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

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

Calculate $\mathbf{SO_2}$ **concentration** using the calculations below:

$$\boldsymbol{A} = 31{,}200 \times [\mathbf{wt\%S_{fuel}}] = 31{,}200 \times \_\_\_\_\_\_\ \% = \_\_\_\_\_\_$$

$$\boldsymbol{B} = 0.148 \times [\mathbf{wt\%S_{fuel}}] = 0.148 \times \_\_\_\_\_\_\ \% = \_\_\_\_\_\_$$

$$\boldsymbol{C} = 0.396 \times [\mathbf{wt\%C_{fuel}}] = 0.396 \times \_\_\_\_\_\_\ \% = \_\_\_\_\_\_$$

$$\boldsymbol{D} = 0.933 \times [\mathbf{wt\%H_{fuel}}] = 0.933 \times \_\_\_\_\_\_\ \% = \_\_\_\_\_\_$$

$$\boldsymbol{E} = \boldsymbol{B} + \boldsymbol{C} + \boldsymbol{D} = \_\_\_\_\_\_ + \_\_\_\_\_\_ + \_\_\_\_\_\_ = \_\_\_\_\_\_$$

$$\boldsymbol{F} = 21\% - [\mathbf{vol\%_{dry}O_{2,\ exhaust}}] = 21\% - \_\_\_\_\_\_\ \% = \_\_\_\_\_\_\ \%$$

$$\boldsymbol{G} = [\mathbf{vol\%_{dry}O_{2,\ exhaust}}] \div \boldsymbol{F} = \_\_\_\_\_\_\ \% \div \_\_\_\_\_\_\ \% = \_\_\_\_\_\_$$

$$\boldsymbol{H} = 1 + \boldsymbol{G} = 1 + \_\_\_\_\_\_ = \_\_\_\_\_\_$$

$$\boldsymbol{I} = \boldsymbol{E} \times \boldsymbol{H} = \_\_\_\_\_\_ \times \_\_\_\_\_\_ = \_\_\_\_\_\_$$

$$\mathbf{SO_2\,concentration} = \mathbf{A} \div \mathbf{I} = \_\_\_\_\_\_ \div \_\_\_\_\_\_ = \_\_\_\_\_\_\mathbf{ppmv}$$

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

SO_2concentration ...exhaust-gas, volumetric, dry SO_2 concentration, 10^6 X *gmole-*SO_2*/gmole-air*$_{exhaust,dry}$ (i.e. *ppmv*)

$vol\%_{dry}O_{2,exhaust}$ ....volume percent O_2 of the dry exhaust gas, 100% X *gmole-*O_2*/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):

- $\mathbf{C_{fuel}}$ = number of gram-moles of the carbon part of a fuel, *gmole-C*
- $\mathbf{H_{2,fuel}}$ = number of gram-moles of the "equivalent H_2" part of a fuel, *gmole-H_2*
- **mol-CO_2** = amount of CO_2 in the exhaust gas, *gmole-CO_2*
- **mol-H_2O** = amount of H_2O 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-H_2O*
- **mol-O_2** = amount of O_2 in the exhaust gas, *gmole-O_2*
- **mol-N_2** = amount of N_2 in the exhaust gas, *gmole-N_2*
- **mol-SO_2** = amount of SO_2 in the exhaust gas, *gmole-SO_2*
- $\mathbf{N_{2,C}}$ = ambient N_2 accompanying $\mathbf{O_{2,C}}$ for combustion, *gmole-N_2*
- $\mathbf{N_{2,H2}}$ = ambient N_2 accompanying $\mathbf{O_{2,H2}}$ for combustion, *gmole-N_2*
- $\mathbf{N_{2,S}}$ = ambient N_2 accompanying $\mathbf{O_{2,S}}$ for combustion, *gmole-N_2*
- $\mathbf{O_{2,C}}$ = ambient O_2 used to combust the carbon part of a fuel, *gmole-O_2*
- $\mathbf{O_{2,H2}}$ = ambient O_2 used to combust the H_2 part of a fuel, *gmole-O_2*
- $\mathbf{O_{2,S}}$ = ambient O_2 used to combust the sulfur part of a fuel, *gmole-O_2*
- $\mathbf{S_{fuel}}$ = number of gram-moles of the sulfur part of a fuel, *gmole-S*
- **SO_2concentration** = exhaust-gas, volumetric, dry SO_2 concentration, 10^6 X *gmole-SO_2/gmole-air$_{exhaust,dry}$* (i.e. *ppmv*)
- **total-N_2** = amount of ambient N_2 accompanying **total-O_2** for combustion, *gmole-N_2*
- **total-O_2** = total amount of ambient O_2 for combustion plus the excess O_2, *gmole-O_2*
- **vol%$_{dry}$$O_{2,exhaust}$** = volume percent O_2 of the dry exhaust gas, 100*% X gmole-O_2/gmole-air$_{exhaust,dry}$*
- **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*

