Determination of a Freeze Point Blending Rule for Jet Fuel Range Hydrocarbons

Allison Coburn

Advisor(s): Joshua Heyne, PhD, and Zhibin Yang

Objective: To develop an accurate freeze point blending rule for jet fuel range hydrocarbons in order to better facilitate the evaluation of the acceptability of novel Sustainable Aviation Fuel (SAF) candidates.

Motivation:

- Aviation sector is responsible for 2% of the worlds CO_2 emissions**.** SAF are a viable option to decrease emissions. [1]
- To date, only 8 fuels have been approved due to their nature of being both cost and volume intensive. Novel SAF needs to go through the industry's standard evaluation process(i.e., ASTM D4054 and D7566) [2]
- Prescreening of a novel SAF can provide feedback on downstream approval issues and de-risking technology development. [4,5]
- Freeze point is one of the key properties in prescreening but the current method from literature used for freeze point prediction is not validated in the ASTM required temperature range (275-350 K) [3]
- Other prediction methods involve experimentally determined interaction coefficients.

Figure 1. Hydrocarbon example images

Methodology

- Hydrocarbons are selected by their neat freeze point being within the temperature range of Phase Technology machine and differing from other hydrocarbons being blended with
- Selected also by price and volume the hydrocarbons can be bought at
- Tridecane, cis-1,2-dimethylcyclohexane, and trans-decahydronaphthalene were mixed at varying compositions to experimentally determine freeze point

