Mechanistic modeling of post-consumption plastic pyrolysis oil purification: Lumping approach for distillation and solvent extraction processes

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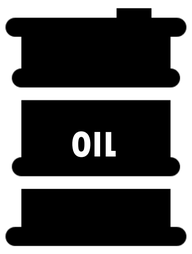
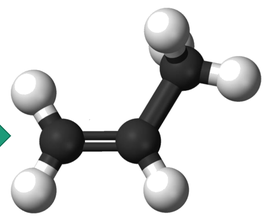
Introduction

Pyrolysis



Steam Cracker



⚠ **Heteroatoms (N, O, Cl, Si)**
Coke formation,
Fouling,
Corrosion
Catalyst poisoning

- Need post-treatment: distillation together with extraction or adsorption process.
- Convert to the ASPEN model for full industrialization.
- Oils created from complex plastic waste are equally complex.
- How to represent it in the ASPEN model?

Bulk properties
- Average liquid density
- Average molar mass
- PONA analysis
- Elemental analysis
- ASTM D1160

Traditional method
- Discretize distillation curve into pseudo components
- Properties of pseudo components were calculated by empirical correlation

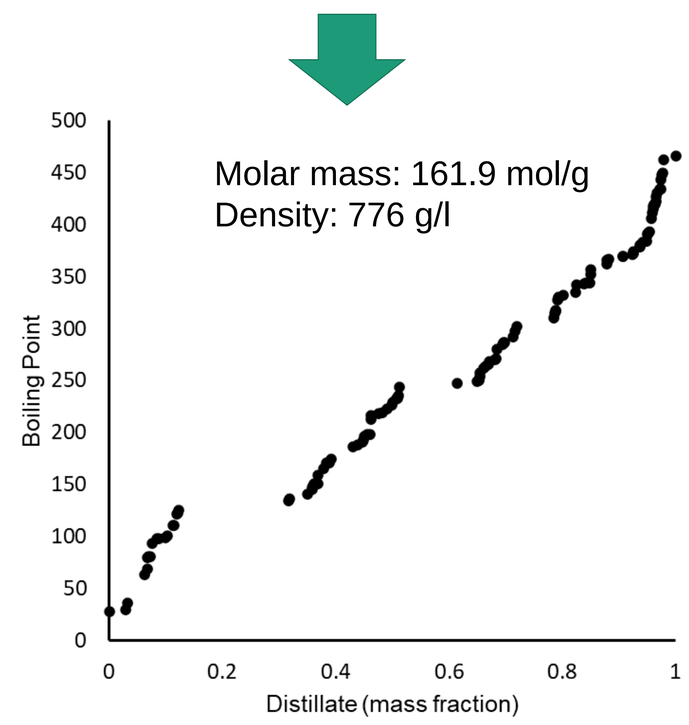
Set of pseudo components
- Only applicable for the distillation process.

'New' method
- Shannon entropy maximization
- $w_i \ln(w_i) \rightarrow MAX,\ \sum w_i = 1$
- $\sum f_{i,j} w_i = 0$

Set of real components
- Suitable for bot distillation and extraction processes.

Modelling approach

FEED from Polypropylene



Lumping by Pseudo Component (A)

Lumping by Entropy maximization (B)

The pseudo component and surrogate mixture constructed by entropy maximization are compared with detailed composition by performing the flash calculation in ASPEN HYSYS. Temperature, the yield of top vapor (TOP stream) and liquid (BOT stream) were blah blah blah

