Pareto Efficient SAF Yield and Blending Project 103

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Project manager: Bahman Habibzadeh, FAA

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ASCENT

Project 103

Pareto Efficient SAF Yield and Blending

Washington State University

PI: Joshua Heyne

PM: Bahman Habibzadeh

Cost Share Partner(s): Air Company, Trinity College Dublin

Objective:

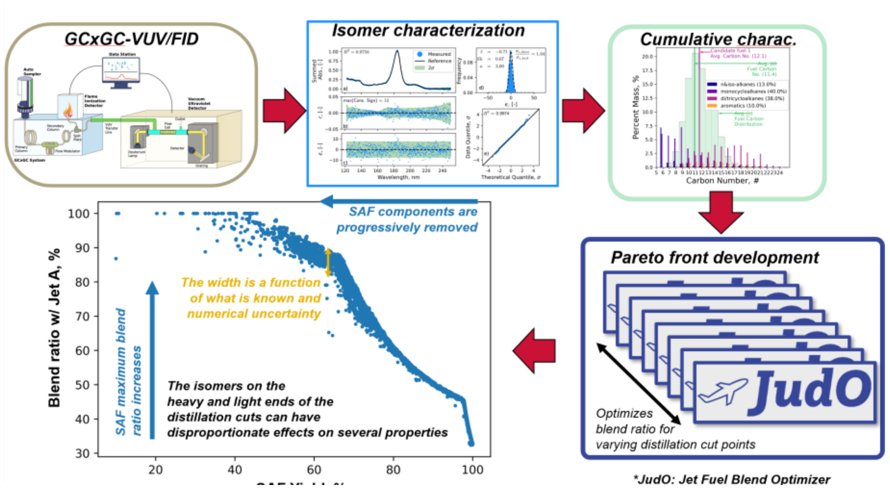
Optimize distillation cut points and blending limit for sustainable aviation fuel candidates.

Project Benefits:

Optimized distillation for new alternative jet fuels improves the potential for meeting ASTM approval criteria while simultaneously optimizing the fraction of renewable carbon into each product stream; synthetic blend component (**SBC**), biodiesel, etc.

Additionally, this work lowers the technology readiness level at which distillation is the final step of fuel finishing before entering ASTM approval process.

Research Approach:



Major Accomplishments (to date):

Early application of methodology: *Upgrading biocrude oil into sustainable aviation fuel using zeolite-supported iron-molybdenum carbide nanocatalysts:* S Yu, H He, S Summers, Z Yang, B Si, R Gao, A Song, J Heyne, Y Zhang, H Yang, Science Advances 11(26) (2025) https://doi.org/10.1126/sciadv.adu5777

19 Synthetic crude oil (**SCO**) candidates have been optimized for distillation cut points since the project started

Future Work / Schedule:

Blend Prediction Model for Vapor Pressure of Jet Fuel Range Hydrocarbons

- Plan to acquire more validation data prior to submitting manuscript

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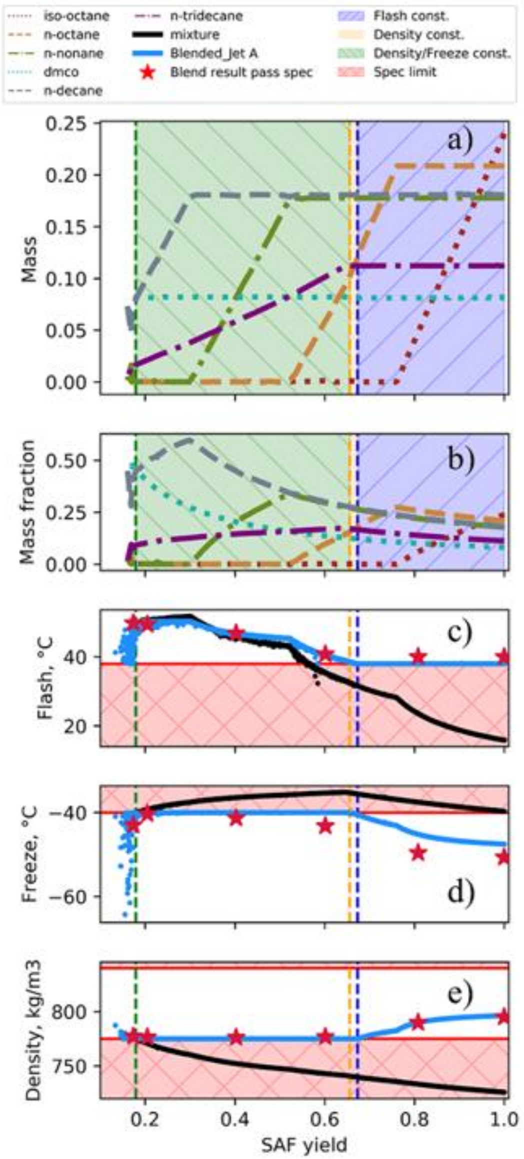
Executive Summary

1. A variety of fuel properties may limit SCO cut points and SBC blend fraction: including most notably
   - Flash point
   - Freeze point
   - Density
   - Viscosity
2. The properties of the conventional jet fuel blend component significantly impacts the SBC; both its definition (cut points) and its maximum blend percentage
3. Optimization of synthetic crude distillation cut points can lead to substantially more synthetic carbon going to high-value jet fuel

Definitions of Figure Axis Terms

- "SAF Yield" is the fraction of synthetic crude going to jet fuel => SBC
- "Blend Limit" is the percentage of SBC going to finished jet fuel