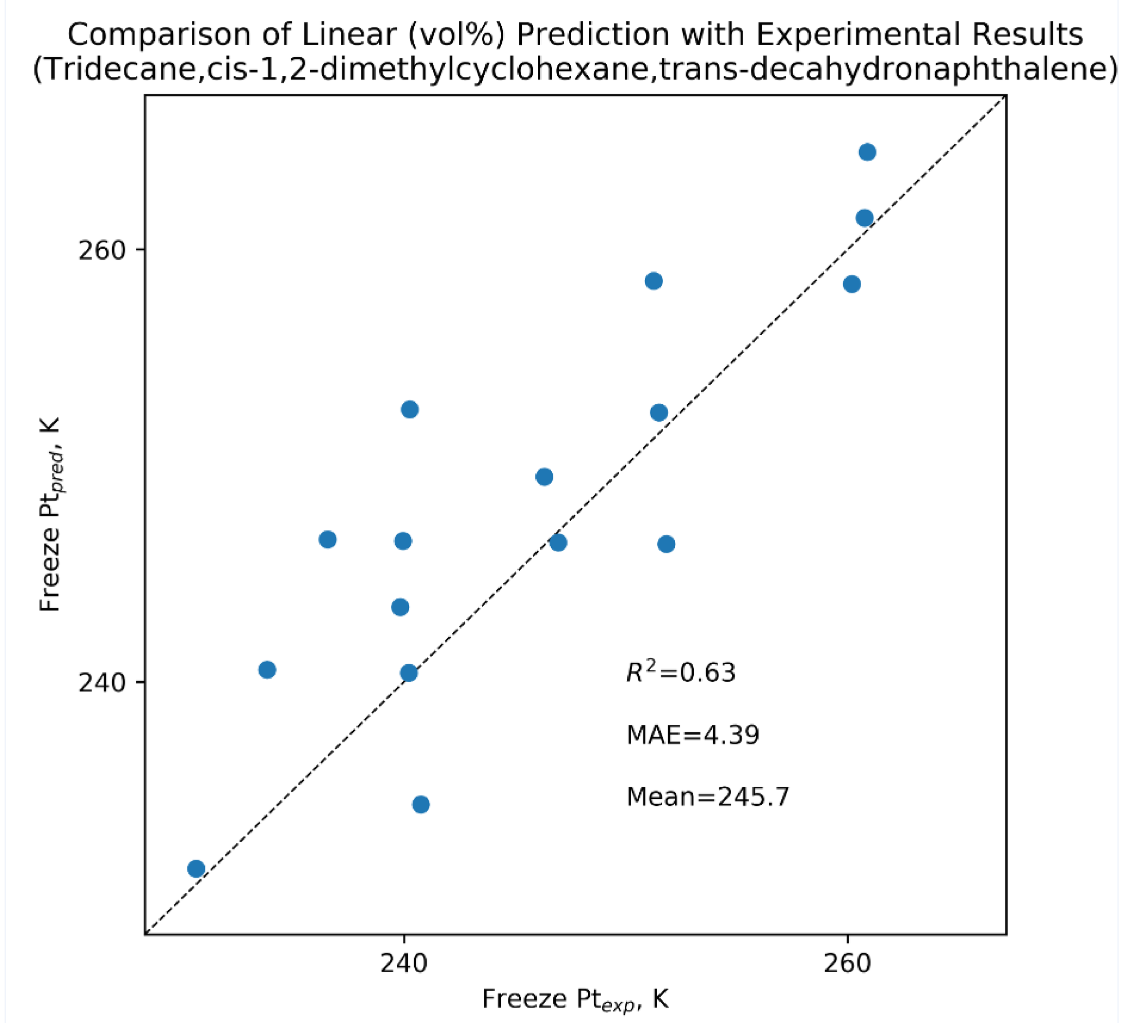


Figure 2. Linear prediction by volume %

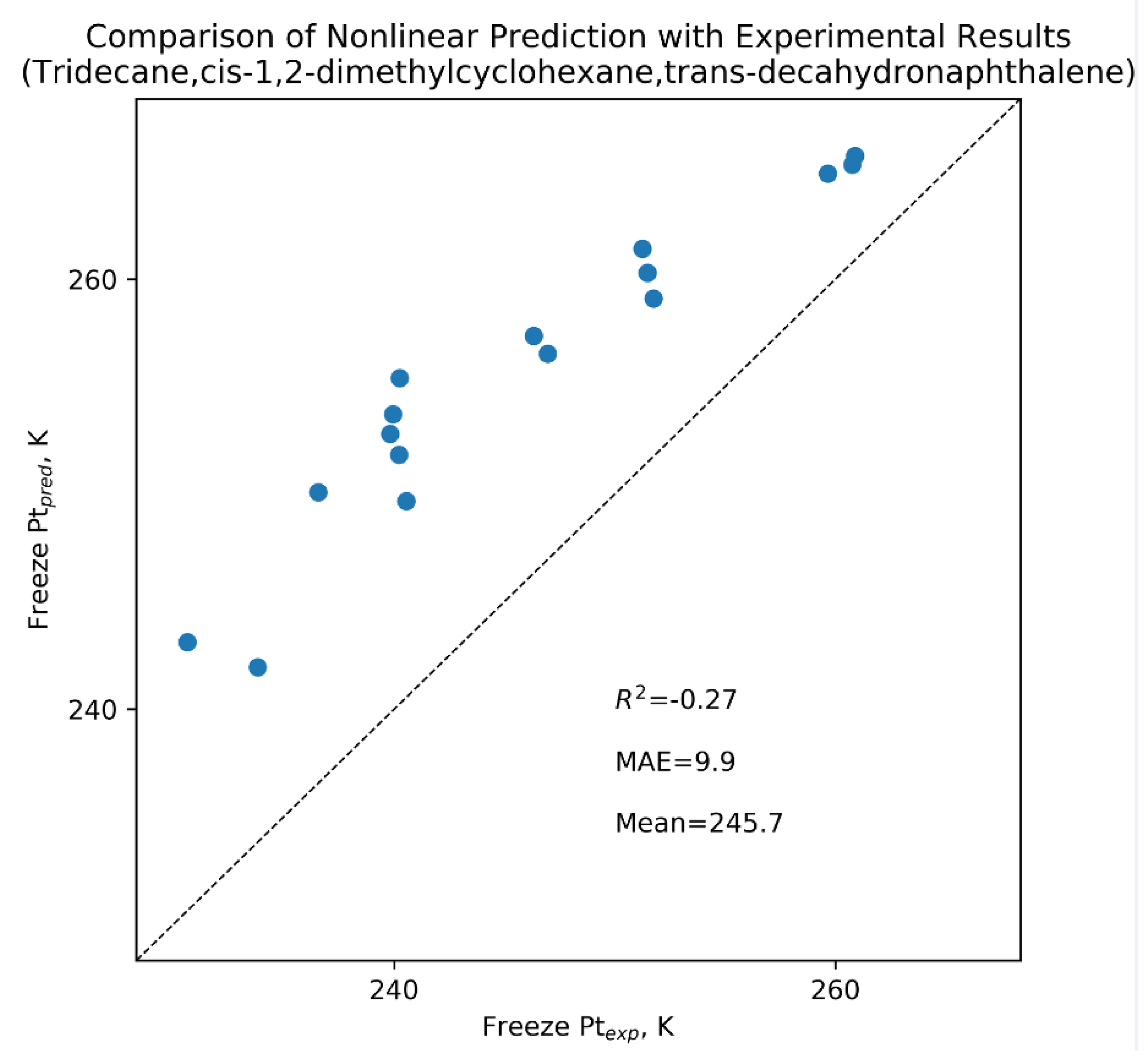


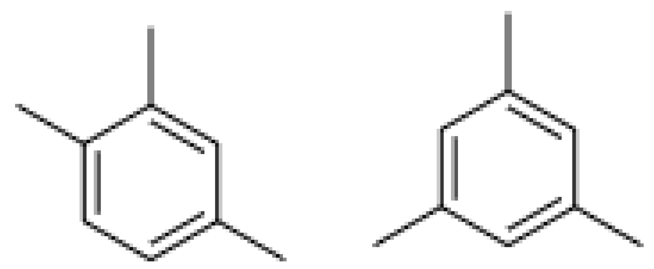
Figure 3. Prediction by current method used

Results:

- Current prediction method is not reliable (figure 3)
- Linear prediction by mole percent and volume percent of data collected were compared with the prediction by the method currently being used (figure 2, 3)
- Some data may need to be run through code to provide more accurate data as seen in figure 4

Conclusion and Next Steps:

