Real-Fluid Modeling for Sustainable Aviation Fuels

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Introduction

- Aviation accounts for 8% of the U.S. transportation sector greenhouse gas (GHG) emissions [1]
- Biofuels provide a means for aviation to reduce GHG emissions
  - Sustainable Aviation Fuel (SAF) is a biofuel with properties compatible with traditional jet fuel
- Challenges: Physical testing of SAFs is challenging
  - Cost prohibitive
  - Wide range of operating conditions represented in aviation
- Project goal: Develop an accurate real-fluid model
  - Characterize SAF thermophysical properties and behavior over jet engine operating conditions
  - Implement the framework in Computational Fluid Dynamics (CFD) software to simulate SAF injection and mixing

Impact

- SAFs reduce the life cycle carbon footprint of aviation because the carbon dioxide emitted from the transportation and fuel combustion is offset by the carbon dioxide sequestered by the feedstock crops
- Modeling addresses the current limits with physical testing of SAFs
  - Analyze operating conditions that are difficult to simulate in a laboratory setup
    - Pressure ranges from 0.4-60 bar
    - Temperature ranges from 233-1000K
- Predictive modeling allows screening and testing of SAFs in realistic configurations through CFD simulations

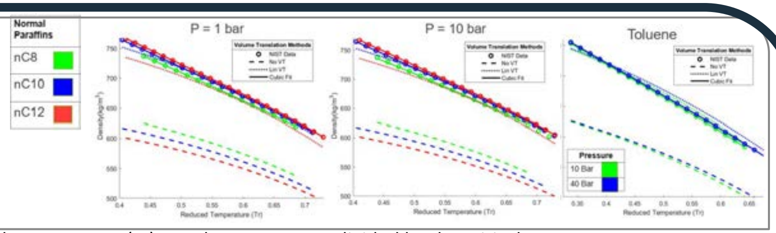
Approach

- Improvement of the **V**olume **T**ranslation (VT) term for **S**oave-**R**edlich-**K**wong (SRK) equation of state (EoS)
  - SRK-VT EoS
  - $$p = \frac{R_u T}{\bar{v} + c - b} - \frac{a}{(\bar{v}+c)(\bar{v}+c+b)}$$
  - Volume Translation term c = f(Tr)

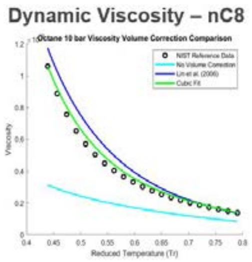
Baseline Model (Lin et al. 2006) [2]	**Cubic Fit**	**Advanced Curve Fit**
$f(T_r) = \beta + (1-\beta)e^{\gamma(1-Tr)}$	$f(Tr) = f(Tr)^3 + g(Tr)^2 + h(Tr) + k$	$f(Tr) = \xi_1 + (1-\xi_2)e^{\gamma(1-Tr)}$ $\xi_1 = a(Tr)^3 + b(Tr)^2 + C(Tr) + d$ $\xi_2 = a(Tr)^3 + b(Tr)^2 + c(Tr) + f$

Results

Density



Reduced temperature (Tr) equals temperature divided by the critical temperature



Comparison of the volume translation methods for the calculation of density and viscosity with respect to NIST reference data at low and high pressure

Conclusion

- The cubic fit best fits the reference data, especially at low temperatures
- Better volume translation methods can improve the fluid property calculations which will yield more accurate results in CFD simulations

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References

[1] U.S. EPA, 2021
[2] Lin et al. *Industrial & engineering chemistry research*, 2006.