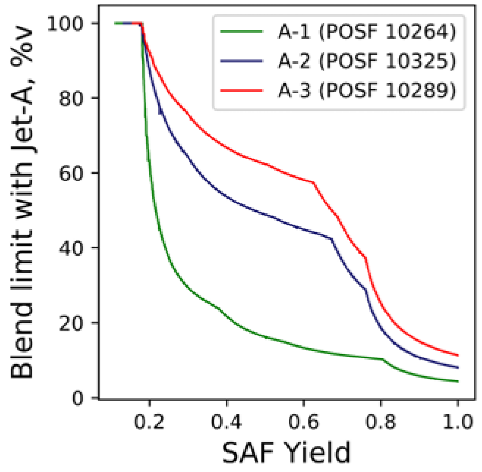
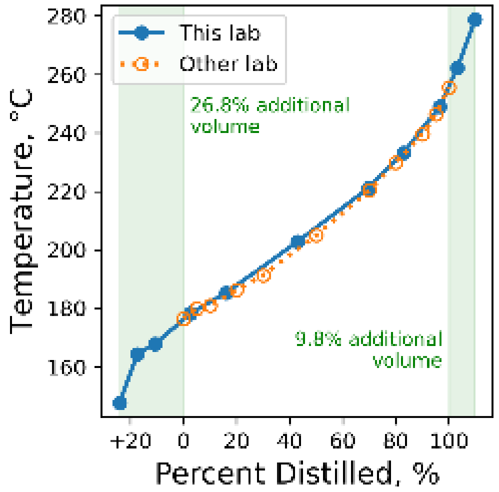
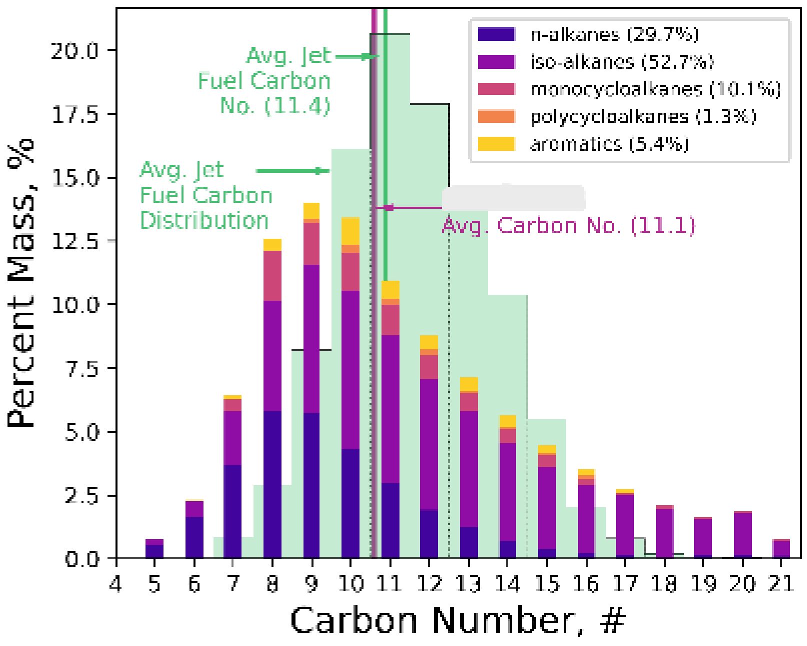
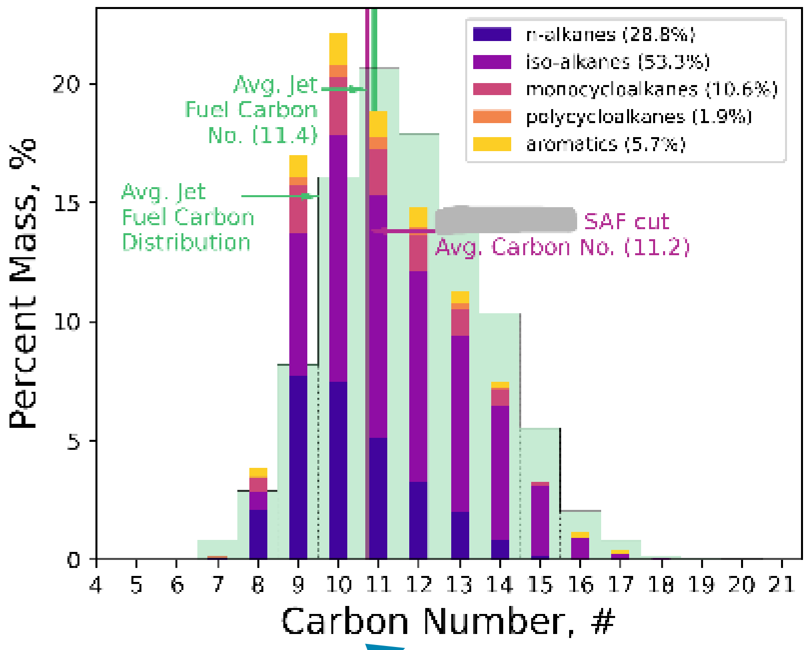


Fig. 4. Pareto fronts of reference conventional jet fuels to illustrate the jet fuel variance effect on SAF blend limit.

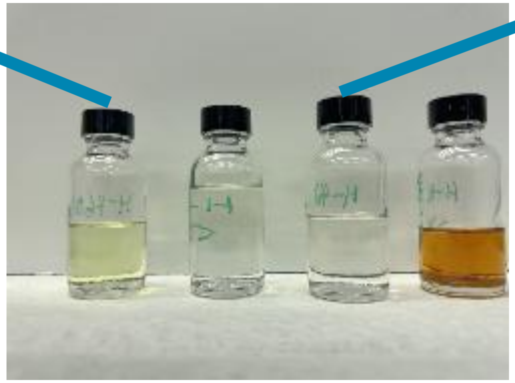


Executive Summary Snapshot





146-265 C cut
SAF yield 55.1%



Method Limitation: Prediction Uncertainty

Uncertainty of SBC composition drives uncertainty of fuel property estimates of pareto-front fuels

- Incomplete knowledge of separation efficiency (theoretical plates) of the refinery or the lab-scale distillation apparatus can be a major contributor to as-modeled SBC composition uncertainty
  - High separation efficiency (high number of plates) is easier to model accurately, but at the refinery this a cost adder
- For low efficiency separations (<3 theoretical plates)
  - Difficult to match plant-scale and lab-scale distillation physics
  - **The composition of the vapor phase and the vapor pressure of the liquid phase is critical-to-quality of the as-modelled SBC composition**
    - <u>Improvement of vapor pressure & composition model is the principal theme of this presentation</u>
    - Vapor pressure & composition also connects with: flash point, lower flammability limit of partially vaporized fuels and other preferential vaporization effects

Other sources of prediction uncertainty include all the usual suspects

- Under-determined isomer concentration in SCO propagates to most of its distillates regardless of separation efficiency
- Relatively small uncertainties from: property blending rules, GCxGC bin concentration determinations, incomplete database, database property inputs

Framework of New Vapor Pressure Model

Daltons Law

$$P = \sum P_i$$

This Model

$$P_i = x_i * P_{vap,i}(x_i)$$

Raoult's Law

Not accurate enough

$$P_i = x_i * P^0_{vap,i}$$

Legacy Model / UNIFAC

Cumbersome for innermost nest in optimization & distillation algorithm

$$P_i = x_i * \boxed{a_i} * P^0_{vap,i}$$

- *Unproven for low x_i*
- *7+ tuned parameters*
- *Van der Walls radii*
- *Convoluted algebraic combinations of terms*

Generalized Clausius-Clapeyron Equation

$$P_{vap,i}(x_i, T) = P_{ref} * \exp[\,(E_{a,i}(x_i, T) / T_{ref,i}(x_i) * (1 - (T_{ref,i}(x_i) / T)\,]$$

$$T_{ref,i}(x_i) = T^0_{ref,i} * (1 + \boldsymbol{c_T} - \boldsymbol{c_T} * x_i)$$

$$E_{a,i}(x_i, T) = E^0_{a,i}(T) * (1 - \boldsymbol{c_E} + \boldsymbol{c_E} * x_i)$$

2 tuned parameters

$$E^0_{a,i}(T) = \ln\left(\frac{P^0_{vap,i}(T)}{P_{ref}}\right) / [\,(1 / T^0_{ref,i}) - (1 / T)\,]$$

$P^0_{vap,i}(T) \equiv$ best available vapor pressure of pure component, i at temperature, T

- Antoine, Wagner, recent measurement, etc.

