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

Hello Joe,

I am sending this letter as a comment to 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 my understanding that this analysis was made available to the public, so that the fair comparison can be made between different types of advanced biofuels produced from renewable raw material sources. In the process of manufacturing various types of fuel derived from renewable materials, it is critically important to take into account the energy content derived from renewable raw material sources, as opposed to content derived from non-renewables (fossil based materials).

The analytical scrutiny is applied to the following fuels: biodiesel, renewable diesel and sustainable aviation fuel (SAF).

Each of the three types of fuel analyzed in this study is using both renewable materials (vegetable oils) and non-renewable materials (hydrogen in case of renewable diesel and SAF and methanol in case of biodiesel). When fuel energy content is calculated, this fact is important to be considered, so that the non-renewable energy content can be subtracted from the total energy content of the fuel in question.

Central to the analysis used in the white paper is so-called equivalence value (EV) which is defined as renewable content relative to ethanol. The reason ethanol is used for this calculation is because EPA is using ethanol for comparison of all advanced biofuels energy contents, and assigns equivalent value for each individual fuel. The calculation of EV uses fraction of the energy in the fuel derived from the renewable portion of the material, this is defined as R value.

Two calculation methods are used to calculate EV in the paper:

a) based on heat of combustion
b) based on bond energy fraction

All calculations were based on a model raw material oleic acid (18 carbon fatty acid with the single double bond).

Biodiesel calculation was based on combustion of methyl oleate as a model compound.

Combustion of methyl oleate was presented in the equation:

$C_{19}H_{36}O_2 + 26O_2 = 19\ CO_2 + 18\ H_2O$

This formula needs to be corrected for properly balancing the formula to:

$C_{19}H_{36}O_2 + 27O_2 = 19\ CO_2 + 18\ H_2O$

In our calculations, obtained methyl oleate total bond energy is shown in the table is different from 22,966 kj/mol used in the paper, we found 22,228 kj/mol and the source we used is: (Bond Energies - Chemistry LibreTexts).

Methyl Oleate Bond Energy Calculation			
Bond	Bond Energy (kJ/mol)	Number of bonds	Bond Energy Sum (kJ/mol)
C-H	413	36	14,868
C-C	347	17	5,899
C-O	358	2	716
C=O	799	1	799
Methyl Oleate Total Bond Energy			**22,282**

Biodiesel heat of combustion is derived from the fatty acid (renewable) and methanol (non-renewable) portion of the fuel. Subtraction of CH3O portion of the molecule of methyl oleate brings the EV of biodiesel to 1.47 and our calculation confirms this (with some minor discrepancies.

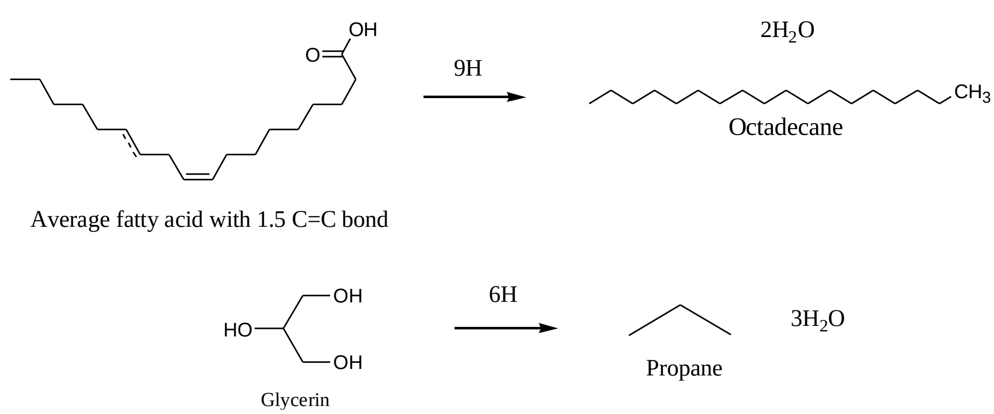
Renewable diesel calculations presented take into account hydrogen used to saturate double bond in oleic acid molecule and also terminal carboxyl group into methyl group.

Non-renewable hydrogen brings renewable diesel EV to 1.53 (relative to ethanol) based on the calculation presented, our values are almost identical.

Similarly, SAF fuel calculation shows EV to be 1.39 and we confirmed validity of calculation.

Observations on Feedstock Selection:

Using oleic acid as a model for calculations is indeed "best case scenario" for renewable diesel and SAF. Most often, tri-glycerides are used as raw materials and among these, soybean oil is frequent. Renewable diesel and SAF are often manufactured from soybean oil or similar vegetable oils, which contain average of 1.5 double bonds per each fatty acid. This increases non-renewable hydrogen required for double bond hydrogenation from 2 to 3 atoms. In addition, the carboxyl group hydrogenation requires 3 H atoms for terminal carbon and additional 3 H atoms for hydrogenation of two oxygen atoms into two molecules of water. Finally, glycerin present in tri-glyceride is being hydrogenated into propane and water and this portion of the bio-renewable molecule is not converted into renewable diesel fuel. As a consequence, glycerin mass is effectively loss for the renewable diesel manufacturing process and this loss could also be taken into consideration. Glycerin hydrogenation consumes additional 3 H atoms for carbon hydrogenation and additional 3 H atoms for oxygen hydrogenation into 3 molecules of water. In summary, each tri-glyceride molecule consumes 9 H atoms for each fatty acid and additional 2 H atoms to hydrogenate 1/3 of glycerin (11 H atoms instead of 5 used in the paper and the mass of glycerin loss).



Conclusion:

Both methods used to calculate energy derived from renewable portion of the raw materials are correct and coherent with the chemical principles and thermodynamics. This white paper analysis is a solid contribution to understanding challenges faced when equivalence value is determined for each advanced renewable fuel. The selection of oleic acid in this white paper provides a higher equivalence value for RD and SAF compared to biodiesel as opposed to other fatty acids which could reasonably have been selected and are present in the most common feedstocks. This demonstrates that the authors have taken a conservative approach in their calculations.

Thank you for opportunity to comment on this valuable white paper.

Best Regards,

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