

# Liquid, hydrocarbon fuel (e.g. diesel) [insert into Title-V Permits]

Note that **wt% $S_{fuel}$** , **wt% $C_{fuel}$** , and **wt% $H_{fuel}$**  must total 100%.

Calculate **SO<sub>2</sub> concentration** using the calculations below:

$$\begin{aligned}
 A &= 31,200 \times [\text{wt}\%S_{fuel}] = 31,200 \times \underline{\hspace{2cm}} \% = \underline{\hspace{2cm}} \\
 B &= 0.148 \times [\text{wt}\%S_{fuel}] = 0.148 \times \underline{\hspace{2cm}} \% = \underline{\hspace{2cm}} \\
 C &= 0.396 \times [\text{wt}\%C_{fuel}] = 0.396 \times \underline{\hspace{2cm}} \% = \underline{\hspace{2cm}} \\
 D &= 0.933 \times [\text{wt}\%H_{fuel}] = 0.933 \times \underline{\hspace{2cm}} \% = \underline{\hspace{2cm}} \\
 E &= B + C + D = \underline{\hspace{2cm}} + \underline{\hspace{2cm}} + \underline{\hspace{2cm}} = \underline{\hspace{2cm}} \\
 F &= 21\% - [\text{vol}\%_{dry}O_{2, exhaust}] = 21\% - \underline{\hspace{2cm}} \% = \underline{\hspace{2cm}} \% \\
 G &= [\text{vol}\%_{dry}O_{2, exhaust}] \div F = \underline{\hspace{2cm}} \% \div \underline{\hspace{2cm}} \% = \underline{\hspace{2cm}} \\
 H &= 1 + G = 1 + \underline{\hspace{2cm}} = \underline{\hspace{2cm}} \\
 I &= E \times H = \underline{\hspace{2cm}} \times \underline{\hspace{2cm}} = \underline{\hspace{2cm}} \\
 \text{SO}_2 \text{ concentration} &= A \div I = \underline{\hspace{2cm}} \div \underline{\hspace{2cm}} = \underline{\hspace{2cm}} \text{ppmv}
 \end{aligned}$$

List of Abbreviations Used in this Permit [insert into Section 1 of Title-V Permits]

- SO<sub>2</sub> concentration ...exhaust-gas, volumetric, dry SO<sub>2</sub> concentration, 10<sup>6</sup> X gmole-SO<sub>2</sub>/gmole-air<sub>exhaust, dry</sub> (i.e. ppmv)
- vol%<sub>dry</sub>O<sub>2, exhaust</sub> ....volume percent O<sub>2</sub> of the dry exhaust gas, 100% X gmole-O<sub>2</sub>/gmole-dryexhaust
- wt% $C_{fuel}$ .....dry weight-percent carbon of a fuel, 100% X g-C/g-fuel
- wt% $H_{fuel}$  .....dry weight-percent hydrogen of a fuel, 100% X g-H/g-fuel
- wt% $S_{fuel}$  .....dry weight-percent sulfur of a fuel, 100% X g-S/g-fuel

ATTACHMENT 1 [insert into Title-V Statements of Bases]

Computational Basis is 100 *gram* liquid, hydrocarbon fuel (e.g. diesel)