$P_{ref} \equiv$ 1 atmosphere

$T^0_{ref,i} \equiv$ normal boiling point of component, i

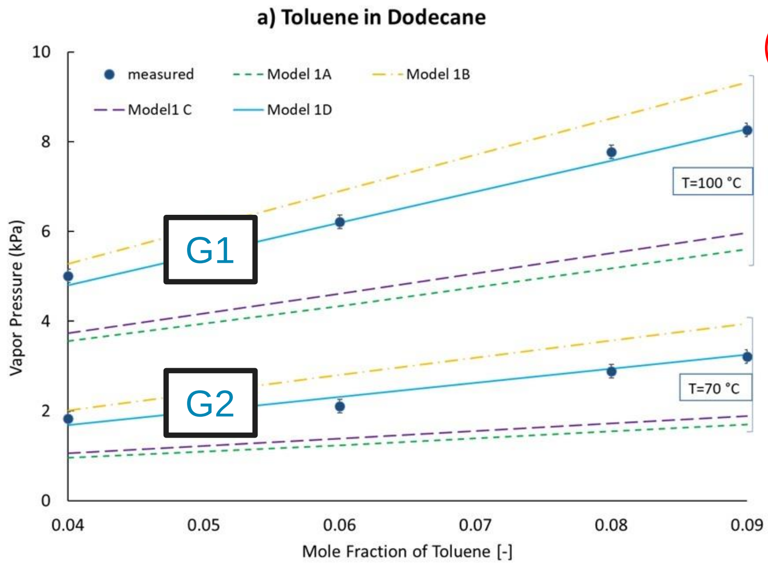
$\boldsymbol{c_T}$ $\boldsymbol{c_E}$

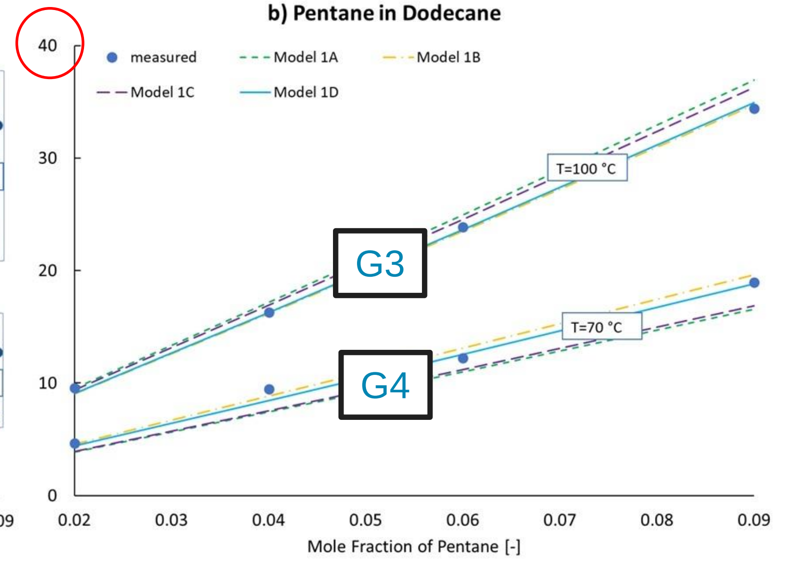
Apply to ALL hydrocarbons

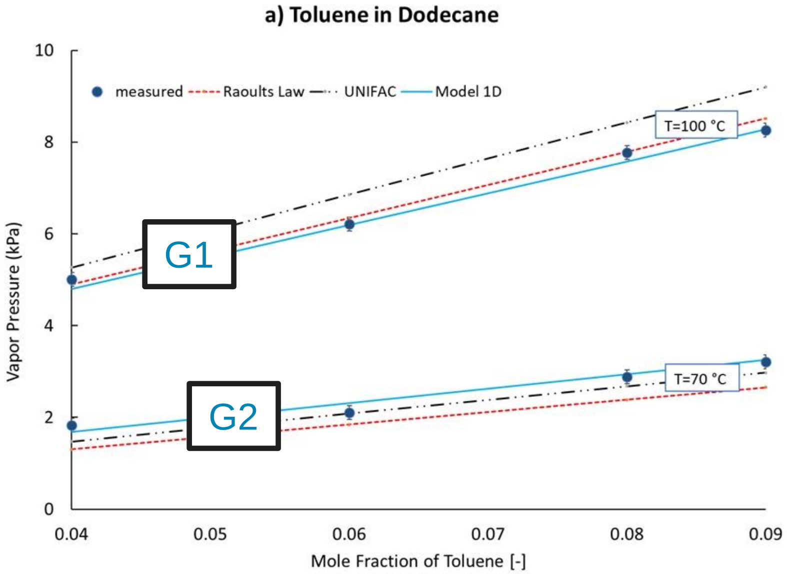
$C_T = C_E = 0$ returns Raoult's Law

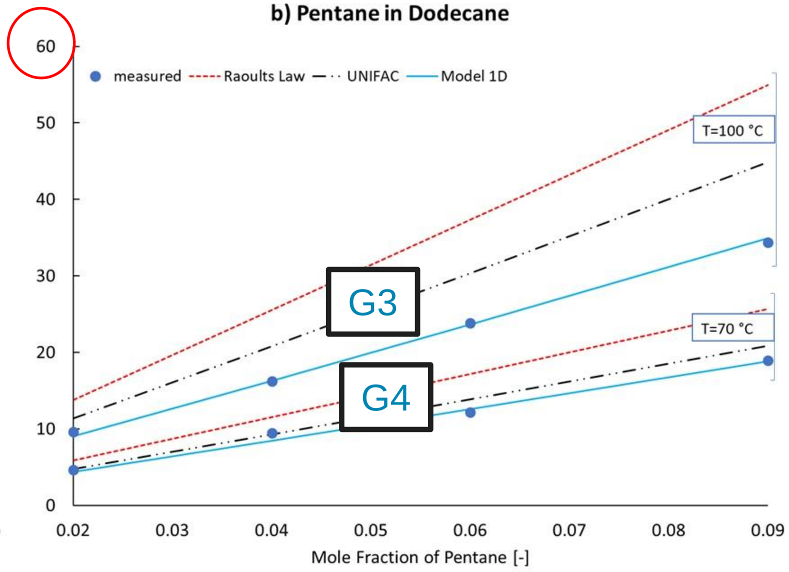
Tuning Results

- Model 1D tracks all four groupings of data with just 2 parameters
- UNIFAC does not track all four in spite of having 7 applicable tuning parameters