Results & Discussion

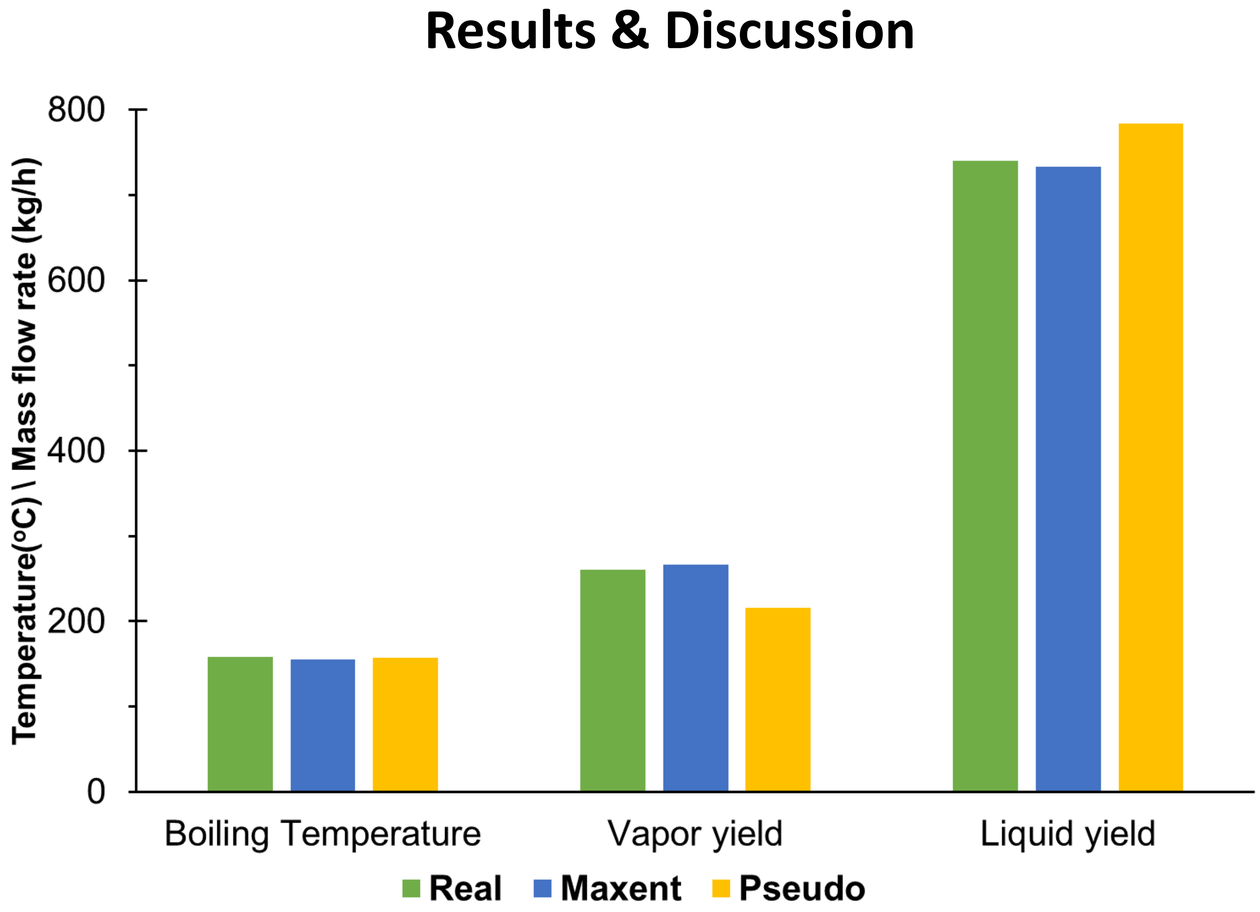


Figure 2: Compare the flash calculation result among detailed composition, lumped by pseudo component and lumped by maximum entropy.

FEED		
Temperature	30.00	C
Pressure	101.3	kPa
Mass Flow	1000	kg/h

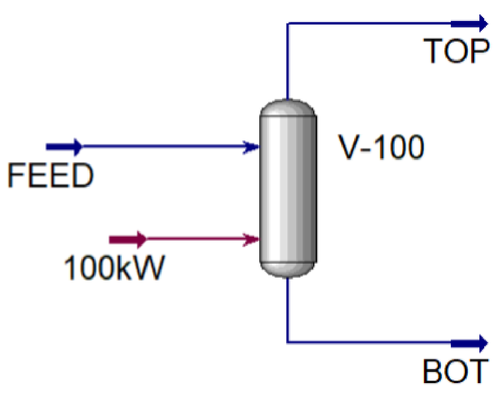


Figure 1: Flash calculation to validate two approaches

The pseudo component and surrogate mixture constructed by entropy maximization are compared with detailed composition by performing the flash calculation in ASPEN HYSYS. Temperature, the yield of top vapor (TOP stream) and liquid (BOT stream) were blah blah blah The pseudo component and surrogate mixture constructed by entropy maximization are compared with detailed composition by performing the flash calculation in ASPEN HYSYS. Temperature, the yield of top vapor (TOP stream) and liquid (BOT stream) were blah blah blah
The pseudo component and surrogate mixture constructed by entropy maximization are compared with detailed composition by performing

Conclusions & Work-in-progress

The pseudo component and surrogate mixture constructed by entropy maximization are compared with detailed composition by performing the flash calculation in ASPEN HYSYS. Temperature, the yield of top vapor (TOP stream) and liquid (BOT stream. The pseudo component and surrogate mixture constructed by entropy maximization are compared with detailed composition by performing the flash calculation in ASPEN HYSYS. Temperature, the yield of top vapor (TOP stream) and liquid (BOT stream The pseudo component and surrogate mixture constructed by entropy maximization are compared with detailed composition by performing the flash calculation in ASPEN HYSYS. Temperature, the yield of top vapor (TOP stream) and liquid (BOT stream