Coal [insert into Title-V Permits]

Note that $wt\%S_{coal}$, $wt\%ash_{coal}$, $wt\%C_{coal}$, $wt\%H_{coal}$, $wt\%N_{coal}$, and $wt\%O_{coal}$ must total 100%.

Calculate SO_2 concentration using the calculations below

$$A = 31,200 \times [\text{wt}\%\text{S}_{\text{coal}}] = 31,200 \times ____\% = ____B = 0.148 \times [\text{wt}\%\text{S}_{\text{coal}}] = 0.148 \times ___\% = ____C = 0.396 \times [\text{wt}\%\text{C}_{\text{coal}}] = 0.396 \times ___\% = ____D = 0.933 \times [\text{wt}\%\text{H}_{\text{coal}}] = 0.933 \times ___\% = ____E = 0.036 \times [\text{wt}\%\text{N}_{\text{coal}}] = 0.036 \times ___\% = ____F = 0.118 \times [\text{wt}\%\text{O}_{\text{coal}}] = 0.118 \times __\% = ____G = B + C + D + E - F = __+ + __+ + __+ + ___- = = ____H = 21\% - [\text{vol}\%\text{dry}\text{O}_2, \text{exhaust}] = 21\% - ___\% = ___\%$$

$$I = [\text{vol}\%\text{dry}\text{O}_2, \text{exhaust}] \div H = ___\% \% = ____\%$$

$$J = 1 + I = 1 + ___= = ____\%$$

$$SO_2 \text{ concentrat ion = A \div K = ___\div = ___ ppmv$$

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

| SO ₂ concentrationexhaust-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 _{coal} dry weight-percent carbon of a fuel, 100% X g-C/g-coal |
| wt%H _{coal} dry weight-percent hydrogen of a fuel, 100% X g-H/g-coal |
| wt%N _{coal} dry weight-percent nitrogen of a fuel, 100% X g-N/g-coal |
| wt%O _{coal} dry weight-percent oxygen of a fuel, 100% X g-O/g-coal |
| wt%S _{coal} dry weight-percent sulfur of a fuel, 100% X g-S/g-coal |

Computational Basis is 100 gram coal

NOMENCLATURE (in alphabetical order):

 C_{coal} = number of gram-moles of the carbon in a coal, gmole-C $H_{2,coal}$ = number of gram-moles of the "equivalent H_2 " in a coal, gmole- H_2 **mol-CO₂** = amount of CO₂ in the exhaust gas, gmole-CO₂ $mol-H_2O$ = amount of H₂O in the exhaust gas supplied by the free hydrogen in the coal, excluding water from the coal and excluding water from the ambient air, gmole- H_2O **mol-O**₂ = amount of O₂ in the exhaust gas, gmole-O₂ **mol-N₂** = amount of N₂ in the exhaust gas, *gmole-N₂* **mol-SO₂** = amount of SO₂ in the exhaust gas, gmole-SO₂ $N_{2,C}$ = ambient N₂ accompanying $O_{2,C}$ for combustion, gmole-N₂ $N_{2,coal}$ = number of gram-moles of the "equivalent N₂" in a coal, gmole-N₂ $N_{2,H2}$ = ambient N₂ accompanying $O_{2,H2}$ for combustion, gmole-N₂ $N_{2,S}$ = ambient N₂ accompanying $O_{2,S}$ for combustion, *gmole-N*₂ $O_{2,C}$ = ambient O_2 used to combust the carbon part of a coal, gmole- O_2 $O_{2,coal}$ = number of gram-moles of the "equivalent O_2 " in a coal, gmole-02 $O_{2,H2}$ = ambient O₂ used to combust the H₂ part of a coal, gmole-O₂ $O_{2,S}$ = ambient O_2 used to combust the sulfur part of a coal, gmole- O_2 S_{coal} = number of gram-moles of the sulfur in a coal, gmole-S **SO**₂**concent** = exhaust-gas, volumetric, dry SO₂ concentration, 10^6 X gmole**ration** SO₂/gmole-air_{exhaust.drv} (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-0₂ **vol** $%_{dry}$ **O**_{2,exh} = volume percent O₂ of the dry exhaust gas, 100% X gmoleaust O₂/qmole-air_{exhaust dry} wt%ash_{coal} = dry weight-percent ash of a coal, 100% X g-C/g-coal wt%C_{coal} = dry weight-percent carbon of a coal, 100% X g-C/g-coal **wt%H**_{coal} = dry weight-percent hydrogen of a coal, 100% X g-H/g-coal wt%N_{coal} = dry weight-percent nitrogen of a coal, 100% X g-N/g-coal **wt%O**_{coal} = dry weight-percent oxygen of a coal, 100% X g-O/g-coal **wt%S**_{coal} = dry weight-percent sulfur of a coal, 100% X g-S/g-coal