**NOMENCLATURE (in alphabetical order):**

- $C_{\text{fuel}}$  = number of gram-moles of the carbon part of a fuel, *gmole-C*  
 $H_{2,\text{fuel}}$  = number of gram-moles of the "equivalent  $H_2$ " part of a fuel, *gmole- $H_2$*   
 $\text{mol-CO}_2$  = amount of  $\text{CO}_2$  in the exhaust gas, *gmole- $\text{CO}_2$*   
 $\text{mol-H}_2\text{O}$  = amount of  $\text{H}_2\text{O}$  in the exhaust gas supplied by the free hydrogen in the fuel, excluding water from the fuel and excluding water from the ambient air, *gmole- $\text{H}_2\text{O}$*   
 $\text{mol-O}_2$  = amount of  $\text{O}_2$  in the exhaust gas, *gmole- $\text{O}_2$*   
 $\text{mol-N}_2$  = amount of  $\text{N}_2$  in the exhaust gas, *gmole- $\text{N}_2$*   
 $\text{mol-SO}_2$  = amount of  $\text{SO}_2$  in the exhaust gas, *gmole- $\text{SO}_2$*   
 $N_{2,\text{C}}$  = ambient  $\text{N}_2$  accompanying  $\text{O}_{2,\text{C}}$  for combustion, *gmole- $\text{N}_2$*   
 $N_{2,\text{H}_2}$  = ambient  $\text{N}_2$  accompanying  $\text{O}_{2,\text{H}_2}$  for combustion, *gmole- $\text{N}_2$*   
 $N_{2,\text{S}}$  = ambient  $\text{N}_2$  accompanying  $\text{O}_{2,\text{S}}$  for combustion, *gmole- $\text{N}_2$*   
 $\text{O}_{2,\text{C}}$  = ambient  $\text{O}_2$  used to combust the carbon part of a fuel, *gmole- $\text{O}_2$*   
 $\text{O}_{2,\text{H}_2}$  = ambient  $\text{O}_2$  used to combust the  $\text{H}_2$  part of a fuel, *gmole- $\text{O}_2$*   
 $\text{O}_{2,\text{S}}$  = ambient  $\text{O}_2$  used to combust the sulfur part of a fuel, *gmole- $\text{O}_2$*   
 $S_{\text{fuel}}$  = number of gram-moles of the sulfur part of a fuel, *gmole-S*  
 $\text{SO}_2\text{concentration}$  = exhaust-gas, volumetric, dry  $\text{SO}_2$  concentration,  $10^6 \times \text{gmole-}SO_2/\text{gmole-air}_{\text{exhaust,dry}}$  (i.e. *ppmv*)  
 $\text{total-N}_2$  = amount of ambient  $\text{N}_2$  accompanying  $\text{total-O}_2$  for combustion, *gmole- $\text{N}_2$*   
 $\text{total-O}_2$  = total amount of ambient  $\text{O}_2$  for combustion plus the excess  $\text{O}_2$ , *gmole- $\text{O}_2$*   
 $\text{vol}\% \text{dry O}_{2,\text{exhaust}}$  = volume percent  $\text{O}_2$  of the dry exhaust gas,  $100\% \times \text{gmole-}O_2/\text{gmole-air}_{\text{exhaust,dry}}$   
 $\text{wt}\% C_{\text{fuel}}$  = dry weight-percent carbon of a fuel,  $100\% \times g-C/g\text{-fuel}$   
 $\text{wt}\% H_{\text{fuel}}$  = dry weight-percent hydrogen of a fuel,  $100\% \times g-H/g\text{-fuel}$   
 $\text{wt}\% S_{\text{fuel}}$  = dry weight-percent sulfur of a fuel,  $100\% \times g-S/g\text{-fuel}$

Note 1: Volume percent and mole percent are equivalent, but neither volume percent nor mole percent are equivalent to weight percent.

Note 2:  $\text{wt}\% H_{\text{fuel}}$  is equivalent to (defined by analogy)  $\text{wt}\% H_{2,\text{fuel}}$ .

**OUTPUT:**

## 1. **SO<sub>2</sub>concentration** on a dry basis for the combustion of diesel fuel

Note 3: Although **SO<sub>2</sub>concentration** is on a dry basis, **mol-H<sub>2</sub>O** is still an important dummy variable that needed to be calculated because **N<sub>2,H<sub>2</sub></sub>** that accompanies **O<sub>2,H<sub>2</sub></sub>** dilutes **SO<sub>2</sub>concentration**.

## INPUTS:

1. **wt%S<sub>fuel</sub>**
2. **wt%C<sub>fuel</sub>**
3. **wt%H<sub>fuel</sub>**
4. **vol% dryO<sub>2,exhaust</sub>**

Note 4: **wt%S<sub>fuel</sub>**, **wt%C<sub>fuel</sub>**, and **wt%H<sub>fuel</sub>** must total 100% by **assumption 2**.

