

# Supplementary Materials

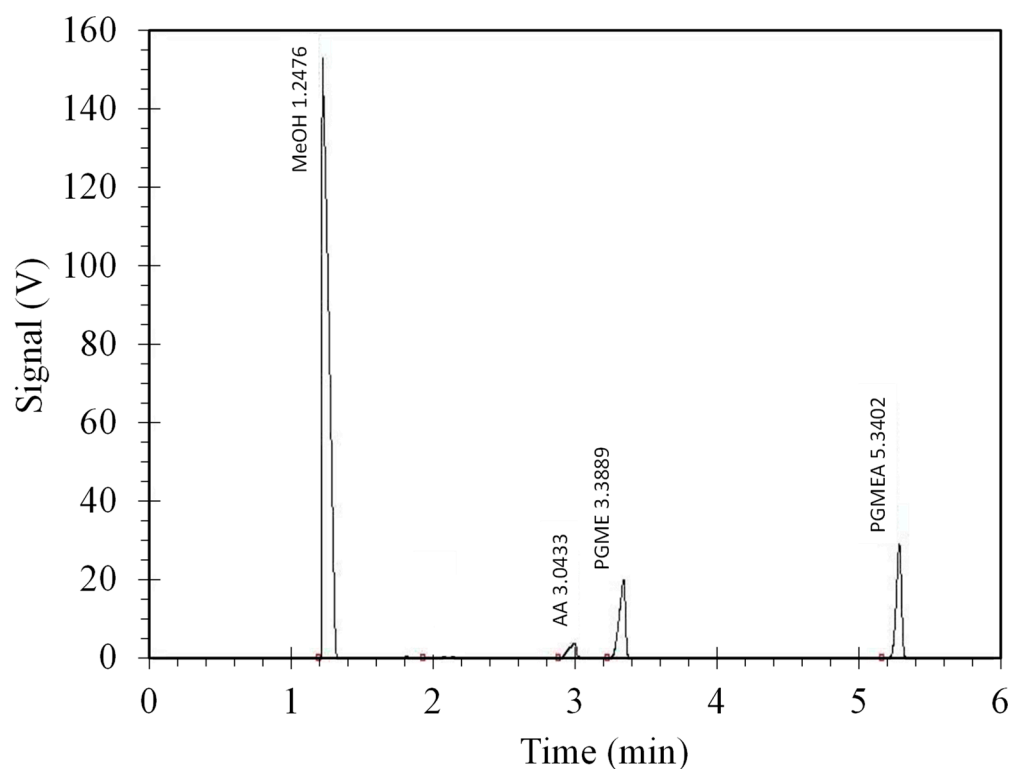


Figure S1. Example of chromatogram.

Reactor type: Reactor with specified temperature

Operating condition

- ☒ Constant at inlet temperature
- ☐ Constant at specified reactor temperature \_\_\_\_\_ K
- ☐ Temperature profile

☒ Catalyst present in reactor

☐ Ignore catalyst volume in rate/residence time calculations

Specifications

Bed voidage 0.3

Particle density 0.5 gm/cc

☐ Multitube reactor Number of tubes: \_\_\_\_\_

☐ Diameter varies along the length of the reactor

Reactor dimensions

Length: 1.5 meter

Diameter: 0.1 meter

Elevation

☒ Reactor rise: 0 meter

☐ Reactor angle: 0 deg

Valid phases

Process stream: Liquid-Only

Coolant stream: Vapor-Liquid

Substream name: MIXED Ref Temperature \_\_\_\_\_

State variables

Temperature 90 C

Pressure 1.2 atm

Total flow: 1.43 Mole kmol/hr

Composition

Mole-Frac

Component	Value
C4H10-01	0.5
C6H12-01	
C2H4O-01	0.5
H2O	
C6H6	

Components

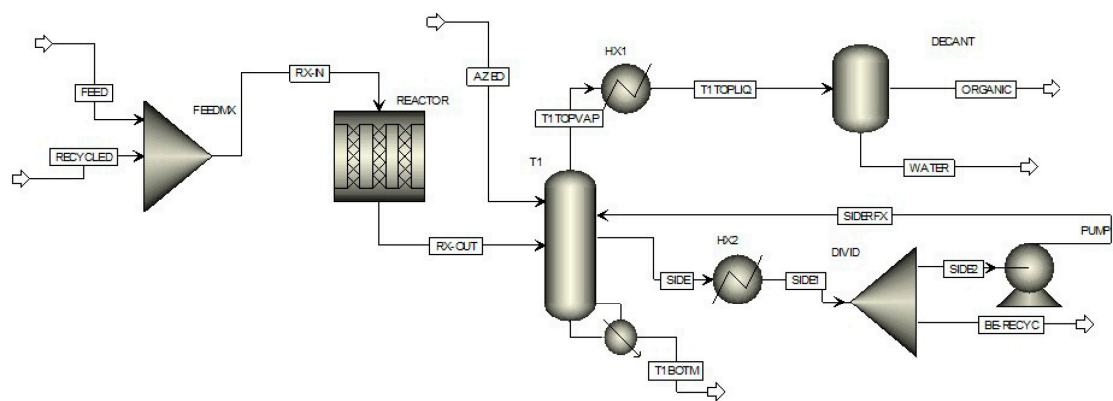
Properties

Flowsheet

Streams

- AZEO
- FEED
- Input
- Results
- EO Variables
- Custom Stream Results
- ORGANIC
- RX-OUT
- T1BOTM
- T1TOP
- T2BOTM

Figure S2. Screen capture of conditions for simulation.



**Figure S3.** Flow sheet of simulation for a PFR system with purification processes.