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

<u>Note 2</u>: **wt%H**_{coal}, **wt%N**_{coal}, and **wt%O**_{coal} are equivalent to (defined by analogy) wt%H_{2,coal}, wt%N_{2,coal}, and wt%O_{2,coal}, respectively.

OUTPUT:

- 1. SO2 concentration on a dry basis for the combustion of coal
- <u>Note 3:</u> Although **SO₂concentration** is on a dry basis, **mol-H₂O** is still an important dummy variable that needed to be calculated because $N_{2,H2}$ that accompanies **O_{2,H2}** dilutes **SO₂concentration**.

INPUTS:

- 1.wt%S_{coal}
- 2.wt%ash_{coal}
- 3. wt%C_{coal}
- 4. wt%H_{coal}
- 5. wt%N_{coal}
- 6.wt%Ocoal
- 7. vol% dryO_{2,exhaust}
- <u>Note 4:</u> wt%S_{coal}, wt%ash_{coal}, wt%C_{coal}, wt%H_{coal}, wt%N_{coal}, and wt%O_{coal} must total 100% by assumption 2. wt%ash_{coal} does not appear in the final equation (i.e. the output) by assumption 6.

ASSUMPTIONS:

- 1. Any and all water in the coal and/or in the ambient air is inert during combustion of the coal.
- 2. All coal only consists of carbon, hydrogen, and oxygen with the only impurities being sulfur, oxygen, nitrogen, and ash, or impurities consisting of those elements (e.g. CO). Any and all water in the coal 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 sources of O_2 for combustion are from the ambient air and from the O_2 contained in the coal.
- 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 N₂ and all excess O₂ is inert in the combustion process.
- 6. The ash occupies a negligible volume of the exhaust gas.

- **7.** For regulatory purposes (i.e. the purpose of developing this output), all of the sulfur in the coal forms SO₂ in the exhaust gas and none of the sulfur is removed by from the exhaust gas.
- <u>Note 5</u>: **Assumptions 1 6** are commonly accepted assumptions for combustion analysis. **Assumption 7** is based on 18 AAC 50.055(c), which states, "sulfur-compound emissions expressed as sulfur dioxide."
- Note 6:total-O2 can not be less than or equal to zero because coal does
not have enough oxygen for clean combustion without some other
oxygen source. Therefore $O_{2,s} + O_{2,C} + O_{2,H2}$ must be greater than
 $O_{2,coal}$ so that $(0.148 \times wt\%S_{coal}) + (0.396 \times wt\%C_{coal}) + (0.933 \times wt\%H_{coal}) + (0.036 \times wt\%N_{coal})$ must be greater than 0.118 X
wt%O_{coal}. Hypothetical coals were not considered.

