Development of a General Kinetic Model based on Chemical Compositions of Lignocellulosic Biomass for Predicting Product Yields from Hydrothermal Liquefaction

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Western Engineering

Chemical and Biochemical Engineering

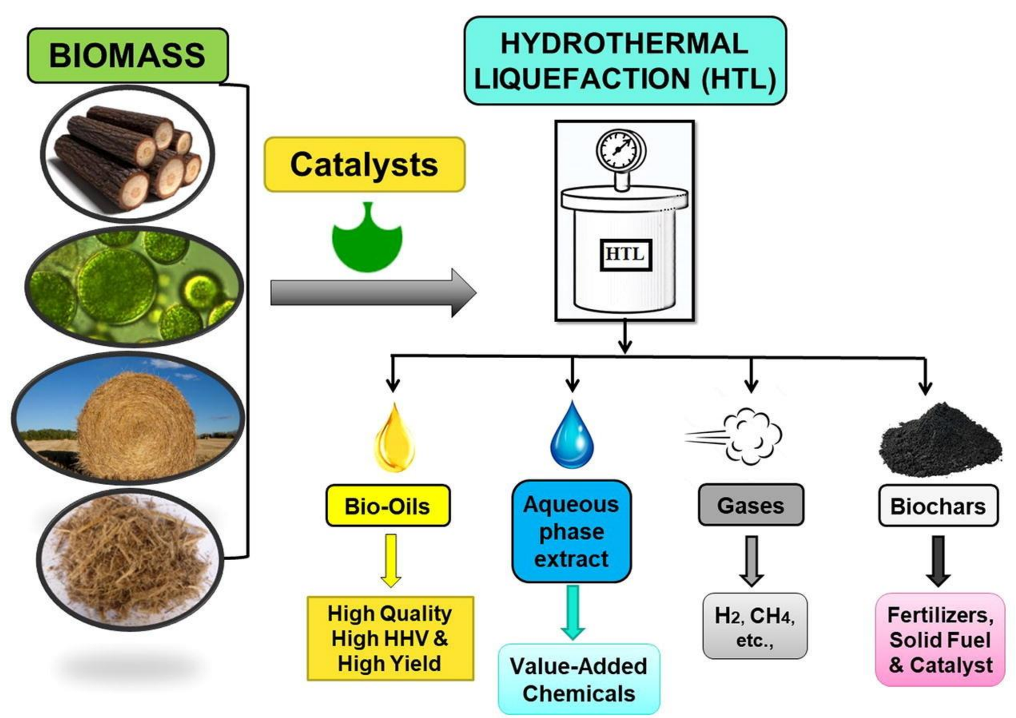
Motivation and Background

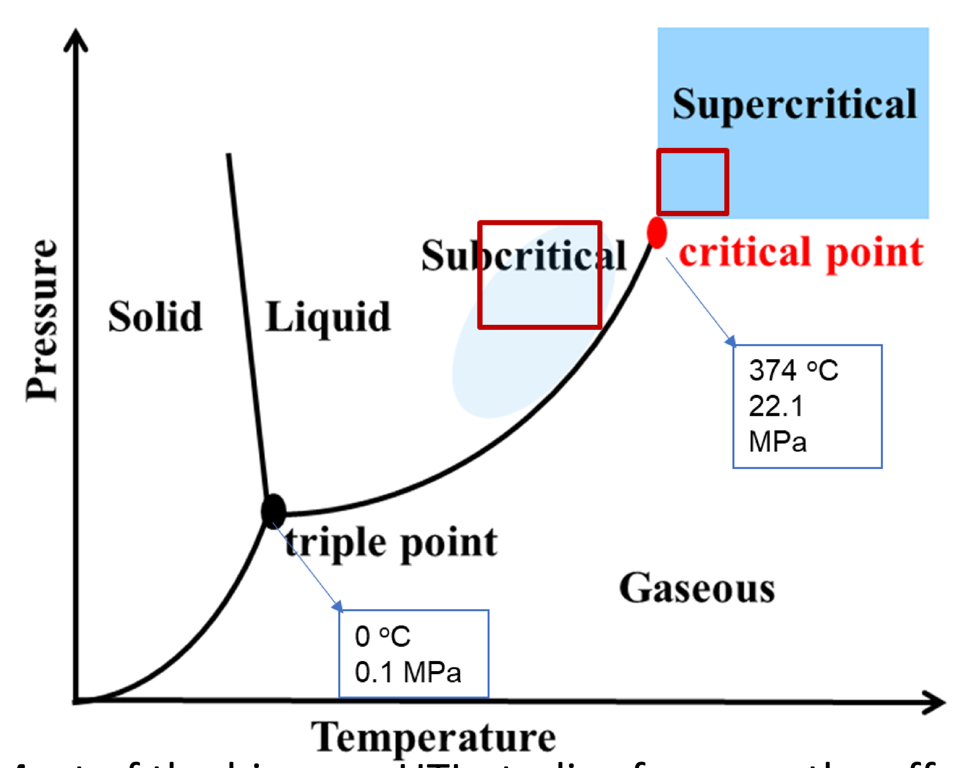
- Energy Demand Growth
- Environmental Impacts
- Fossil Fuel Depletion

