# ***Equivalence Value (EV) Determination for Biodiesel, Renewable Diesel, and Sustainable Aviation Fuel (SAF) from Fats and Oils*** [1]

## Introduction:

Equivalence value or EV are used by EPA to compare renewable energy content of all the advanced biofuels against ethanol on a volumetric basis. The EV formula considers the renewable content of a renewable fuel in comparison to that for ethanol, and the energy content of the renewable fuel relative to that of ethanol. Therefore, the formula used by EPA for calculating the EV is:

$EV = (R_{RF}/ R_{Eth}) \times (EC_{RF}/ EC_{Eth})$

Where,

EV = Equivalence Value for the renewable fuel
$R_{RF}$ = Renewable content of the renewable fuel, in percent
$R_{Eth}$ = Renewable content of ethanol, in percent
$EC_{RF}$ = Energy content of the renewable fuel, in Btu per Gallon (LHV)
$EC_{Eth}$ = Energy content of ethanol, in Btu per Gallon (LHV)

R is the measure of that portion of a single renewable fuel molecule which can be considered to have come from the renewable source. Since R is being combined with relative energy content in the formula above, the value of R cannot be based on the mass fraction of the renewable content. This paper determines the EVs of biodiesel, renewable diesel and SAF using EPA's formula and using two different approaches to account for renewable energy content fraction or R in these fuels.

## ***Equivalence Value Calculation Based on Heat of Combustion***

The energy content of a fuel can be determined using heat of combustion values of the overall fuel molecule.[i] In calculating Equivalence Values (EV) of renewable fuel, R is the percentage renewable content of the renewable fuel. More specifically, R is the measure of the fraction of energy content of the fuel molecule released from the renewable part of molecule and should not include the energy released due to the non-renewable part of the molecule. Hence the heat of combustion of the non-renewable atoms in each fuel molecule should not be taken into account while determining the R values.

During the production process of renewable diesel (RD) and sustainable aviation fuel (SAF) via HEFA route from renewable molecules like vegetable oil, the non-renewable H2 molecule reacts with oxygen containing sites and the naturally occurring C=C bond in the molecule. As a result, the naturally occurring C=O, C-OH, and C=C bonds get broken and new C-H gets formed in the RD molecule. For one molecule of fatty acid from natural source as represented by oleic acid, 5 hydrogen atoms get added per molecule of renewable diesel (three H atoms to the terminal Carbon and two H atoms to Carbon $\pi$ bonds) and 6

[1] Cite this article as *"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*

hydrogen atoms per molecule of SAF. In the case of biodiesel one atom of C and O and 3 H atoms get added per molecule from non-renewable methanol molecule.

## ***Energy Content, R, and EV Value Calculation for Biodiesel:***

Biodiesel modeled as C18 Methyl Ester produced from oleic acid esterification.

The combustion equation of BD is as below:

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

Heat of Combustion Rxn = Total Energies of Bond Formation in Product – Total Energies of Bond Formation in Reactant

= (19x2x799 + 18x2x463) – (22966 + 26x495) kJ/mol
= 11, 194 kJ/mol
= (11, 350 x 1000x 3.76 x 0.88) / (1.055 x 296.5) BTU/Gal
= 118,400 BTU/Gal (Vs 118,000 Btu/Gal EPA)

Non-Renewable Fraction in BD is $CH_3O$. The combustion equation for non-renewable part is

$CH_3O + 1.25\ O_2 = CO_2 + 1.5\ H_2O$

Heat of Combustion = (2x799 + 1.5x2x463) – (3*413+358 + 1.25x495) kJ/mol
= 771.3 kJ/mol

R = (1- Heat of combustion from Non Renewable fraction/ Total heat of combustion of fuel)
= (1- 771.3/11,194) *100 %
= 93.11%

EQ Value = (93.11/97.2) * (118,400/77000)
BD EQ value = 1.47 RIN value

## ***Energy Content, R, and EV Value Calculation for Renewable Diesel (RD):***

Renewable Diesel modeled as C18 Alkane as a product from oleic acid by deoxygenation.