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

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

OUTPUT:

1. **SO_2concentration** on a dry basis for the combustion of diesel fuel

Note 3: Although **SO_2concentration** is on a dry basis, **mol-H_2O** is still an important dummy variable that needed to be calculated because **$N_{2,H2}$** that accompanies **$O_{2,H2}$** dilutes **SO_2concentration**.

INPUTS:

1. **wt%S_{fuel}**
2. **wt%C_{fuel}**
3. **wt%H_{fuel}**
4. **vol%$_{dry}O_{2,exhaust}$**

Note 4: **wt%S_{fuel}**, **wt%C_{fuel}**, and **wt%H_{fuel}** 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_2 and N_2—has 3.76 moles of N_2 per mole of O_2. Therefore, there are 4.76 moles of air per mole of O_2. 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_2 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_x in the exhaust gas. Therefore, **vol%$_{dry}O_{2,exhaust}$** must be greater than or equal to zero while all N_2 and all excess O_2 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_2 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).

Eq. (1-1) $\mathbf{S_{fuel}}$ = **dummy-fuel** X **wt%**$\mathbf{S_{fuel}}$ / 32.06

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

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

<u>Note 7</u>: **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_2 supplied by the ambient air minus the O_2 consumed in **eqs. (2-1) – (2-3)** is the O_2 in the exhaust gas. **Eq. (2-5)** shows that the N_2 supplied by the ambient air is the N_2 in the exhaust gas without any chemical change (e.g. zero NO_x from **assumption 4**). The double arrows in **eqs. (2-4) – (2-5)** show no chemical reactions (i.e. inert from **assumption 5**).

Eq. (2-1) $\mathbf{S_{fuel} + O_{2,S} + N_{2,S} \Rightarrow mol\text{-}SO_2 + N_{2,S}}$

Eq. (2-2) $\mathbf{C_{fuel} + O_{2,C} + N_{2,C} \Rightarrow mol\text{-}CO_2 + N_{2,C}}$

Eq. (2-3) $\mathbf{H_{2,fuel} + O_{2,H2} + N_{2,H2} \Rightarrow mol\text{-}H_2O + N_{2,H2}}$

Eq. (2-4) $\mathbf{total\text{-}O_2 - O_{2,S} - O_{2,C} - O_{2,H2} \Leftrightarrow mol\text{-}O_2}$

Eq. (2-5) $\mathbf{total\text{-}N_2 \Leftrightarrow mol\text{-}N_2}$

<u>Note 8</u>: **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)**.

Eq. (3-1) $\mathbf{mol\text{-}SO_2 = S_{fuel} = O_{2,S}}$

Eq. (3-2) $\mathbf{mol\text{-}CO_2 = C_{fuel} = O_{2,C}}$

Eq. (3-3) $\mathbf{mol\text{-}H_2O = H_{2,fuel}} = 2 \times \mathbf{O_{2,H2}}$

Eq. (3-4) $\mathbf{mol\text{-}O_2 = total\text{-}O_2 - O_{2,S} - O_{2,C} - O_{2,H2} = total\text{-}O_2 - mol\text{-}SO_2 - mol\text{-}CO_2} - (0.5 \times \mathbf{mol\text{-}H_2O})$

Eq. (3-5) $\mathbf{mol\text{-}N_2 = total\text{-}N_2} = 3.76 \times \mathbf{total\text{-}O_2} = 3.76 \times (\mathbf{mol\text{-}SO_2 + mol\text{-}CO_2} + (0.5 \times \mathbf{mol\text{-}H_2O}) + \mathbf{mol\text{-}O_2}) = (3.76 \times \mathbf{mol\text{-}SO_2}) + (3.76 \times \mathbf{mol\text{-}CO_2}) + (1.88 \times \mathbf{mol\text{-}H_2O}) + (3.76 \times \mathbf{mol\text{-}O_2})$

