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

Note that \( \text{wt}\% S_{\text{fuel}}, \text{wt}\% C_{\text{fuel}}, \) and \( \text{wt}\% H_{\text{fuel}} \) must total 100%.

Calculate \( \text{SO}_2 \) concentration using the calculations below:

\[
A = 31.200 \times [\text{wt}\% S_{\text{fuel}}] = 31.200 \times \text{______} \% = \text{______}
\]
\[
B = 0.148 \times [\text{wt}\% S_{\text{fuel}}] = 0.148 \times \text{______} \% = \text{______}
\]
\[
C = 0.396 \times [\text{wt}\% C_{\text{fuel}}] = 0.396 \times \text{______} \% = \text{______}
\]
\[
D = 0.933 \times [\text{wt}\% H_{\text{fuel}}] = 0.933 \times \text{______} \% = \text{______}
\]
\[
E = B + C + D = \text{______} + \text{______} + \text{______} = \text{______}
\]
\[
F = 21\% - [\text{vol}\% \text{dry} O_2, \text{exhaust}] = 21\% - \text{______} \% = \text{______} \%
\]
\[
G = [\text{vol}\% \text{dry} O_2, \text{exhaust}] \div F = \text{______} \% \div \text{______} \% = \text{______} \%
\]
\[
H = 1 + G = 1 + \text{______} = \text{______}
\]
\[
I = E \times H = \text{______} \times \text{______} = \text{______}
\]
\[
\text{SO}_2 \text{concentration} = A \div I = \text{______} \div \text{______} = \text{______ppmv}
\]

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

\( \text{SO}_2 \text{concentration} \) ...exhaust-gas, volumetric, dry \( \text{SO}_2 \) concentration, \( 10^6 \times \text{g mole-} \)
\( \text{SO}_2/\text{g mole-air, exhaust, dry (i.e. ppmv)} \)
\( \text{vol}\% \text{dry} O_2, \text{exhaust} \) ...volume percent \( O_2 \) of the dry exhaust gas, \( 100\% \times \text{g mole-} \)
\( O_2/\text{g mole-dry exhaust} \)
\( \text{wt}\% C_{\text{fuel}} \) ...............dry weight-percent carbon of a fuel, \( 100\% \times \text{g-C/g-fuel} \)
\( \text{wt}\% H_{\text{fuel}} \) ...............dry weight-percent hydrogen of a fuel, \( 100\% \times \text{g-H/g-fuel} \)
\( \text{wt}\% S_{\text{fuel}} \) ...............dry weight-percent sulfur of a fuel, \( 100\% \times \text{g-S/g-fuel} \)
ATTACHMENT 1 [insert into Title-V Statements of Bases]

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

NOMENCLATURE (in alphabetical order):

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

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

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

**OUTPUT:**
1. **SO\textsubscript{2} concentration** on a dry basis for the combustion of diesel fuel

**Note 3:** Although **SO\textsubscript{2} concentration** is on a dry basis, mol-H\textsubscript{2}O is still an important dummy variable that needed to be calculated because N\textsubscript{2,H2} that accompanies O\textsubscript{2,H2} dilutes **SO\textsubscript{2} concentration**.

**INPUTS:**

1. wt\%S\textsubscript{fuel}
2. wt\%C\textsubscript{fuel}
3. wt\%H\textsubscript{fuel}
4. vol\%\textsubscript{dry}O\textsubscript{2,exhaust}

**Note 4:** wt\%S\textsubscript{fuel}, wt\%C\textsubscript{fuel}, and wt\%H\textsubscript{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\textsubscript{2} and N\textsubscript{2}—has 3.76 moles of N\textsubscript{2} per mole of O\textsubscript{2}. Therefore, there are 4.76 moles of air per mole of O\textsubscript{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\textsubscript{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\textsubscript{x} in the exhaust gas. Therefore, vol\%\textsubscript{dry}O\textsubscript{2,exhaust} must be greater than or equal to zero while all N\textsubscript{2} and all excess O\textsubscript{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\textsubscript{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) \[ S_{\text{fuel}} = \text{dummy-fuel} \times \text{wt}\% S_{\text{fuel}} / 32.06 \]

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

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

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 \( O_2 \) 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 \( \text{NO}_x \) 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) \[ S_{\text{fuel}} + O_{2,S} + N_{2,S} \iff \text{mol-SO}_2 + N_{2,S} \]

Eq. (2-2) \[ C_{\text{fuel}} + O_{2,C} + N_{2,C} \iff \text{mol-CO}_2 + N_{2,C} \]

Eq. (2-3) \[ H_{2,\text{fuel}} + O_{2,H2} + N_{2,H2} \iff \text{mol-H}_2\text{O} + N_{2,H2} \]

Eq. (2-4) \[ \text{total-}O_2 - O_{2,S} - O_{2,C} - O_{2,H2} \iff \text{mol-O}_2 \]

Eq. (2-5) \[ \text{total-}N_2 \iff \text{mol-N}_2 \]

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).