## ASSUMPTIONS:

1. Any and all water in the diesel fuel and/or in the ambient air is inert during combustion of the fuel.
2. All diesel fuel only consists of carbon, hydrogen, and sulfur. Any and all water in the diesel fuel is negligible because the output is on a dry basis and because of **assumption 1**.
3. Ambient air— only O<sub>2</sub> and N<sub>2</sub>—has 3.76 moles of N<sub>2</sub> per mole of O<sub>2</sub>. Therefore, there are 4.76 moles of air per mole of O<sub>2</sub>. Any and all water in the ambient air is negligible because the output is on a dry basis and because of **assumption 1**.
4. The only source of O<sub>2</sub> for combustion is from the ambient air.
5. Perfect combustion is combustion that is complete and clean with no soot, PM, HC, VOC, CO, and NO<sub>x</sub> in the exhaust gas. Therefore, **vol% dryO<sub>2,exhaust</sub>** must be greater than or equal to zero while all N<sub>2</sub> and all excess O<sub>2</sub> is inert in the combustion process.
6. For regulatory purposes (i.e. the purpose of developing this output), all of the sulfur in the diesel fuel forms SO<sub>2</sub> in the exhaust gas and none of the sulfur is removed by from the exhaust gas.

Note 5: **Assumptions 1 – 5** are commonly accepted assumptions for combustion analysis. **Assumption 6** is based on 18 AAC 50.055(c), which states, “sulfur-compound emissions expressed as sulfur dioxide.”

## SOLUTION:

Note 6: **Eqs. (1-1) – (1-3)** are definitions of variables as functions of inputs

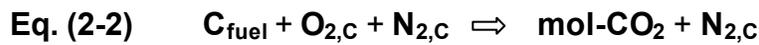
and molecular weights, whereas the 100 *grams* (from the 100-*gram* computational basis) and the 100% from the weight percents cancel each other. (These units were not shown).

$$\text{Eq. (1-1)} \quad \mathbf{S_{fuel} = \text{dummy-fuel} \times \text{wt}\%S_{fuel} / 32.06}$$

$$\text{Eq. (1-2)} \quad \mathbf{C_{fuel} = \text{dummy-fuel} \times \text{wt}\%C_{fuel} / 12.01}$$

$$\text{Eq. (1-3)} \quad \mathbf{H_{2,fuel} = \text{dummy-fuel} \times \text{wt}\%H_{fuel} / 2.016}$$

Note 7: **Eqs. (2-1) – (2-3)** are the stoichiometric combustion equations for sulfur, carbon, and hydrogen, whereas the right arrows show exothermic chemical reactions. **Eq. (2-4)** shows that the O<sub>2</sub> supplied by the ambient air minus the O<sub>2</sub> consumed in **eqs. (2-1) – (2-3)** is the O<sub>2</sub> in the exhaust gas. **Eq. (2-5)** shows that the N<sub>2</sub> supplied by the ambient air is the N<sub>2</sub> in the exhaust gas without any chemical change (e.g. zero NO<sub>x</sub> from **assumption 4**). The double arrows in **eqs. (2-4) – (2-5)** show no chemical reactions (i.e. inert from **assumption 5**).



Note 8: **Eqs. (3-1) – (3-3)** are corollaries of **eqs. (2-1) – (2-3)**, respectively. **Eq. (3-4)** is a corollary of **eq. (2-4)** and of **eqs. (3-1) – (3-3)**. **Eq. (3-5)** is a corollary of **eq. (2-5)**, of **assumption 3**, and of **eq. (3-4)**.