Note 9: **Eq. (4-1)** is the definition of **$vol\%_{dry}O_{2,exhaust}$**. **Eq. (4-2)** is the solution of **eq. (4-1)** as a function of **mol-O_2**. **Eq. (4-3)** is the result of substituting **mol-N_2** 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_2** term on the right side of **eq. (4-4)** to the left side and then factoring out **mol-O_2**. **Eq. (4-6)** is the result of multiplying both sides of **eq. (4-5)** by "100% - **$vol\%_{dry}O_{2,exhaust}$**." **Eq. (4-7)** is the result of combining the two **$vol\%_{dry}O_{2,exhaust}$** terms on the left side of **eq. (4-6)** and isolating the **mol-O_2** 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)**.

Eq. (4-1) $vol\%_{dry}O_{2,exhaust} = 100\% \times \text{mol-}O_2 / (\text{mol-}SO_2 + \text{mol-}CO_2 + \text{mol-}O_2 + \text{mol-}N_2)$

Eq. (4-2) $\text{mol-}O_2 = vol\%_{dry}O_{2,exhaust} \times (\text{mol-}SO_2 + \text{mol-}CO_2 + \text{mol-}N_2) / (100\% - vol\%_{dry}O_{2,exhaust})$

Eq. (4-3) $\text{mol-}O_2 = vol\%_{dry}O_{2,exhaust} \times (\text{mol-}SO_2 + \text{mol-}CO_2 + ((3.76 \times \text{mol-}SO_2) + (3.76 \times \text{mol-}CO_2) + (1.88 \times \text{mol-}H_2O) + (3.76 \times \text{mol-}O_2))) / (100\% - vol\%_{dry}O_{2,exhaust})$

Eq. (4-4) $\text{mol-}O_2 = vol\%_{dry}O_{2,exhaust} \times ((4.76 \times \text{mol-}SO_2) + (4.76 \times \text{mol-}CO_2) + (1.88 \times \text{mol-}H_2O) + (3.76 \times \text{mol-}O_2)) / (100\% - vol\%_{dry}O_{2,exhaust})$

Eq. (4-5) $\text{mol-}O_2 \times (1 - (3.76 \times vol\%_{dry}O_{2,exhaust} / (100\% - vol\%_{dry}O_{2,exhaust}))) = vol\%_{dry}O_{2,exhaust} \times ((4.76 \times \text{mol-}SO_2) + (4.76 \times \text{mol-}CO_2) + (1.88 \times \text{mol-}H_2O)) / (100\% - vol\%_{dry}O_{2,exhaust})$

Eq. (4-6) $\text{mol-}O_2 \times ((100\% - vol\%_{dry}O_{2,exhaust}) - (3.76 \times vol\%_{dry}O_{2,exhaust})) = vol\%_{dry}O_{2,exhaust} \times ((4.76 \times \text{mol-}SO_2) + (4.76 \times \text{mol-}CO_2) + (1.88 \times \text{mol-}H_2O))$

Eq. (4-7) $\text{mol-}O_2 = vol\%_{dry}O_{2,exhaust} \times ((4.76 \times \text{mol-}SO_2) + (4.76 \times \text{mol-}CO_2) + (1.88 \times \text{mol-}H_2O)) / (100\% - (4.76 \times vol\%_{dry}O_{2,exhaust}))$

Eq. (4-8) $\text{mol-}O_2 = vol\%_{dry}O_{2,exhaust} \times ((4.76 \times \text{mol-}SO_2) + (4.76 \times \text{mol-}CO_2) + (1.88 \times \text{mol-}H_2O)) / (4.76 \times (21\% - vol\%_{dry}O_{2,exhaust}))$

Note 10: **Eq. (5-1)** is the definition of **SO_2 concentration**. **Eq. (5-2)** is the result of substituting **mol-N_2** 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_2** from **eq. (4-8)** into **eq. (5-3)**. **Eq. (5-5)** is the result of combining terms in **eq. (5-4)**.