Intensive research on exploring alternatives to fossil resources for both energy and chemical production.

Bioresources, such as lignocellulosic biomass, food waste and algal biomass, are promising candidates to produce bioenergy and bio-based chemicals.

Hydrothermal liquefaction is one of the promising method to convert biomass into valuable products.





Most of the biomass HTL studies focus on the effects of catalysts, operating parameters (e.g., temperature, time, etc.) on production efficiency and chemical properties of the products.

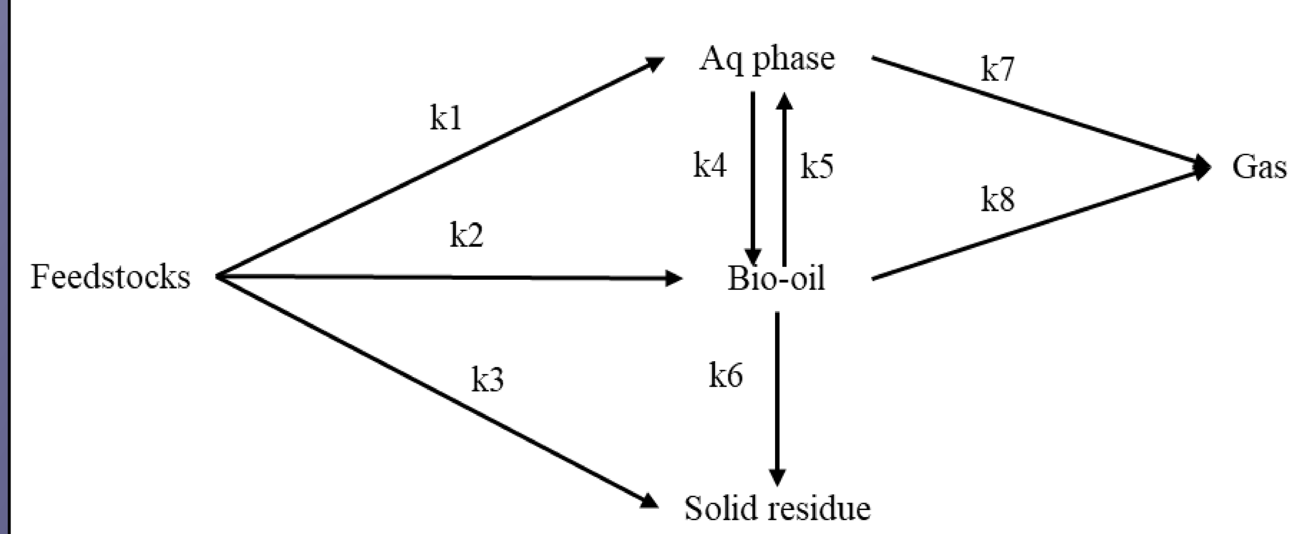
No kinetic model involving detailed reaction pathways for predicting product yields in HTL of lignocellulosic biomass.

Objectives

To develop a general kinetic model based on the chemical compositions (cellulose, hemicellulose, and lignin) of lignocellulosic biomass to predict product yields (gas, liquid, and solid residue) and elucidate the reaction pathways and mechanisms in HTL of lignocellulosic biomass.