SOLUTION:

| <u>Note 7</u> : | Eqs. (1-1) – (1-5) 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 _{coal} = dummy-coal X wt%S _{coal} / 32.06 |
| Eq. (1-2) | C _{coal} = dummy-coal X wt%C _{coal} / 12.01 |
| Eq. (1-3) | H _{2,coal} = dummy-coal X wt%H _{coal} / 2.016 |
| Eq. (1-4) | O _{2,coal} = dummy-coal X wt%O _{coal} / 32.00 |
| Eq. (1-5) | N _{2,coal} = dummy-coal X wt%N _{coal} / 28.01 |
| <u>Note 8</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 coal plus 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 all of the N_2 supplied by the coal plus 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) – (2-6) show no chemical reactions (i.e. inert from assumption 5). |

Eq. (2-1) $S_{coal} + O_{2,S} + N_{2,S} \implies mol-SO_2 + N_{2,S}$

- Eq. (2-2) $C_{coal} + O_{2,C} + N_{2,C} \implies mol-CO_2 + N_{2,C}$
- Eq. (2-3) $H_{2,coal} + O_{2,H2} + N_{2,H2} \implies mol-H_2O + N_{2,H2}$
- Eq. (2-4) $O_{2,coal}$ + total- O_2 $O_{2,S}$ $O_{2,C}$ $O_{2,H2}$ \iff mol- O_2
- Eq. (2-5) $N_{2,coal} + total-N_2 \iff mol-N_2$
- <u>Note 9:</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) $mol-SO_2 = S_{coal} = O_{2,S}$
- Eq. (3-2) $mol-CO_2 = C_{coal} = O_{2,C}$
- Eq. (3-3) mol- $H_2O = H_{2,coal} = 2 \times O_{2,H2}$
- Eq. (3-4) $mol-O_2 = O_{2,coal} + total-O_2 O_{2,S} O_{2,C} O_{2,H2} = O_{2,coal} + total-O_2 mol-SO_2 mol-CO_2 (0.5 \times mol-H_2O)$
- Eq. (3-5) $mol-N_2 = N_{2,coal} + total-N_2 = N_{2,coal} + (3.76 \times total-O_2) = N_{2,coal} + (3.76 \times (mol-SO_2 + mol-CO_2 + (0.5 \times mol-H_2O) + mol-O_2 O_{2,coal})) = N_{2,coal} + (3.76 \times mol-SO_2) + (3.76 \times mol-CO_2) + (1.88 \times mol-H_2O) + (3.76 \times mol-O_2) (3.76 \times O_{2,coal})$
- Note 10: 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-O₂. Eq. (4-3) is the result of substituting mol-N₂ 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-O₂ term on the right side of eq. (4-4) to the left side and then factoring out mol-O₂. Eq. (4-6) is the result of multiplying both sides of eq. (4-5) by "100% vol% dryO_{2,exhaust}." Eq. (4-7) is the result of combining the two vol% dryO_{2,exhaust} terms on the left side of eq. (4-8) is the result of a constant in the denominator of eq. (4-7).
- Eq. (4-1) $vol_{dry}O_{2,exhaust} = 100\% \times mol-O_2 / (mol-SO_2 + mol-CO_2 + mol-O_2 + mol-O_2 + mol-N_2)$
- Eq. (4-2) $mol-O_2 = vol_{dry}O_{2,exhaust} \times (mol-SO_2 + mol-CO_2 + mol-N_2) / (100\% vol_{dry}O_{2,exhaust})$
- Eq. (4-3) $mol-O_2 = vol\%_{dry}O_{2,exhaust} \times (mol-SO_2 + mol-CO_2 + (N_{2,coal} + (3.76 \times mol-SO_2) + (3.76 \times mol-CO_2) + (1.88 \times mol-H_2O) + (3.76 \times mol-O_2) (3.76 \times O_{2,coal}))) / (100\% vol\%_{dry}O_{2,exhaust})$