Eq. (5-1) $\mathbf{SO_2concentration} = 10^6 \text{ X } \mathbf{mol\text{-}SO_2} / (\mathbf{mol\text{-}SO_2} + \mathbf{mol\text{-}CO_2} + \mathbf{mol\text{-}O_2} + \mathbf{mol\text{-}N_2})$

Eq. (5-2) $\mathbf{SO_2concentration} = 10^6 \text{ X } \mathbf{mol\text{-}SO_2} / (\mathbf{mol\text{-}SO_2} + \mathbf{mol\text{-}CO_2} + \mathbf{mol\text{-}O_2} + (3.76 \text{ X } \mathbf{mol\text{-}SO_2}) + (3.76 \text{ X } \mathbf{mol\text{-}CO_2}) + (1.88 \text{ X } \mathbf{mol\text{-}H_2O}) + (3.76 \text{ X } \mathbf{mol\text{-}O_2}))$

Eq. (5-3) $\mathbf{SO_2concentration} = 10^6 \text{ X } \mathbf{mol\text{-}SO_2} / ((4.76 \text{ X } \mathbf{mol\text{-}SO_2}) + (4.76 \text{ X } \mathbf{mol\text{-}CO_2}) + (1.88 \text{ X } \mathbf{mol\text{-}H_2O}) + (4.76 \text{ X } \mathbf{mol\text{-}O_2}))$

Eq. (5-4) $\mathbf{SO_2concentration} = 10^6 \text{ X } \mathbf{mol\text{-}SO_2} / ((4.76 \text{ X } \mathbf{mol\text{-}SO_2}) + (4.76 \text{ X } \mathbf{mol\text{-}CO_2}) + (1.88 \text{ X } \mathbf{mol\text{-}H_2O}) + (\mathbf{vol\%_{dry}O_{2,exhaust}} \text{ X } ((4.76 \text{ X } \mathbf{mol\text{-}SO_2}) + (4.76 \text{ X } \mathbf{mol\text{-}CO_2}) + (1.88 \text{ X } \mathbf{mol\text{-}H_2O})) / (21\% - \mathbf{vol\%_{dry}O_{2,exhaust}})))$

Eq. (5-5) $\mathbf{SO_2concentration} = 10^6 \text{ X } \mathbf{mol\text{-}SO_2} / ((1 + (\mathbf{vol\%_{dry}O_{2,exhaust}} / (21\% - \mathbf{vol\%_{dry}O_{2,exhaust}}))) \text{ X } ((4.76 \text{ X } \mathbf{mol\text{-}SO_2}) + (4.76 \text{ X } \mathbf{mol\text{-}CO_2}) + (1.88 \text{ X } \mathbf{mol\text{-}H_2O})))$

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 $\mathbf{mol\text{-}SO_2}$, $\mathbf{mol\text{-}CO_2}$, and $\mathbf{mol\text{-}H_2O}$ into **eqs. (3-1) – (3-3)** and then substituting $\mathbf{S_{fuel}}$, $\mathbf{C_{fuel}}$, and $\mathbf{H_{2,fuel}}$ into **eqs. (1-1) – (1-3)**. **Eq. (6-2)** is the result of combining some constants in **eq. (6-1)**.

Eq. (6-1) $\mathbf{SO_2concentration} = (10^6 \text{ X } \mathbf{wt\%S_{fuel}} / 32.06) / ((1 + (\mathbf{vol\%_{dry}O_{2,exhaust}} / (21\% - \mathbf{vol\%_{dry}O_{2,exhaust}}))) \text{ X } ((4.76 \text{ X } \mathbf{wt\%S_{fuel}} / 32.06) + (4.76 \text{ X } \mathbf{wt\%C_{fuel}} / 12.01) + (1.88 \text{ X } \mathbf{wt\%H_{fuel}} / 2.016)))$

Eq. (6-2) $\mathbf{SO_2concentration} = (31{,}200 \text{ X } \mathbf{wt\%S_{fuel}}) / ((1 + (\mathbf{vol\%_{dry}O_{2,exhaust}} / (21\% - \mathbf{vol\%_{dry}O_{2,exhaust}}))) \text{ X } ((0.148 \text{ X } \mathbf{wt\%S_{fuel}}) + (0.396 \text{ X } \mathbf{wt\%C_{fuel}}) + (0.933 \text{ X } \mathbf{wt\%H_{fuel}})))$

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.