- Linear prediction by either volume or mole percent have potential but need to be improved
- Further testing is being conducted on hydrocarbons with similar structure but varying neat freeze points



Left: 1,2,4-trimethylbenzene, Right: 1,3,5-trimethylbenzene

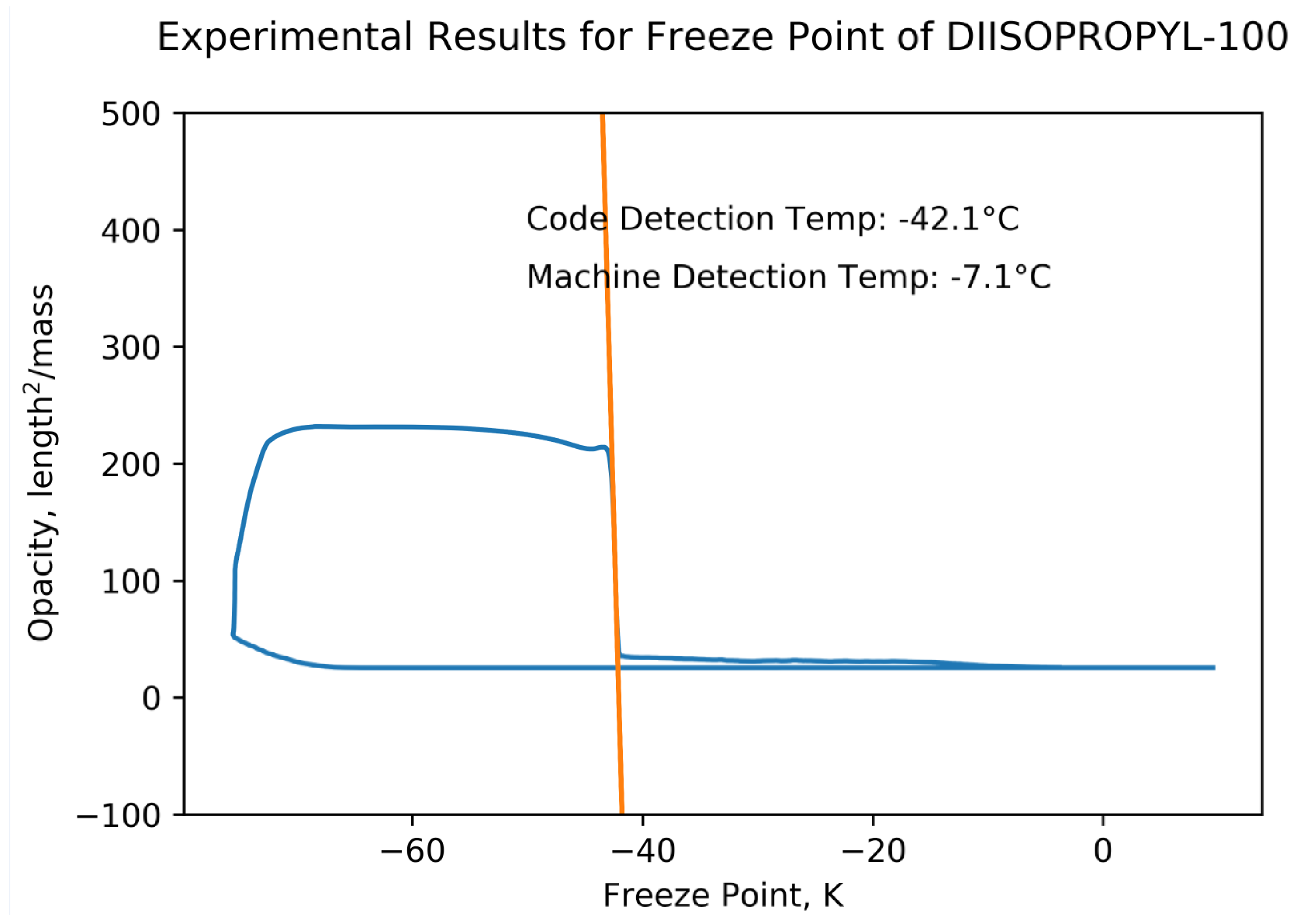


Figure 4. Example graph output from machine with code detection shown in orange

References

1.“Aviation and Climate Change”, Aviation Benefits Beyond Borders
2.ASTM International. (2016). *D5972-16 Standard Test Method for Freezing Point of Aviation Fuels (Automatic Phase Transition Method).*
3.Hessa A. AlMulla & Tareq A. Albahri (2017) Predicting the properties of petroleum blends, Petroleum science and Technology, 35:8, 775-782
4. Zhibin Yang, Shane Kosir, Robert Stachler, Linda Shafer, Carlie Anderson, Joshua S. Heyne, A GC × GC Tier α combustor operability prescreening method for sustainable aviation fuel candidates, Fuel, Volume 292, 2021.
5. Joshua Heyne, Bastian Rauch, Patrick Le Clercq, Meredith Colket, Sustainable aviation fuel prescreening tools and procedures, Fuel, Volume 290, 2021.