The combustion equation of RD is as below:

$C_{18}H_{38} + 27.5O_2 = 18\ CO_2 + 19\ H_2O$

Heat of Combustion Rxn = Total Energies of Bond Formation in Product – Total Energies of Bond Formation in Reactant

= (18x2x799 + 19x2x463) – (18*348+38*413 + 27.5x495) kJ/mol
= 11,135.5 kJ/mol
= (11, 135.5 x 1000x 3.76 x 0.78) / (1.055 x 254) BTU/Gal
= 121,873 BTU/Gal (Vs 122,000 Btu/Gal EPA)

Non-Renewable Fraction in RD is 5 H atoms. The combustion equation for non-renewable part is

2.5 H2 + 1.25 O2 = 2.5 H2O

Heat of Combustion = (5x463) – (2.5x432+1.25x495) kJ/mol
= 616.3 kJ/mol

R = (1- Heat of combustion from Non Renewable fraction/ Total heat of combustion of fuel)
= (1- 616.3/11,135) *100 %
= 94.47%

EQ Value = (94.47/97.2) * (121,873/77000)

RD EQ value = 1.53 RIN value

***Energy Content, R, and EV Value Calculation for SAF:***

SAF modeled as C12 Alkane as a product from oleic acid by deoxygenation and cracking.

The combustion equation of RD is as below:

C12H26 + 18.5O2 = 12 CO2 + 13 H2O

Heat of combustion for this reaction is: 7,491 Kj/mol

Non-Renewable Fraction in SAF is 6 H atoms. The combustion equation for non-renewable part is

3 H2 + 1.5 O2 = 3 H2O

Heat of Combustion = (6x463) – (3x432+1.5x495) kJ/mol
= 739.5 kJ/mol

R = (1- Heat of combustion from Non Renewable fraction/ Total heat of combustion of fuel)
= (1- 739.5/7,491) *100 %
= 90.13%

EQ Value = (90.13/97.2) * (115611/77000)

EQ value = 1.39 RIN value (or 1.41 based on energy content per EPA)

**Table 1: Calculated Equivalence Values of BD, RD, and SAF Using Heat of Combustion**

| *Fuel* | *Modeled Energy content, Btu/gal* | *Energy Content per EPA* | *Current EV* | *R (Heat of Combustion based)* | *EV (Heat of Combustion based)* |
|---|---|---|---|---|---|
| Biodiesel | 118,400 | 118,000 | 1.54 | 93.11% | 1.47 (~1.5) |
| Renewable Diesel | 121,900 | 122,000 | 1.69 | 94.47% | 1.53(~1.5) |
| SAF | 115,600 | 117,210 | 1.6* | 90.26% | 1.41(~1.4) |

**1.6 used as a surrogate for illustration*

## *Equivalence Value Calculation Based on Bond Energy Fraction*

The energy content of the fuel molecule is the measure of the total bond energy of all the atoms in the molecules that take part in combustion.[ii] For the purpose of calculating R, the energy released due to the bonds involving non-renewable portion of the molecules (H atoms in case of RD and SAF and CH3O for BD) should not be considered as renewable energy fraction of the molecule. Therefore the energy of the bonds formed with non-renewable portion in the renewable molecule (C-H in RD and SAF) should be considered as non-renewable energy fraction of the total energy content of the renewable molecule. The calculations below demonstrate the R value and corresponding EV calculation based on the bond energy fraction of bonds involving non-renewable atoms in the fuel molecule which were not present in the original renewable feed stock molecule.

### Renewable Diesel: Modeled as C18 Alkane as a product from oleic acid by deoxygenation

Energy from C18 Alkane = 17 C-C bonds + 38 C-H bonds
= 17* 348 + 38 * 413
=21,610 KJ/Mol

Non-Renewable Content/Bonds = 2 C-H bonds (From saturation) + 3 C-H bonds (Terminal carbon CH3)
= 5 * 413
=2065 KJ of non-renewable energy

R = (21,610 – 2065) * 100/21,610
R = 90.44%

EQ Value = (90.44/97.2) * (122000/77000)
RD EQ value = 1.47 RIN value

### SAF: Modeled as C12 Alkane as a product from oleic acid by deoxygenation and cracking

Total Bond Energy from C12 Alkane = 11 C-C bonds + 26 C-H bonds
= 11* 348 + 26 * 413
=14,566 KJ/Mol