Research Methodology

Reaction Network



Reaction Rate

(1) $\frac{dX_{feed}}{dt} = -(k_1 + k_2 + k_3)X_{feed}$

(2) $\frac{dX_{AP}}{dt} = k_1X_{feed} + k_5X_{oil} - (k_4 + k_7)X_{AP}$

(3) $\frac{dX_{oil}}{dt} = k_2X_{feed} + k_4X_{AP} - (k_5 + k_6 + k_8)X_{oil}$

(4) $\frac{dX_{SR}}{dt} = k_3X_{feed} + k_6X_{oil}$

(5) $\frac{dX_{gas}}{dt} = k_7X_{AP} + k_8X_{oil}$

(6) $f = \min \sum_{i=1}^{N}(X_{cal} - X_{exp})^2$

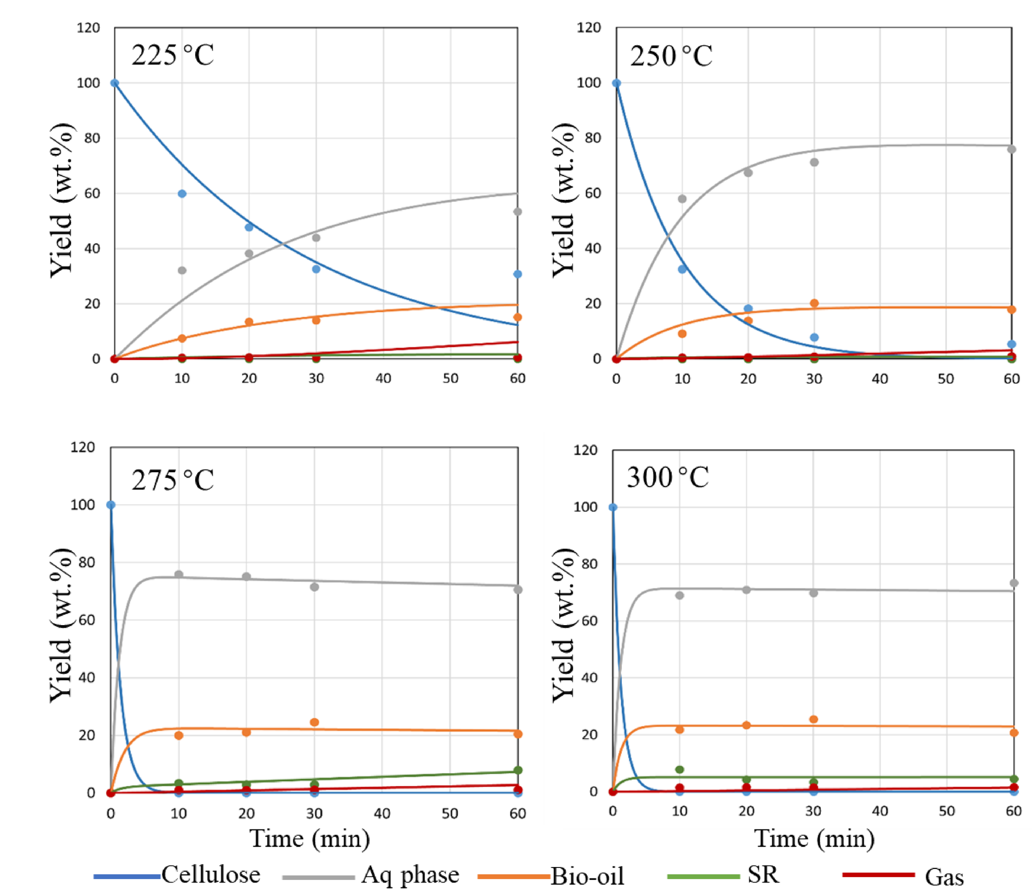
(7) $k = A\exp\frac{-E}{RT}$

(8) $Y_i = \sum_i y_i x_i$

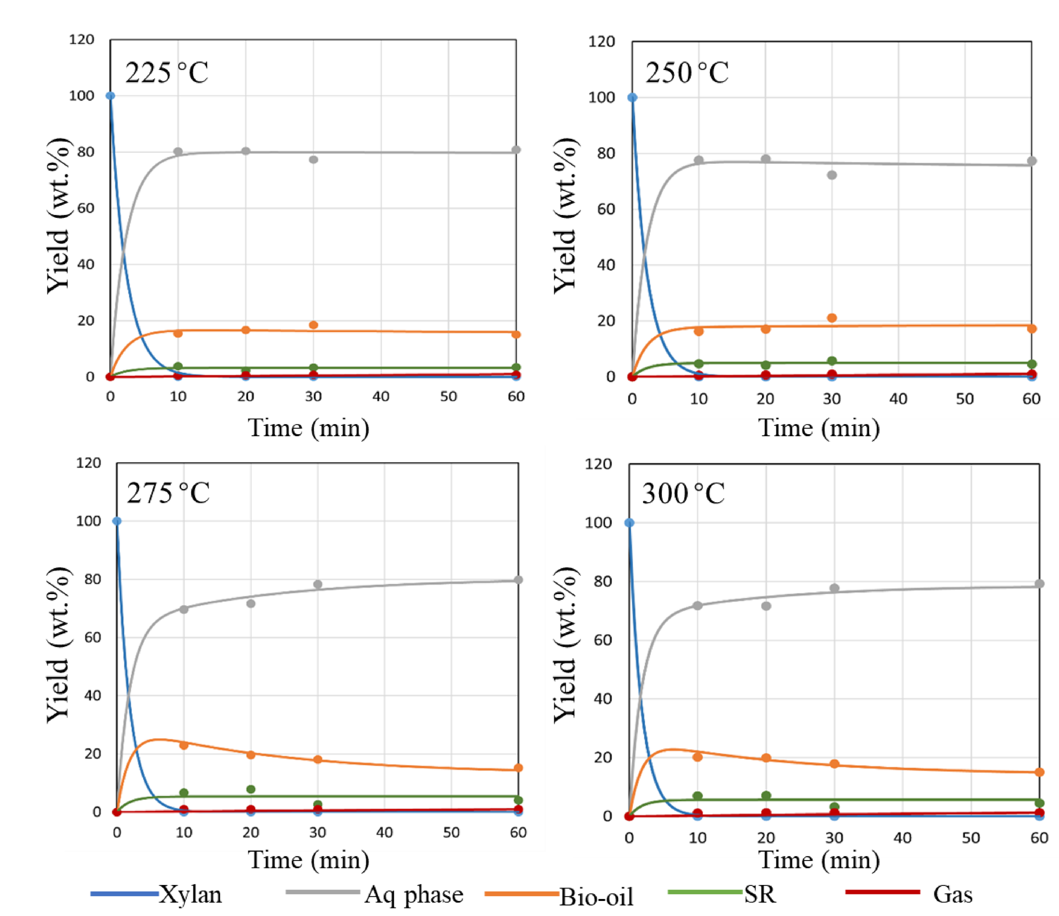