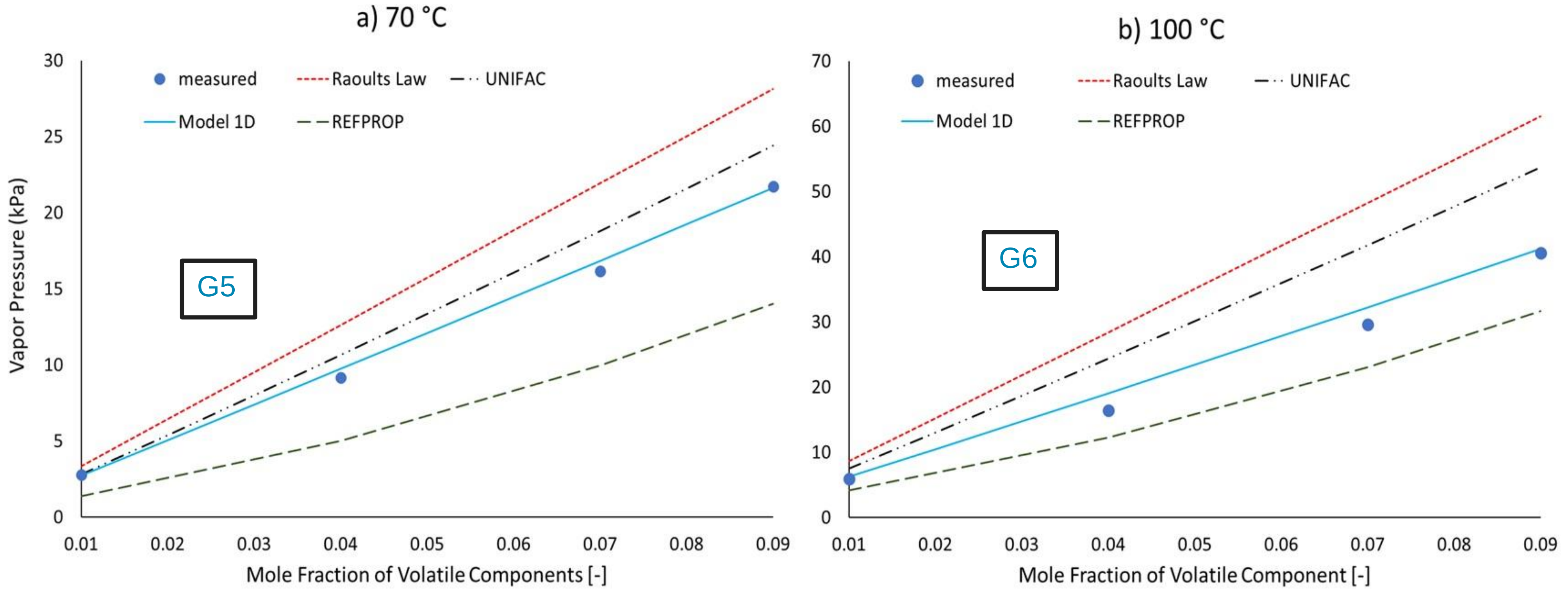


Validation Step 1

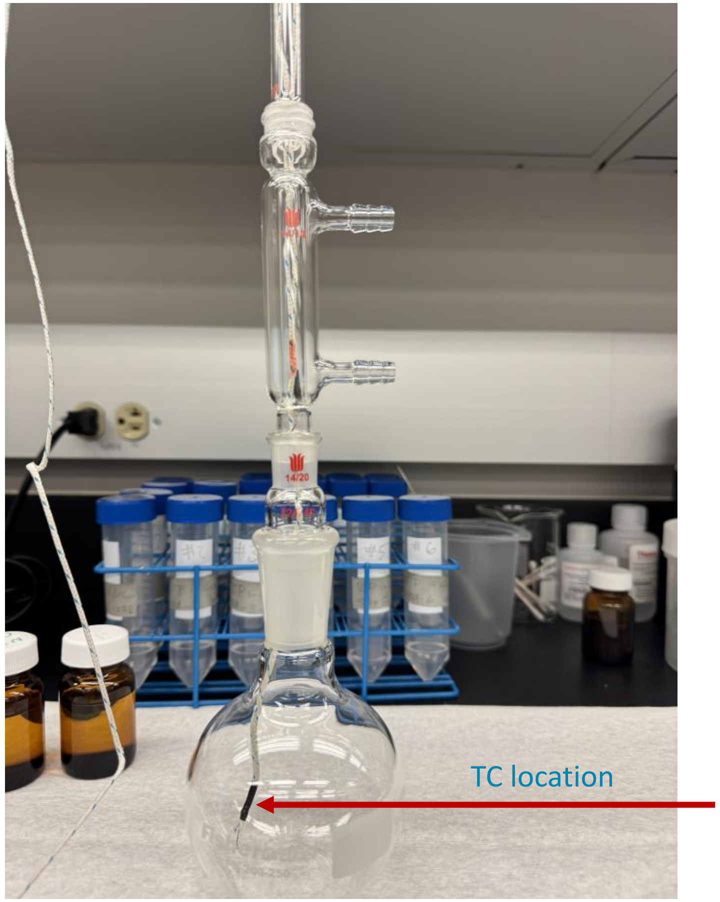
- The tuning holds when all three training materials are present
  - Pentane, toluene and dodecane
- Total solute concentration range doubled relative to training mixtures

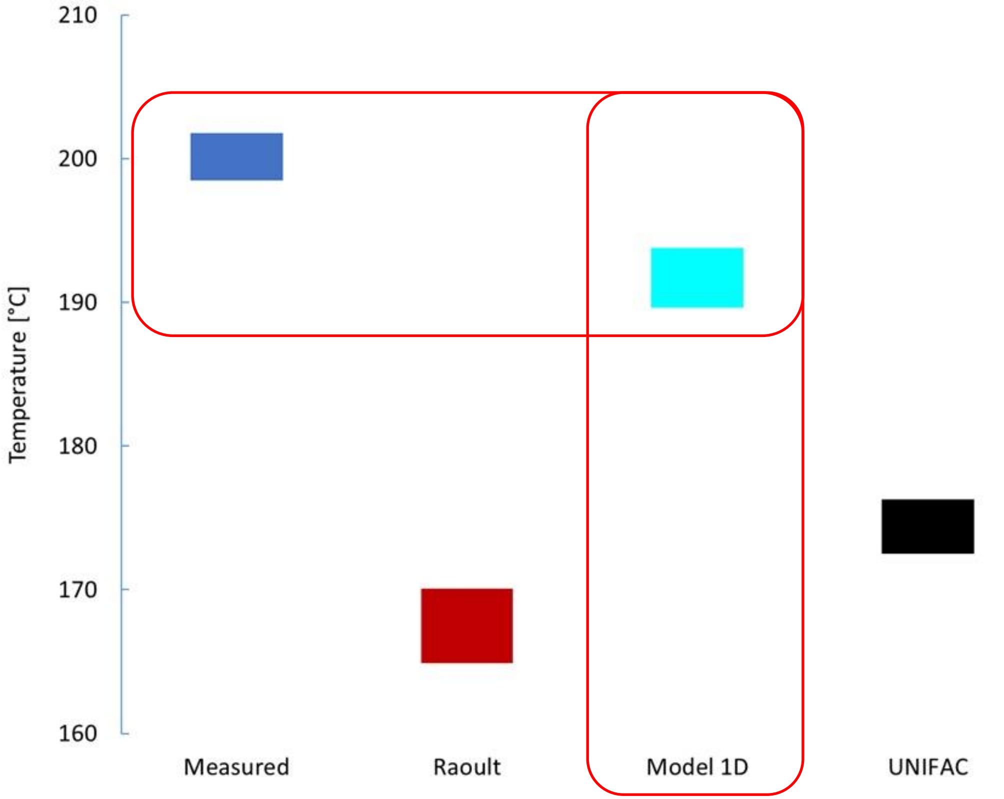
REFPROP

- Added per comment received at the Spring meeting
- Predictions provided by REFPROP technical support
- Based equation-of-state model with inputs derived from prescribed blending rules [Kunz, O and Wagner, W (2012)]



Validation Step 2





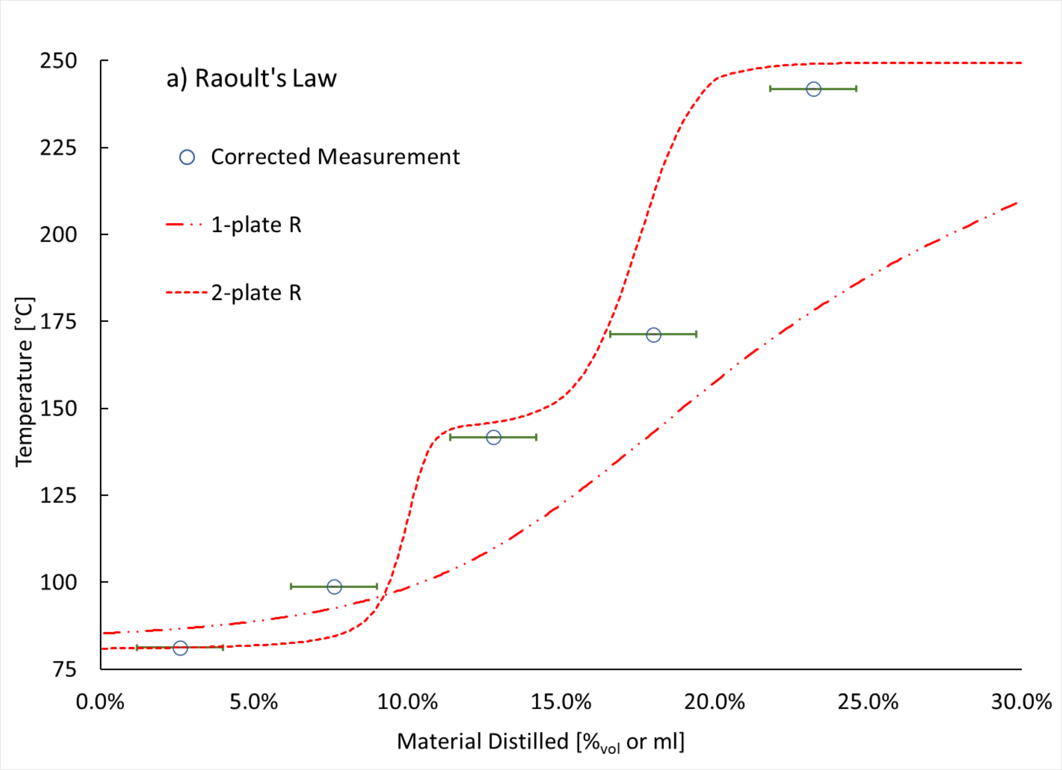
PREDICTED AND MEASURED LIQUID TEMPERATURE OF REFLUXING MIXTURE OF CYCLOHEXANE AND O-XYLENE IN TETRADECANE