Non-Renewable Content/Bonds = 2 C-H bonds (From saturation) + 4 C-H bonds (Terminal carbon CH3)
= 6 * 413
=2478 KJ of non-renewable energy

R = (14,566 – 2478) * 100/14,566
R = 82.99%

EQ Value = (82.99/97.2) * (115,611/77000)
SAF EQ value = 1.28 RIN value (or 1.43 based on energy content per EPA)

### Biodiesel: Modeled as C18 Methyl Ester produced from oleic acid esterification

Energy from C18 Methyl Ester = 1 C=C bond + 16 C-C bonds + 1 C=O bond + 2 C-O bonds + 37 C-H bonds
= 1*602 + 16 * 348 + 1 * 799 + 2 * 358 + 37 * 413
= 22,966 KJ/Mol

Non-Renewable Content/Bonds = 1 C-O + 3 C-H (Terminal carbon CH3)
= 1 * 358 + 3 * 413
=1,597 KJ of non-renewable energy

R = (22,966 – 1,597) *100/22,966
R = 93.05%

EQ Value = (93.05/97.2) * (118,000/77000)
BD EQ value = 1.47 RIN value

**Table 2: Calculated Equivalence Values of BD, RD, and SAF Using Bond Energy**

| *Fuel* | *Current R* | *Energy Content Btu/gal* | *Current EV* | *Bond Energy Based R* | *Bond Energy Based EV* |
|---|---|---|---|---|---|
| Biodiesel | 94.20% | 118,000 | 1.54 | 93.03% | 1.47 (~1.5) |
| Renewable Diesel | 100% | 122,000 | 1.69 | 90.44% | 1.47 (~1.5) |
| SAF | NA | 117,200 | 1.6 | 82.99% | 1.3 |

## ***References:***


[i] https://www.engineeringtoolbox.com/standard-heat-of-combustion-energy-content-d_1987.html

[ii] Bond Energies - Chemistry LibreTexts

## *Appendix1: Bond Energy Values in Kj/Mol*

| *Bond Type* | *Energy* |
|---|---|
| C-H | 413 |
| C-C | 348 |
| C-O | 358 |
| C=O | 799 |
| C=C | 602 |
| H-H | 432 |
| O=O | 495 |
| O-H | 463 |

## *Appendix2: Simplified Molecular Structure for Bond Energy Calculations*

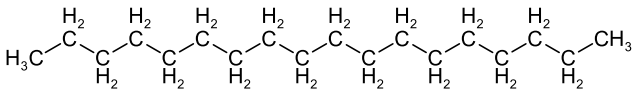

**Figure 1. Molecular Structure of RD molecule (C18)**

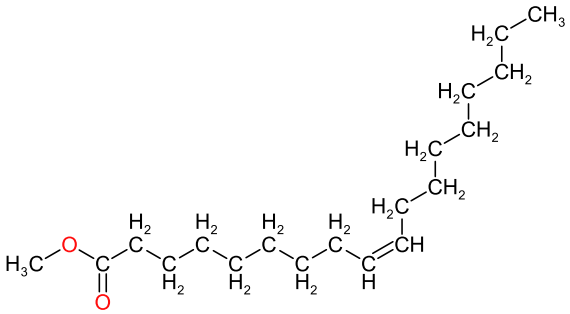

**Figure 2. Molecular Structure of BD molecule (Methyl Oleate)**

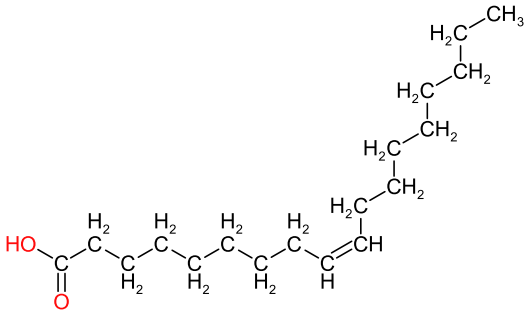

**Figure 3. Molecular Structure of Oleic acid**