Equipment and Tools

Key Results-Curve fitting of experimental data

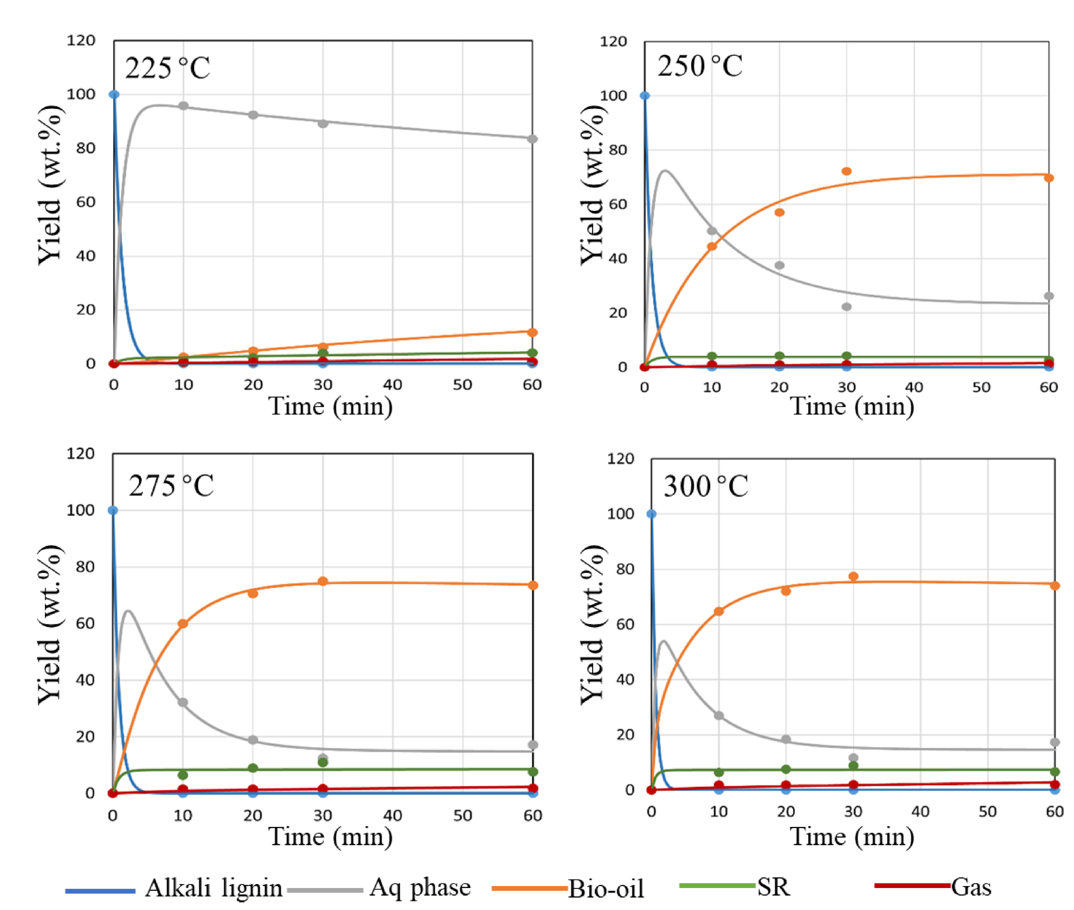
Cellulose



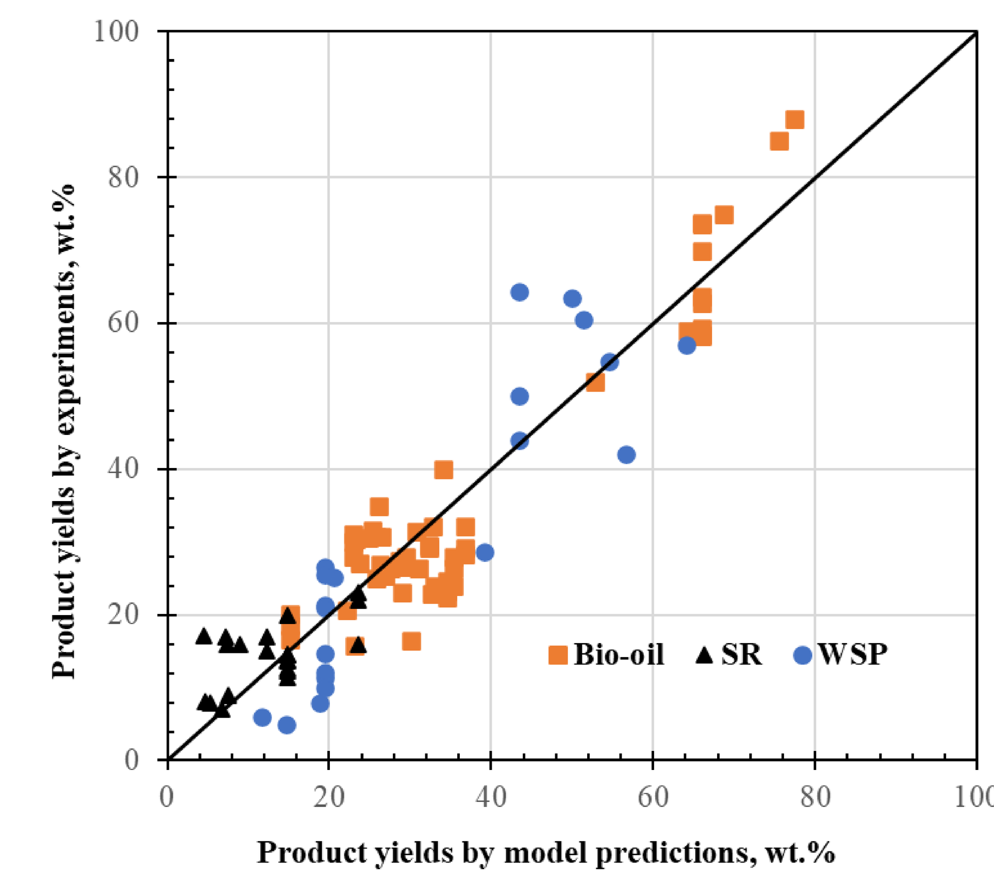
Xylan



Alkali Lignin



Key Results-Comparison of HTL product yields obtained by model predictions and by experiments reported in literature



Key Conclusions

- Lignin was found to be the main contributor to bio-oil formation from HTL of lignocellulosic biomass.
- The formations of bio-oil and aqueous-phase products from decomposition of cellulose, xylan, and lignin are the dominant steps in HTL conversion.
- A general kinetic model was successfully developed based on the experimental results obtained from HTL of biomass model compounds and validated using the publicly available data in literature from HTL of various lignocellulosic biomass feedstocks.

Acknowledgment of Sponsors

NSERC CRSNG
FPInnovations
Natural Resources Canada / Ressources naturelles Canada
Canada
CanmetMATERIALS / CanmetMATÉRIAUX
Western University · Canada
Ontario
Ministry of Economic Development and Innovation
INNOVATION Canada Foundation for Innovation / Fondation canadienne pour l'innovation