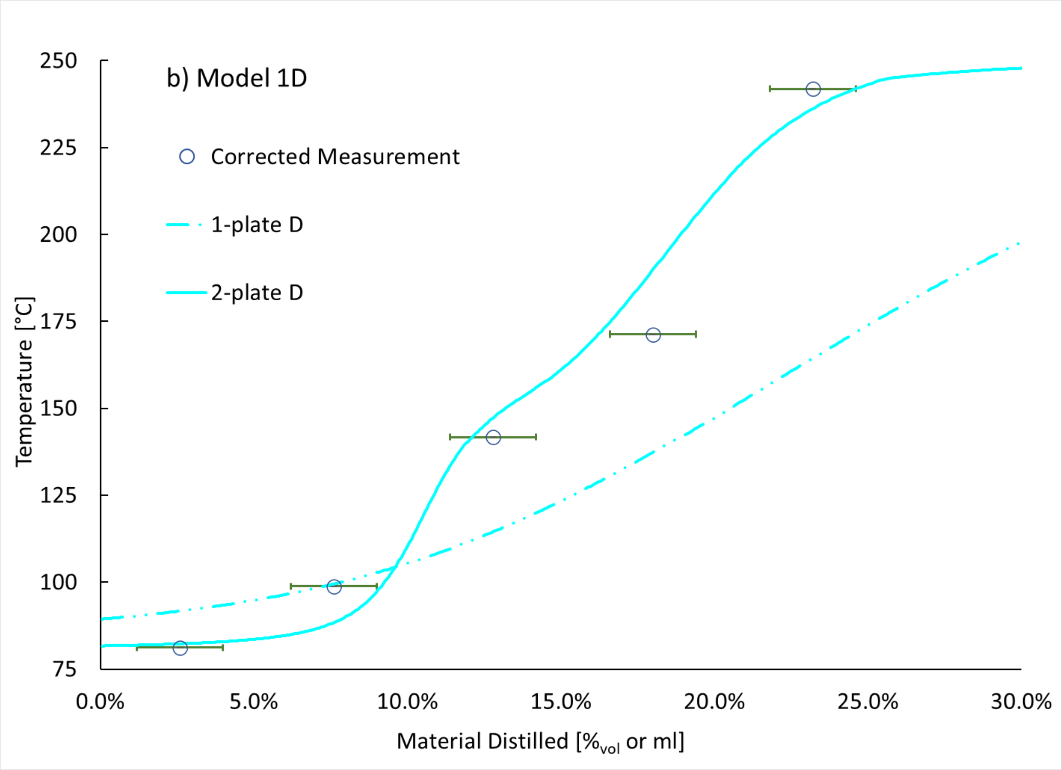
- Prediction ranges are IBP & 1% distilled
- Measured range is first bubble observed & steady-state

This model matches the refluxing temperature of a randomly chosen ternary mixture much more accurately than UNIFAC

Validation Step 3

Part 1: Predicted and measured distillation curve of mixture A: cyclohexane and o-xylene in tetradecane