- Eq. (4-4) $mol-O_2 = vol\%_{dry}O_{2,exhaust} \times (N_{2,coal} + (4.76 \times mol-SO_2) + (4.76 \times mol-CO_2) + (1.88 \times mol-H_2O) + (3.76 \times mol-O_2) (3.76 \times O_{2,coal})) / (100\% vol\%_{dry}O_{2,exhaust})$
- Eq. (4-5) $mol-O_2 \times (1 (3.76 \times vol\%_{dry}O_{2,exhaust} / (100\% vol\%_{dry}O_{2,exhaust}))) = vol\%_{dry}O_{2,exhaust} \times (N_{2,coal} + (4.76 \times mol-SO_2) + (4.76 \times mol-CO_2) + (1.88 \times mol-H_2O) (3.76 \times O_{2,coal})) / (100\% vol\%_{dry}O_{2,exhaust})$
- Eq. (4-6) $mol-O_2 \times ((100\% vol\%_{dry}O_{2,exhaust}) (3.76 \times vol\%_{dry}O_{2,exhaust})) = vol\%_{dry}O_{2,exhaust} \times (N_{2,coal} + (4.76 \times mol-SO_2) + (4.76 \times mol-CO_2) + (1.88 \times mol-H_2O) (3.76 \times O_{2,coal}))$
- Eq. (4-7) $mol-O_2 = vol\%_{dry}O_{2,exhaust} \times (N_{2,coal} + (4.76 \times mol-SO_2) + (4.76 \times mol-CO_2) + (1.88 \times mol-H_2O) (3.76 \times O_{2,coal})) / (100\% (4.76 \times vol\%_{dry}O_{2,exhaust}))$
- Eq. (4-8) $mol-O_2 = vol_{dry}O_{2,exhaust} \times (N_{2,coal} + (4.76 \times mol-SO_2) + (4.76 \times mol-CO_2) + (1.88 \times mol-H_2O) (3.76 \times O_{2,coal})) / (4.76 \times (21\% vol_{dry}O_{2,exhaust}))$
- <u>Note 11</u>: Eq. (5-1) is the definition of SO₂concentration. Eq. (5-2) is the result of substituting mol-N₂ 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-O₂ from eq. (4-8) into eq. (5-3). Eq. (5-5) is the result of combining terms in eq. (5-4).
- **<u>Eq. (5-1)</u>** SO₂concentration = $10^6 \times \text{mol-SO}_2 / (\text{mol-SO}_2 + \text{mol-CO}_2 + \text{mol-O}_2 + \text{mol-N}_2)$
- **Eq. (5-2)** SO₂concentration = $10^6 \times \text{mol-SO}_2 / (\text{mol-SO}_2 + \text{mol-CO}_2 + \text{mol-O}_2) + (3.76 \times \text{mol-SO}_2) + (3.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) + (3.76 \times \text{mol-O}_2) (3.76 \times \text{O}_{2,\text{coal}}))$
- **<u>Eq. (5-3)</u>** SO₂concentration = $10^6 \times \text{mol-SO}_2 / (N_{2,coal} + (4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) + (4.76 \times \text{mol-O}_2) (3.76 \times \text{O}_{2,coal}))$
- **<u>Eq. (5-5)</u>** SO₂concentration = $10^6 \times \text{mol-SO}_2 / ((1 + (vol\%_{dry}O_{2,exhaust}))) (21\% vol\%_{dry}O_{2,exhaust}))) \times (N_{2,coal} + (4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-SO}_$

 $mol-CO_2$) + (1.88 X mol-H₂O) - (3.76 X O_{2,coal})))

- Note 12: 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-SO₂, mol-CO₂, and mol-H₂O into eqs. (3-1) (3-3) and then substituting S_{coal} , C_{coal} , and $H_{2,coal}$ into eqs. (1-1) (1-3). The $N_{2,coal}$ and $O_{2,coal}$ terms in eq. (6-1) were replaced by wt% N_{coal} and wt% O_{coal} via substituting into eqs. (1-4) (1-5). Eq. (6-2) is the result of combining some constants in eq. (6-1).

- <u>Note 13</u>: **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 twelve simple steps.