenated compounds.

The reference section at the end of the paper should be edited based on the following:

## References

- [1] Marre, S.; Adamo, A.; Basak, S.; Aymonier, C.; Jensen, K. F. Design and Packaging of Microreactors for High Pressure and High Temperature Applications. *Ind. Eng. Chem. Res.* [Online] 2010, 49 (22), 11310–11320.
- [2] B. Pinho, S. Girardon, F. Bazer-Bachi, G. Bergeot, S. Marre, C. Aymonier, Microfluidic Investigation of Multicomponent Systems at high pressure and high temperature, *Lab Chip*, 2014, 14, 3843-3849
- [3] T. Gavaille, N. Pannacci, G. Bergeot, C. Marlière, S. Marre, Microfluidics approaches for accessing thermophysical properties of fluids systems, *Reaction Chemistry and Engineering*, 2019, 4, 1721-.1739