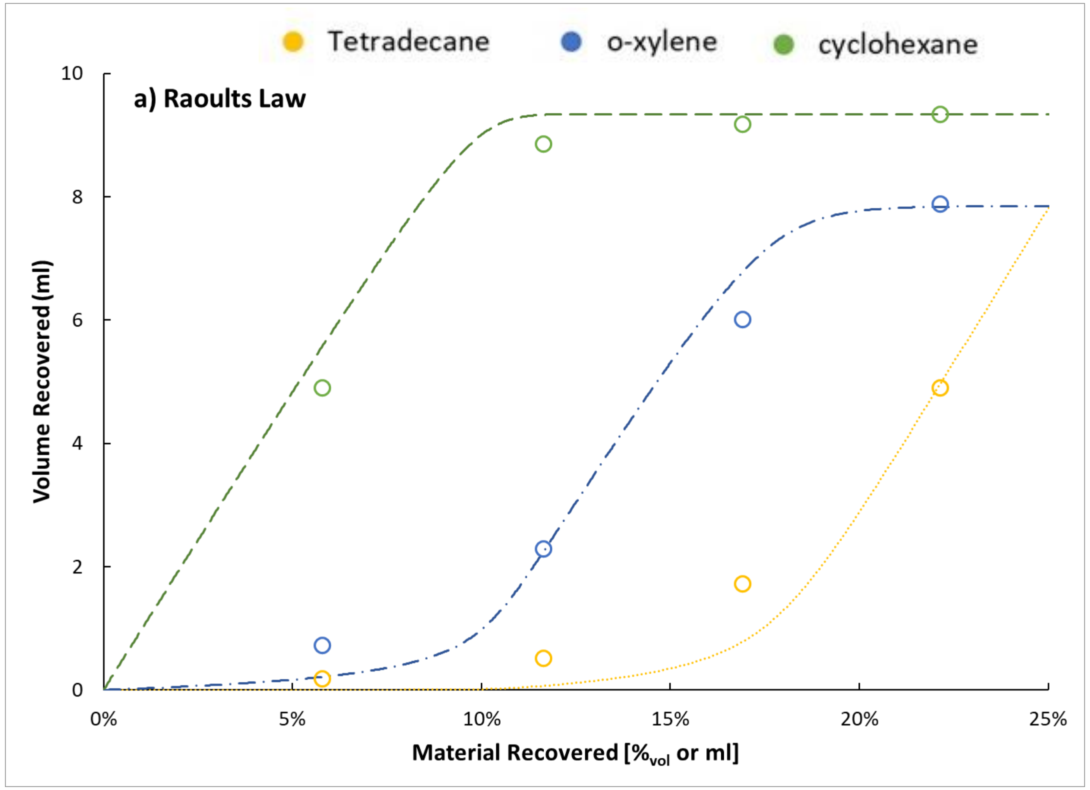


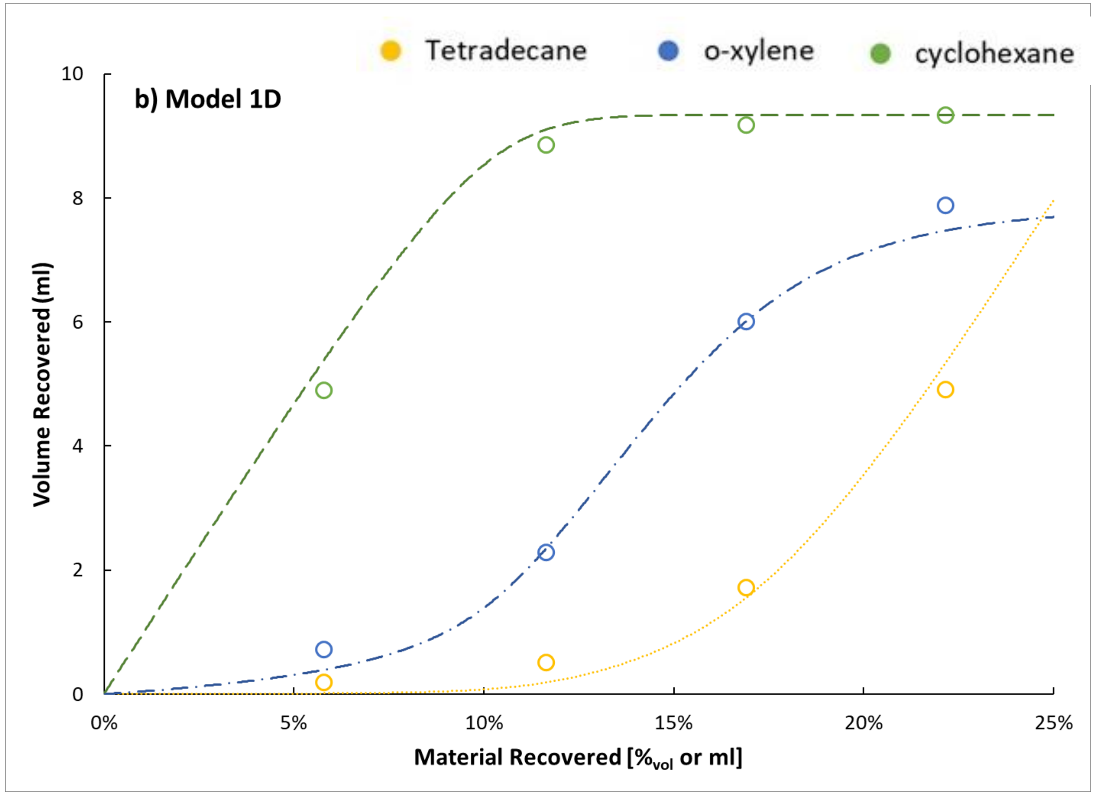


- Neither vapor pressure model reproduces the distillation curve, but Model D is closer than Raoult's Law
  - The open symbols shown here account for dynamic holdup but not distillation loss
- The shape of the predicted distillation curve is sensitive to the vapor pressure model

Validation Step 3

Part 2: Predicted and measured distillate composition of mixture A: cyclohexane and o-xylene in tetradecane



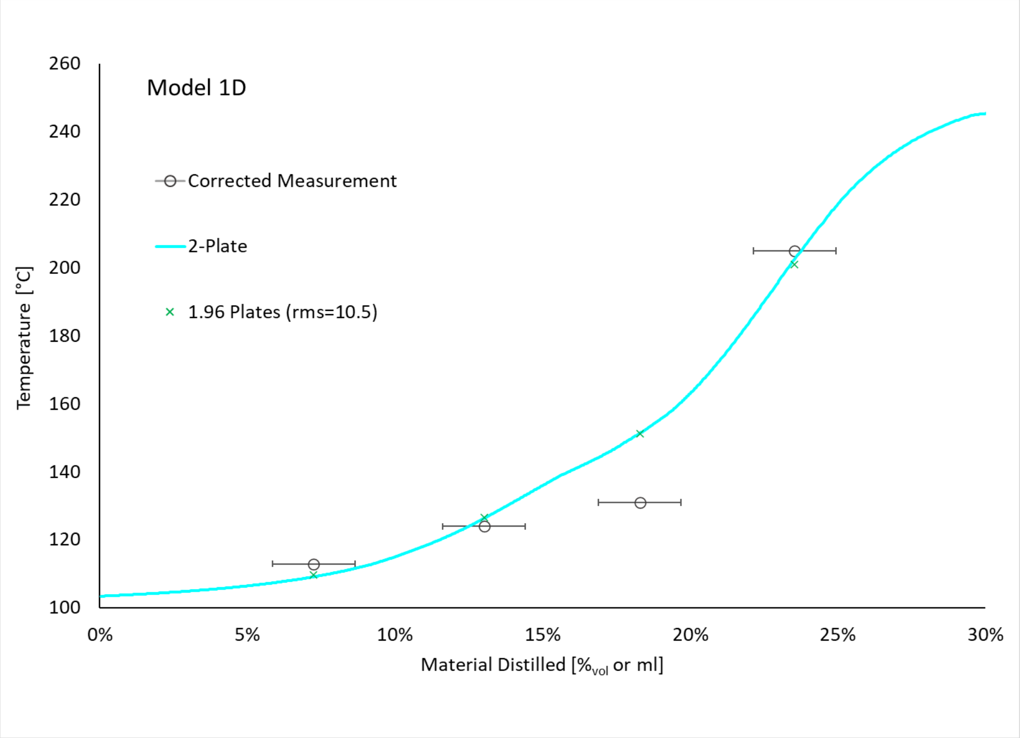


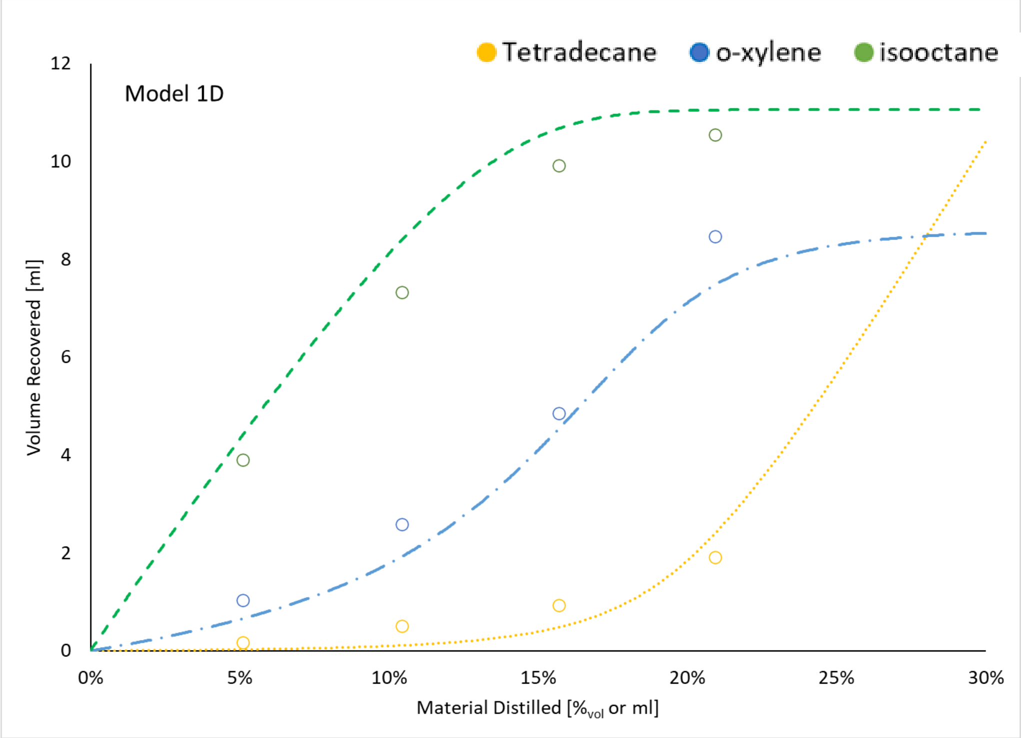
The open symbols here account for distillation loss

