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Joe Jobe

Rock House Advisors

Re: Calculation of R-values for biodiesel, renewable diesel and HEFA-SPK SAF

Dear Joe

Thank you for asking me to review and comment on the white paper:

> *"Equivalence Value Determination for Biodiesel, Renewable diesel, and Sustainable Aviation Fuel (SAF) from Fats and Oils", Shah Parag, More Amol, Jobe Joe,* www.sabrcoalition.org/news, 2023

It is critically important that the fraction of energy in a renewable fuel that comes from renewable biomass be accurately accounted for. As you point out, currently this accounting is not accurate for diesel and jet fuel blendstocks made by hydrogenation of renewable fats, oils and greases. This is because fossil-derived hydrogen (from natural gas) is used in the production of renewable diesel (RD) or sustainable aviation fuel (SAF) and this portion is not deducted from the fuel energy content.

The white paper describes calculation of the R-value – the fraction of energy in the fuel from renewable biomass – and the use of this to calculate an equivalence value (EV) which is the renewable content relative to ethanol. I will confine my remarks to the calculation of the R-value. The paper shows calculation of R for biodiesel, RD, and SAF using two different methods. One is based on heat of combustion that are calculated from bond energy (BE), the other based on the energy content of the molecule and is also calculated from BE.

I have repeated all these calculations and have found some minor errors that I will point out. These do not change the overall conclusions of the analysis.

*Heat of Combustion Basis*

Here the total heat of combustion is calculated based on the BE for all the bonds in the combustion reactants (methyl oleate and O2) and all of the BE in the products (CO2 and H2O). The heat of combustion is total BE in the products minus total BE in the reactants. The combustion reaction in the white paper is stated as:

$C19H36O2 + 26\ O2 = 19\ CO2 + 18\ H2O$

However, the correct balanced combustion equation is:

$C19H36O2 + 27\ O2 = 19\ CO2 + 18\ H2O$

In the calculation of the heat of combustion the number 22,966 appears which should be the total BE in methyl oleate. I could not reproduce this number. Here is a table of my calculation:

| Number of Bonds | Bond Type | BE, kJ/mol | Total BE, kJ/mol |
|---|---|---|---|
| 17 | C-C | 348 | 5,916 |
| 36 | C-H | 413 | 14,868 |
| 2 | C-O | 358 | 716 |
| 1 | C=O | 799 | 799 |
| Total Methyl Oleate Energy | | | 22,299 |

Using my total energy for methyl oleate and the correct stoichiometry yields a lower heating value of 11,366 kJ/mol. My calculation of the CH3O non-renewable portion heat of combustion yields the same value in the white paper 771.3 kJ/mol. I obtain an R-value of 0.932, very close to that in the white paper of 0.931.

For RD on this basis my calculations exactly replicate the numbers in the white paper. I note that the first equation in this section implies that there are 18 C-C bonds in C18H38 but in fact there are only 17. This must have been what was used in the calculation as it is what I used and we get the same answer to several decimal places. I am also able to replicate the combustion-based calculation for SAF.

*Bond Energy Fraction Basis*

In my opinion the BE fraction calculations take a cleaner approach, with fewer assumptions – but yields very similar results to the calculations on a heat of combustion basis.

In repeating the calculations, I noted one minor error in the biodiesel calculation, there are 36 C-H bonds, not 37. This changes the calculate R-value by less than 1%. I can reproduce the calculations from RD and SAF exactly.

*Summary*

Both approaches to calculating the fraction of energy in the fuel derived from renewable biomass are valid. Both are consistent with the basic principles of chemistry and the first law of thermodynamics. The use of methyl oleate, octadecane, and dodecane as surrogates, respectively, for biodiesel, RD, and SAF is very reasonable – but other molecules could be chosen and would produce very similar results. The calculations take a conservative approach to estimating the fraction of energy in the fuel that comes from renewable biomass in terms of the assumptions as to what parts of the molecules are non-renewable. The BE fraction-based calculation requires no assumptions about what the non-renewable portion of the molecule is (CH3O, or CH3, or CH3OH for biodiesel, for example), and therefore seems more straightforward and easier to implement.

Thank you again for the opportunity to comment on this important question.

Best regards,

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