Use of Thermodynamic Models for Optimizing Fuel Treatment Processes

Shawn Kirby, Andrew Guenthner
Rocket Propulsion Division, Aerospace Systems Directorate, Air Force Research Laboratory, Edwards AFB, CA

Abstract

The IRS and EPA require certain fuels to be dyed for tax purposes, however dyes can be detrimental to fuel performance. It would be advantageous to remove the dyes prior to their use in critical aerospace applications. Many dyes are unable to be removed from fuels using current technologies. We used Hansen Solubility Parameters to develop an "ideal solvent" to extract these dyes from fuel.

A similar approach will also be applied to removal of sulfur compounds from fuels. Sulfur compounds in fuels create sulfates during combustion, which in turn react with water to make sulfuric acid. Sulfuric acid damages engine components and the environment.

Background

According to the Hansen Solubility Parameters, there are three main molecular forces that affect solubility: the dispersion component, \( \delta_D \), the polar component \( \delta_P \), and the hydrogen bonding component, \( \delta_H \).

All three components must be somewhat close in order for the solute to dissolve. Thus, if we know the solubility parameters of several solvents, we can use "pass/fail" solubility tests with a solute to determine its solubility parameters.

Experimental

Compounds were tested in approximately 40 different solvents for solubility.

They were classified as "pass" or "fail", this data was then entered into a custom Microsoft Excel program which then calculated approximate values for \( \delta_D \), \( \delta_P \), and \( \delta_H \). A "radius of solubility" was also calculated to create a sphere, to determine how far the solvents values of \( \delta_D \), \( \delta_P \), \( \delta_H \) could vary and still allow dissolution.

Based on this data, an ideal solvent, that was immiscible with the fuel, and that would dissolve the dyes easily, was formulated using the calculated values of \( \delta_D \), \( \delta_P \), \( \delta_H \).

The dye removal performance of the ideal solvent was then tested.

Results

Current Method: Using a 10:1 Isopropyl Alcohol to Water solution, dodecane containing dye Oil Red B4 was run through an extraction. As can be seen, most of the dye stayed in the dodecane.

The solubility parameters of Oil Red O (ORO) were determined experimentally. Then, topological methods were used to calculate the solubility parameters of Oil Red B4, which is similar to ORO except for a side chain. Using a custom program in Excel, it was determined that a 4:1 mixture of 1,1,2,2-tetrabromoethane and dimethylformamide would be an ideal solvent. This mixture was used in an extraction of Oil Red B4 from dodecane. By visual inspection, far more of the dye was removed.

New Method: The solubility parameters of Oil Red O (ORO) were determined experimentally. Then, topological methods were used to calculate the solubility parameters of Oil Red B4, which is similar to ORO except for a side chain. Using a custom program in Excel, it was determined that a 4:1 mixture of 1,1,2,2-tetrabromoethane and dimethylformamide would be an ideal solvent. This mixture was used in an extraction of Oil Red B4 from dodecane. By visual inspection, far more of the dye was removed.

Conclusion

We have demonstrated that Hansen Solubility Parameters can be used to formulate effective extraction fluids for fuel treatment. This eliminates the previous need for "trial and error" experiments. This can be applied to new technologies to clean fuels before usage.