- (dashed lines) 2-plates of separation used to model the distillation
  - Raoult’s Law case clearly over-separates by a lot, Model D case is closer but underpredicts tetradecane content in the front end

Validation Step 4

Predicted and measured distillation curve and distillate composition of mixture B: isooctane and o-xylene in tetradecane





- (dashed lines) 2-plates of separation used to model the distillation
  - Under-predicts tetradecane (yellow) in the front end, under-predicts o-xylene (blue) everywhere, over-predicts isooctane (green) everywhere

Summary

- 2-parameter, vapor pressure model has been developed
  - Much more accurate than Raoult's Law
  - Significantly easier to implement than UNIFAC
  - May be more accurate than UNIFAC as well
  - Much easier to implement than equation-of-state models (and more accurate)
- Modeling the physical process of evaporation and distillation introduces a lot of uncertainty
  - Unless the theoretical plate count is high, in which case the vapor pressure model is of low consequence
- Some hints have indicated that UNIFAC may represent the volatility of some aromatic components more accurately than Model D
  - If this turns out to be true and significant, then a third parameter (say two c_E's instead of one) could be added to further improve the model.

Acknowledgements

- U.S. Federal Aviation Administration Office of Environment and Energy
- Trinity College Dublin
  - Robert Parker (vapor pressure data collection)
  - Stephan Dooley

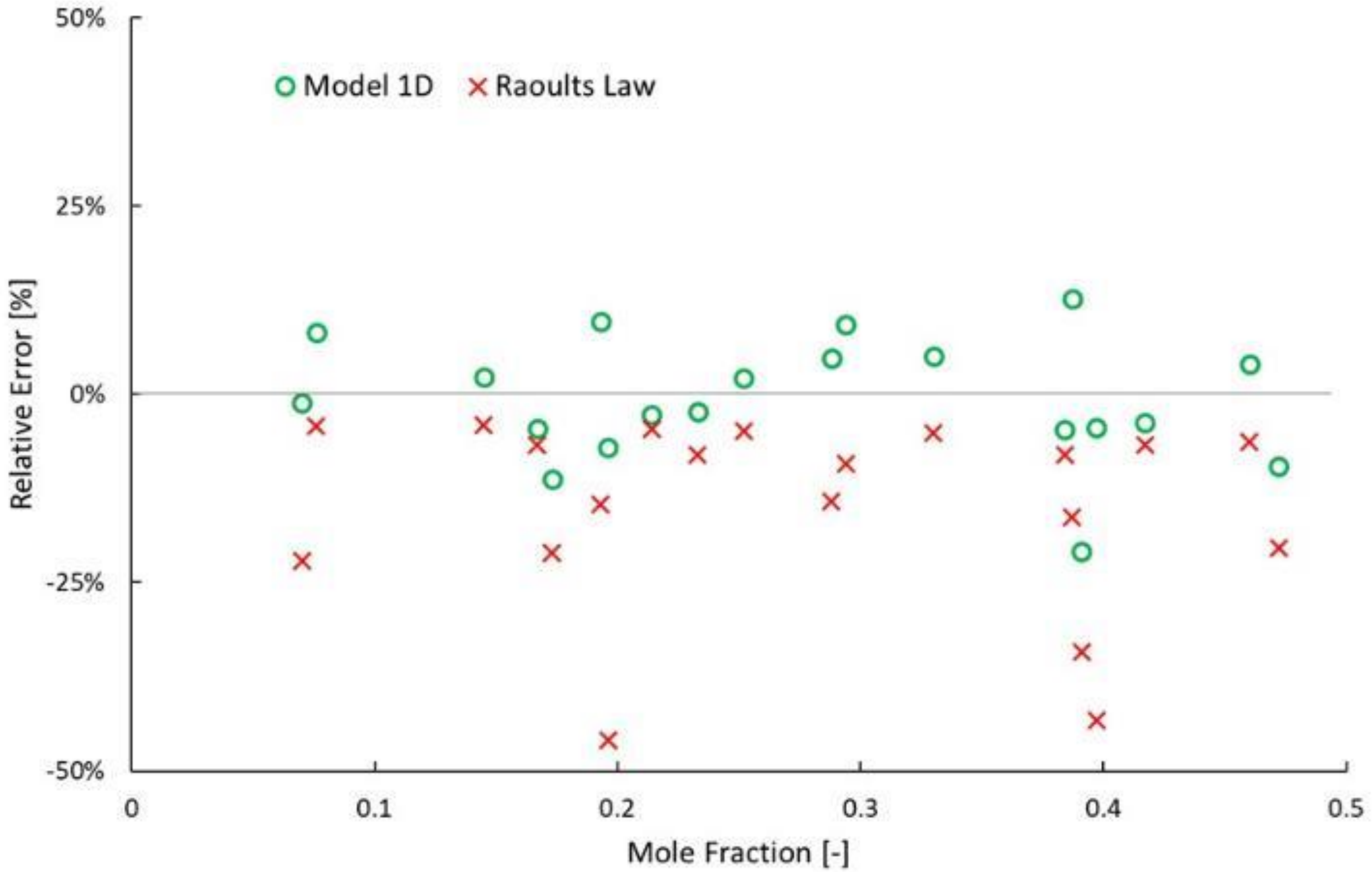
WSU Participants

- Zhibin Yang
- Joshua Heyne
- Randall Boehm
- Alexander Kelly

Appendix

Validation Step 5 (Literature Data)

Hung Y-C, Su S-W, Yan J-W, Hong G-B. Vapor-liquid equilibrium for binary systems containing n-alkanes and cycloalkanes. Fluid Phase Equilib 2024;578:114004. https://doi.org/https://doi.org/10.1016/j.fluid.2023.114004.



Relative Error of Vapor Pressure Predictions of Assorted Binary Mixtures of n-Nonane, n-Octane, Methylcyclohexane or Methylcyclopentane.

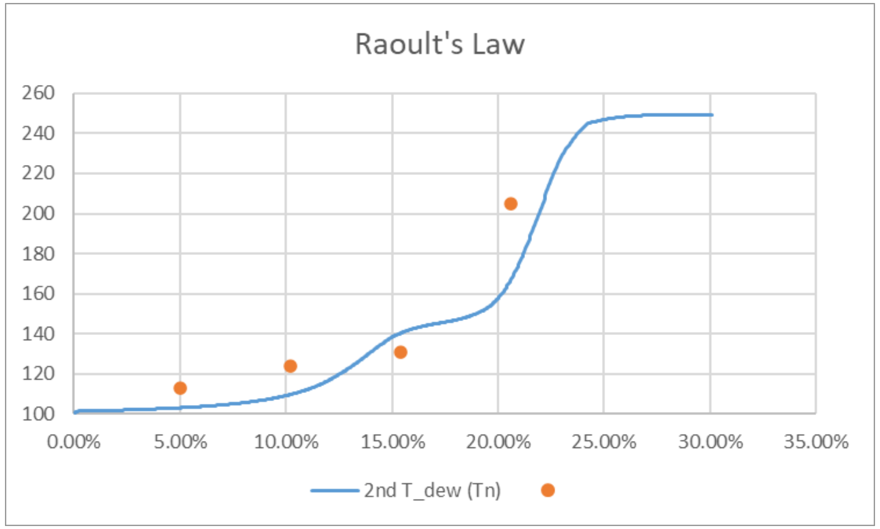
The measurements were taken from the vapor-liquid equilibrium work by Hung et al.