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

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

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

Eq. (3-4) \[ \text{mol-O}_2 = \text{total-}O_2 - O_{2,S} - O_{2,C} - O_{2,H2} = \text{total-}O_2 - \text{mol-SO}_2 - \text{mol-CO}_2 - (0.5 \times \text{mol-H}_2\text{O}) \]

Eq. (3-5) \[ \text{mol-N}_2 = \text{total-N}_2 = 3.76 \times \text{total-}O_2 = 3.76 \times (\text{mol-SO}_2 + \text{mol-CO}_2 + (0.5 \times \text{mol-H}_2\text{O}) + \text{mol-O}_2) = (3.76 \times \text{mol-SO}_2) + (3.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) + (3.76 \times \text{mol-O}_2) \]
Note 9: Eq. (4-1) is the definition of \( \text{vol}\%_{\text{dry}, \text{exhaust}} \). Eq. (4-2) is the solution of eq. (4-1) as a function of \( \text{mol-}O_2 \). Eq. (4-3) is the result of substituting \( \text{mol-N}_2 \) 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 \( \text{mol-}O_2 \) term on the right side of eq. (4-4) to the left side and then factoring out \( \text{mol-}O_2 \). Eq. (4-6) is the result of multiplying both sides of eq. (4-5) by “100% - \( \text{vol}\%_{\text{dry}, \text{exhaust}} \).” Eq. (4-7) is the result of combining the two \( \text{vol}\%_{\text{dry}, \text{exhaust}} \) terms on the left side of eq. (4-6) and isolating the \( \text{mol-}O_2 \) 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) \( \text{vol}\%_{\text{dry}, \text{exhaust}} = 100\% \times \text{mol-}O_2 / (\text{mol-SO}_2 + \text{mol-CO}_2 + \text{mol-}O_2 + \text{mol-N}_2) \)

Eq. (4-2) \( \text{mol-}O_2 = \text{vol}\%_{\text{dry}, \text{exhaust}} \times (\text{mol-SO}_2 + \text{mol-CO}_2 + \text{mol-N}_2) / (100\% - \text{vol}\%_{\text{dry}, \text{exhaust}}) \)

Eq. (4-3) \( \text{mol-}O_2 = \text{vol}\%_{\text{dry}, \text{exhaust}} \times (\text{mol-SO}_2 + \text{mol-CO}_2 + ((3.76 \times \text{mol-SO}_2) + (3.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) + (3.76 \times \text{mol-}O_2))) / (100\% - \text{vol}\%_{\text{dry}, \text{exhaust}}) \)

Eq. (4-4) \( \text{mol-}O_2 = \text{vol}\%_{\text{dry}, \text{exhaust}} \times ((4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) + (3.76 \times \text{mol-}O_2) / (100\% - \text{vol}\%_{\text{dry}, \text{exhaust}}) \)

Eq. (4-5) \( \text{mol-}O_2 = \text{vol}\%_{\text{dry}, \text{exhaust}} \times (1 - (3.76 \times \text{vol}\%_{\text{dry}, \text{exhaust}}) / (100\% - \text{vol}\%_{\text{dry}, \text{exhaust}})) = \text{vol}\%_{\text{dry}, \text{exhaust}} \times ((4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) / (100\% - \text{vol}\%_{\text{dry}, \text{exhaust}}) \)

Eq. (4-6) \( \text{mol-}O_2 = (100\% - \text{vol}\%_{\text{dry}, \text{exhaust}}) - (3.76 \times \text{vol}\%_{\text{dry}, \text{exhaust}}) = \text{vol}\%_{\text{dry}, \text{exhaust}} \times ((4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) \)

Eq. (4-7) \( \text{mol-}O_2 = \text{vol}\%_{\text{dry}, \text{exhaust}} \times ((4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) / (100\% - (4.76 \times \text{vol}\%_{\text{dry}, \text{exhaust}}) \)

Eq. (4-8) \( \text{mol-}O_2 = \text{vol}\%_{\text{dry}, \text{exhaust}} \times ((4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) / (4.76 \times (21\% - \text{vol}\%_{\text{dry}, \text{exhaust}}) \)

Note 10: Eq. (5-1) is the definition of \( \text{SO}_2 \) concentration. Eq. (5-2) is the result of substituting \( \text{mol-N}_2 \) 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 \( \text{mol-}O_2 \) from eq. (4-8) into eq. (5-3). Eq. (5-5) is the result of combining terms in eq. (5-4).
**Eq. (5-1)** \[ \text{SO}_2 \text{concentration} = 10^6 \times \frac{\text{mol-} \text{SO}_2}{(\text{mol-} \text{SO}_2 + \text{mol-} \text{CO}_2 + \text{mol-} \text{O}_2 + \text{mol-} \text{N}_2)} \]

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

**Eq. (5-3)** \[ \text{SO}_2 \text{concentration} = 10^6 \times \frac{\text{mol-} \text{SO}_2}{((4.76 \times \text{mol-} \text{SO}_2) + (4.76 \times \text{mol-} \text{CO}_2) + (1.88 \times \text{mol-} \text{H}_2\text{O}) + (3.76 \times \text{mol-} \text{O}_2))} \]

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

**Eq. (5-5)** \[ \text{SO}_2 \text{concentration} = 10^6 \times \frac{\text{mol-} \text{SO}_2}{((1 + (\text{vol-} \text{dry} \text{O}_2, \text{exhaust} / (21\% - \text{vol-} \text{dry} \text{O}_2, \text{exhaust}))) \times ((4.76 \times \text{wt-} \text{S}_\text{fuel}) / (32.06) + (4.76 \times \text{wt-} \text{C}_\text{fuel}) / (12.01) + (1.88 \times \text{wt-} \text{H}_\text{fuel}) / (2.016)))} \]

**Note 11:** Eqs. (6-1) – (6-2) were derived such that the eq. (6-2) depends only on constants and inputs. **Eq. (6-1)** is the result of substituting mol-SO\(_2\), mol-CO\(_2\), and mol-H\(_2\)O into eqs. (3-1) – (3-3) and then substituting S\(_{\text{fuel}}\), C\(_{\text{fuel}}\), and H\(_{\text{2,fuel}}\) into eqs. (1-1) – (1-3). Eq. (6-2) is the result of combining some constants in eq. (6-1).

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

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

**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.