$$\text{Eq. (3-1)} \quad \mathbf{\text{mol-SO}_2 = S_{fuel} = O_{2,S}}$$

$$\text{Eq. (3-2)} \quad \mathbf{\text{mol-CO}_2 = C_{fuel} = O_{2,C}}$$

$$\text{Eq. (3-3)} \quad \mathbf{\text{mol-H}_2\text{O} = H_{2,fuel} = 2 \times O_{2,H2}}$$

$$\text{Eq. (3-4)} \quad \mathbf{\text{mol-O}_2 = \text{total-O}_2 - O_{2,S} - O_{2,C} - O_{2,H2} = \text{total-O}_2 - \text{mol-SO}_2 - \text{mol-CO}_2 - (0.5 \times \text{mol-H}_2\text{O})}$$

$$\text{Eq. (3-5)} \quad \mathbf{\text{mol-N}_2 = \text{total-N}_2 = 3.76 \times \text{total-O}_2 = 3.76 \times (\text{mol-SO}_2 + \text{mol-CO}_2 + (0.5 \times \text{mol-H}_2\text{O}) + \text{mol-O}_2) = (3.76 \times \text{mol-SO}_2) + (3.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) + (3.76 \times \text{mol-O}_2)}$$

Note 9: **Eq. (4-1)** is the definition of **vol%<sub>dry</sub>O<sub>2,exhaust</sub>**. **Eq. (4-2)** is the solution of **eq. (4-1)** as a function of **mol-O<sub>2</sub>**. **Eq. (4-3)** is the result of substituting **mol-N<sub>2</sub>** from **eq. (3-5)** into **eq. (4-2)**. **Eq. (4-4)** is the result of combining terms on the right side of **eq. (4-3)**. **Eq. (4-5)** is the result of moving the **mol-O<sub>2</sub>** term on the right side of **eq. (4-4)** to the left side and then factoring out **mol-O<sub>2</sub>**. **Eq. (4-6)** is the result of multiplying both sides of **eq. (4-5)** by “100% - **vol%<sub>dry</sub>O<sub>2,exhaust</sub>**.” **Eq. (4-7)** is the result of combining the two **vol%<sub>dry</sub>O<sub>2,exhaust</sub>** terms on the left side of **eq. (4-6)** and isolating the **mol-O<sub>2</sub>** term on the left side by division. **Eq. (4-8)** is the result of factoring out a constant in the denominator of **eq. (4-7)**.

$$\text{Eq. (4-1)} \quad \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}} = 100\% \times \text{mol-O}_2 / (\text{mol-SO}_2 + \text{mol-CO}_2 + \text{mol-O}_2 + \text{mol-N}_2)$$

$$\text{Eq. (4-2)} \quad \text{mol-O}_2 = \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}} \times (\text{mol-SO}_2 + \text{mol-CO}_2 + \text{mol-N}_2) / (100\% - \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}})$$

$$\text{Eq. (4-3)} \quad \text{mol-O}_2 = \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}} \times (\text{mol-SO}_2 + \text{mol-CO}_2 + ((3.76 \times \text{mol-SO}_2) + (3.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) + (3.76 \times \text{mol-O}_2))) / (100\% - \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}})$$

$$\text{Eq. (4-4)} \quad \text{mol-O}_2 = \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}} \times ((4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) + (3.76 \times \text{mol-O}_2)) / (100\% - \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}})$$

$$\text{Eq. (4-5)} \quad \text{mol-O}_2 \times (1 - (3.76 \times \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}} / (100\% - \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}}))) = \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}} \times ((4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O})) / (100\% - \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}})$$

$$\text{Eq. (4-6)} \quad \text{mol-O}_2 \times ((100\% - \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}}) - (3.76 \times \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}})) = \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}} \times ((4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}))$$

$$\text{Eq. (4-7)} \quad \text{mol-O}_2 = \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}} \times ((4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O})) / (100\% - (4.76 \times \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}}))$$

$$\text{Eq. (4-8)} \quad \text{mol-O}_2 = \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}} \times ((4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O})) / (4.76 \times (21\% - \text{vol\%}_{\text{dry}}\text{O}_{2,\text{exhaust}}))$$

Note 10: **Eq. (5-1)** is the definition of **SO<sub>2</sub> concentration**. **Eq. (5-2)** is the result of substituting **mol-N<sub>2</sub>** from **eq. (3-5)** into **eq. (5-1)**. **Eq. (5-3)** is the result of combining terms on the right side of **eq. (5-2)**. **Eq. (5-4)** is the result of substituting **mol-O<sub>2</sub>** from **eq. (4-8)** into **eq. (5-3)**. **Eq. (5-5)** is the result of combining terms in **eq. (5-4)**.