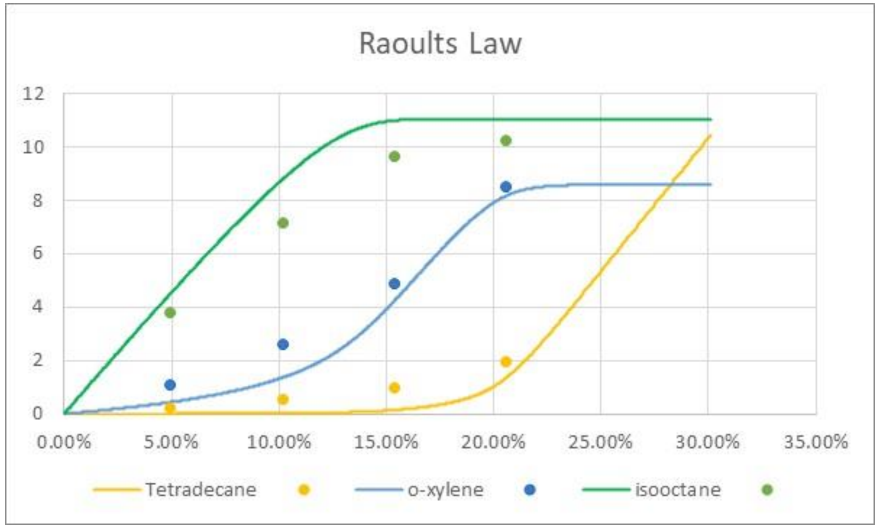
Temperature filtered to 120 °C where vapor pressure equals 45.9 - 261.1 kPa.

Relative error defined as
(measurement – prediction) divided by measurement.

Validation Step 4 supplemental

Predicted and measured distillation curve and distillate composition of mixture B: isooctane and o-xylene in tetradecane





Validation Step 3

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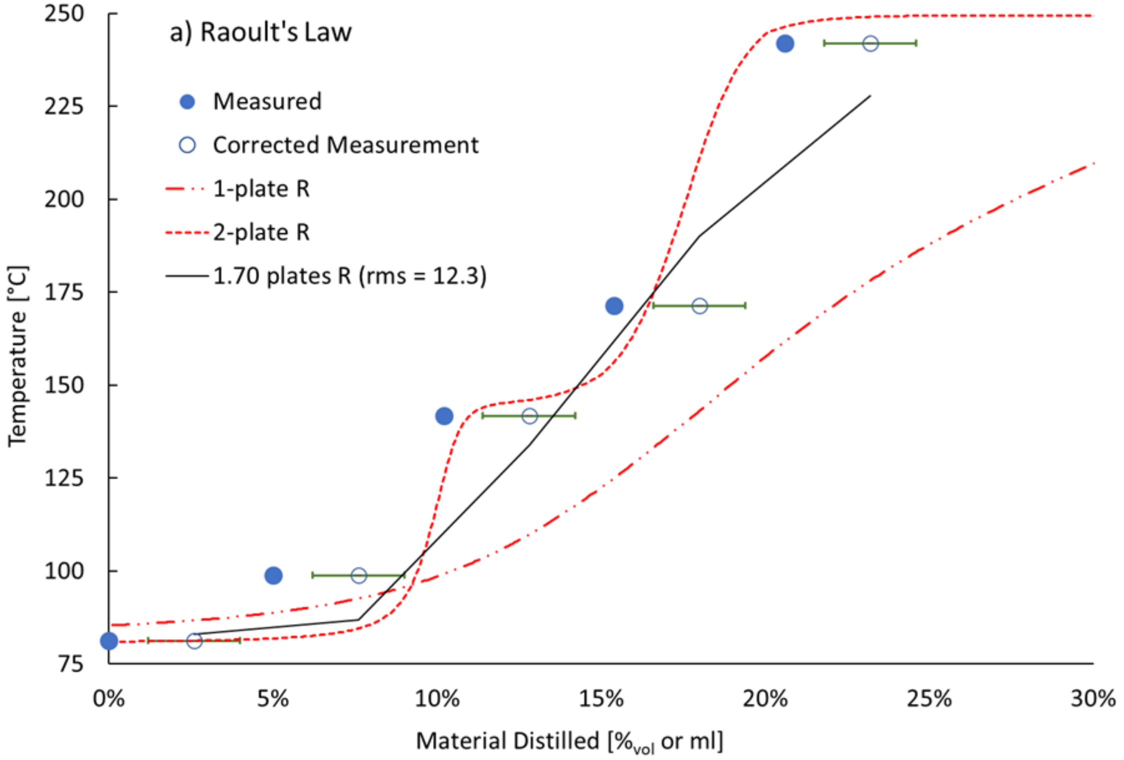

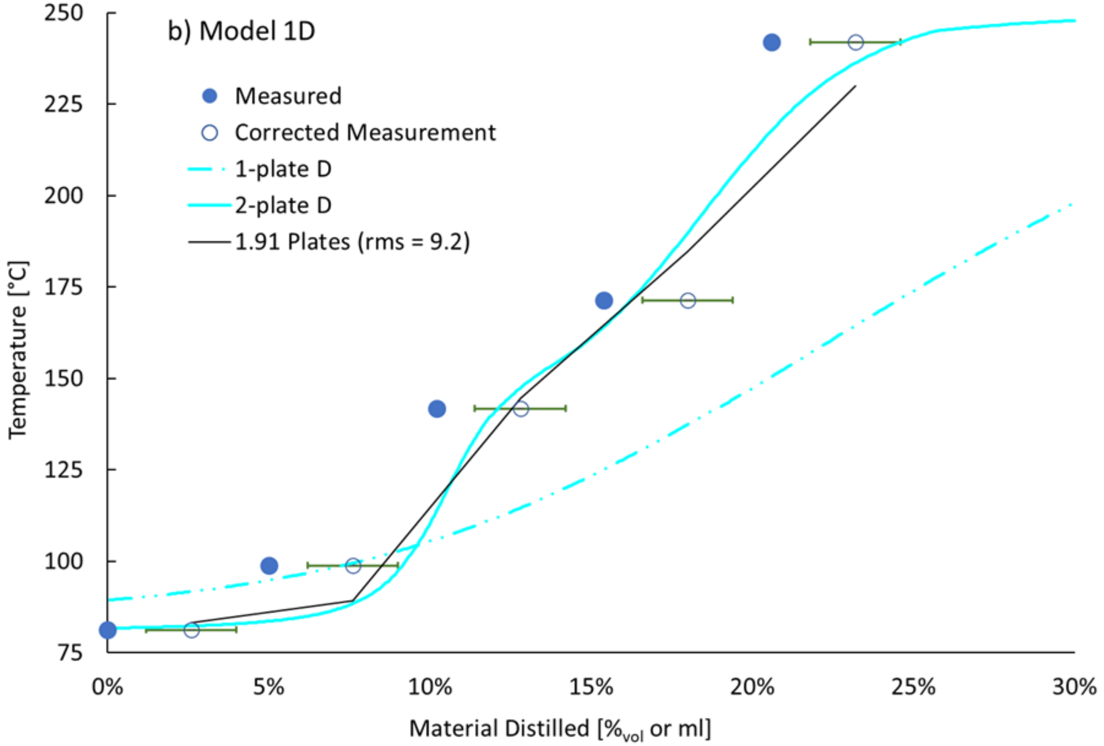

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