**Eq. (5-1)** 
$$\text{SO}_2\text{concentration} = 10^6 \times \text{mol-SO}_2 / (\text{mol-SO}_2 + \text{mol-CO}_2 + \text{mol-O}_2 + \text{mol-N}_2)$$

**Eq. (5-2)** 
$$\text{SO}_2\text{concentration} = 10^6 \times \text{mol-SO}_2 / (\text{mol-SO}_2 + \text{mol-CO}_2 + \text{mol-O}_2 + (3.76 \times \text{mol-SO}_2) + (3.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) + (3.76 \times \text{mol-O}_2))$$

**Eq. (5-3)** 
$$\text{SO}_2\text{concentration} = 10^6 \times \text{mol-SO}_2 / ((4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) + (4.76 \times \text{mol-O}_2))$$

**Eq. (5-4)** 
$$\text{SO}_2\text{concentration} = 10^6 \times \text{mol-SO}_2 / ((4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) + (\text{vol}\%_{\text{dry O}_2, \text{exhaust}} \times ((4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}))) / (21\% - \text{vol}\%_{\text{dry O}_2, \text{exhaust}}))$$

**Eq. (5-5)** 
$$\text{SO}_2\text{concentration} = 10^6 \times \text{mol-SO}_2 / ((1 + (\text{vol}\%_{\text{dry O}_2, \text{exhaust}} / (21\% - \text{vol}\%_{\text{dry O}_2, \text{exhaust}}))) \times ((4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O})))$$

Note 11: **Eqs. (6-1) – (6-2)** were derived such that the **eq. (6-2)** depends on only constants and inputs. **Eq. (6-1)** is the result of substituting **mol-SO<sub>2</sub>**, **mol-CO<sub>2</sub>**, and **mol-H<sub>2</sub>O** into **eqs. (3-1) – (3-3)** and then substituting **S<sub>fuel</sub>**, **C<sub>fuel</sub>**, and **H<sub>2, fuel</sub>** into **eqs. (1-1) – (1-3)**. **Eq. (6-2)** is the result of combining some constants in **eq. (6-1)**.

**Eq. (6-1)** 
$$\text{SO}_2\text{concentration} = (10^6 \times \text{wt}\% \mathbf{S}_{\text{fuel}} / 32.06) / ((1 + (\text{vol}\%_{\text{dry O}_2, \text{exhaust}} / (21\% - \text{vol}\%_{\text{dry O}_2, \text{exhaust}}))) \times ((4.76 \times \text{wt}\% \mathbf{S}_{\text{fuel}} / 32.06) + (4.76 \times \text{wt}\% \mathbf{C}_{\text{fuel}} / 12.01) + (1.88 \times \text{wt}\% \mathbf{H}_{\text{fuel}} / 2.016)))$$

**Eq. (6-2)** 
$$\text{SO}_2\text{concentration} = (31,200 \times \text{wt}\% \mathbf{S}_{\text{fuel}}) / ((1 + (\text{vol}\%_{\text{dry O}_2, \text{exhaust}} / (21\% - \text{vol}\%_{\text{dry O}_2, \text{exhaust}}))) \times ((0.148 \times \text{wt}\% \mathbf{S}_{\text{fuel}}) + (0.396 \times \text{wt}\% \mathbf{C}_{\text{fuel}}) + (0.933 \times \text{wt}\% \mathbf{H}_{\text{fuel}})))$$

Note 12: **Eq. (6-2)** is relatively long and could confuse some people needing to use this equation. To resolve this potential problem, **eq. (6-2)** was simplified in the permit by breaking it into ten simple steps.