Hydrocarbon Fuel Gas [insert into Title-V Permits]

Calculate **SO₂concentration** using the equations below:

$$A = [H_2Sconcentration] + 1,000,000 = _____ ppmv + 1,000,000 = _____B = 6.64 × A = 6.64 × _____ = ____C = [vol%inertgastuel] + 100% = _____ % + 100% = ____D = [vol%HCuel] + 100% = ____ % + 100% = ____E = [wt%Cuc] + 100% = ____ % + 100% = ____F = 0.396 × E = 0.396 × ___ = ___G = [wt%Huc] + 100% = ___ % + 100% = ____H = 0.933 × G = 0.933 × ___ = ___I = F + H = ___ + ___ = ___J = D × I × [MW uc] = ___ × ___ × __ = ___K = B + C + J = ___ + ___ + + __ = ___L = 21% - [vol%dryO_2, exhaust] = 21% - ___ % = ___ %M = [vol%dryO_2, exhaust] + L = ___ % + ___ % = ___ %N = 1 + M = 1 + ___ = ___SO_2concentration = [H_2Sconcentration] + O = ___ ppmv + ___ = ___ ppmv$$

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

- **H₂Sconcentration** is the volumetric H₂S concentration of a fuel gas on a dry or wet basis, 10^6 X *gmole-H₂S/gmole-fuel* (i.e. *ppmv*)
- MW_{HC} is the molecular weight of the hydrocarbon portion of the fuel gas, *g*-*HC/gmole-HC*
- **SO₂concentration** is the volumetric SO₂ concentration of the exhaust gas on a dry basis, 10⁶ X *gmole-SO₂/gmole-air_{exhaust,dry}* (i.e. *ppmv*)
- **vol%**_{dry}**O**_{2,exhaust} is the volume percent O₂ of the exhaust gas on a dry basis, 100% X gmole-O₂/gmole-dryexhaust
- **vol%HC**_{fuel} is the volume percent hydrocarbons of a fuel gas, 100% X gmole-HC/gmole-fuel
- vol%H₂O_{fuel} is the volume percent water vapor of a fuel gas (equals zero if on a dry basis), 100% X gmole-H₂O/gmole-fuel
- **vol%inertgas_{fuel}** is the volume percent inert gas (e.g. N₂ and CO₂) of a fuel gas, excluding water vapor, 100% X *gmole-inertgas/gmole-fuel*
- **wt%C**_{HC} is the weight-percent carbon of the hydrocarbon portion of a fuel gas, 100% X g-C/g-HC
- **wt%H**_{HC} is the weight-percent hydrogen of the hydrocarbon portion of a fuel gas, 100% X *g-H/g-HC*

For example, a fuel gas on a dry basis is 50-ppm H₂S, 2% CO₂, 3% N₂, and 95% CH₄ (i.e. methane) with **vol%**_{dry}O_{2,exhaust} = 15%. The inputs are: **H₂Sconcentration** = 50 ppm; **MW**_{HC} = 16; **vol%inertgas**_{fuel} = 2 + 3 = 5%; **vol%HC**_{fuel} = 95%; **wt%C**_{HC} = 75%; and **wt%H**_{HC} = 25%. (Note that vol%H₂S_{fuel} = 50 / 10,000 = 0.005%, that **vol%H₂O**_{fuel} = 0%.) **SO**₂**concentration** =1.8 ppmv.

Note that the sum of the following four terms must total 100%: 1) H_2 Sconcentration converted to a percent by dividing by 10,000 (i.e. vol%H₂S_{fuel}); 2) vol%inertgas_{fuel}; 3) vol%HC_{fuel}; and 4) vol%H₂O_{fuel}. Note that the sum of wt%C_{HC} and wt%H_{HC} must total 100%.

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

Computational Basis is 1 gmole hydrocarbon fuel gas

NOMENCLATURE (in alphabetical order):

 C_{fuel} = number of gram-moles of the carbon part of a fuel gas, *gmole-C* $H_{2,fuel}$ = number of gram-moles of the "equivalent H₂" part of a fuel gas, $qmole-H_2$ H_2 Sconcent = volumetric H_2 S concentration of a fuel gas on a dry or wet basis, **ration** 10^6 X gmole-H₂S/gmole-fuel (i.e. ppmv) **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 fuel gas, excluding water vapor from the fuel gas and excluding water vapor 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, excluding N₂ from the fuel gas, $gmole-N_2$ **mol-SO₂** = amount of SO₂ in the exhaust gas, *qmole-SO*₂ MW_{HC} = molecular weight of the hydrocarbon part of a fuel gas. q-HC/gmole-HC $N_{2,C}$ = ambient N₂ accompanying $O_{2,C}$ for combustion, *gmole-N*₂ $N_{2,H2}$ = ambient N₂ accompanying $O_{2,H2}$ for combustion, gmole-N₂ $N_{2,S}$ = ambient N₂ accompanying $O_{2,S}$ for combustion, gmole-N₂ $O_{2,C}$ = ambient O_2 used to combust the carbon part of a fuel gas, gmole-O₂ $O_{2,H2}$ = ambient O_2 used to combust the H_2 part of a fuel gas, gmole- O_2 $O_{2,S}$ = ambient O_2 used to combust the sulfur part of a fuel gas, *qmole*-02 **part-H**₂**S** = fraction of hydrogen-sulfide of a fuel gas, gmole- H_2 S/gmole-fuel **part-HC** = fraction hydrocarbon of a fuel gas, *gmole-HC/gmole-fuel* **part-** = fraction inert gas (e.g. N_2 and CO_2) of a fuel gas, gmoleinertgas inertgas/gmole-fuel S_{fuel} = number of gram-moles of the sulfur part of a fuel gas, gmole-S SO_2 concent = volumetric SO_2 concentration of the exhaust gas on a dry basis, ration 10^6 X gmole-SO₂/gmole-dryexhaust (i.e. ppmv) total- N_2 = amount of ambient N_2 accompanying total- O_2 for combustion, $gmole-N_2$ **total-O₂** = total amount of ambient O_2 for combustion plus the excess O_2 , gmole-O₂ **vol** $%_{dry}$ **O**_{2,ex} = volume percent O₂ of the exhaust gas on a dry basis, 100 % X haust gmole-O₂/gmole-dryexhaust **vol%H₂O_{fuel}** = volume percent water vapor of a fuel gas (equals zero if on a dry basis), 100% X gmole-H₂O/gmole-fuel

- **vol%HC**_{fuel} = volume percent hydrocarbons of a fuel gas, 100% X gmole-HC/gmole-fuel
- **vol%inertga** = volume percent inert gas (e.g. N₂ and CO₂) of a fuel gas, **s**_{fuel} excluding water vapor, 100% X gmole-inertgas/gmole-fuel
 - $wt\%C_{HC}$ = dry weight-percent carbon of the hydrocarbon part of a fuel gas (not weight percent carbon of the total fuel gas), 100% X g-C/g-HC
 - **wt%H_{HC}** = dry weight-percent hydrogen of hydrocarbon part of a fuel gas (not weight percent carbon of the total fuel gas),100% X *g-H/g-HC*
- <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_{HC}** is equivalent to (defined by analogy) wt%H_{2,HC}. **partinertgas** is equivalent to both (defined by analogy) inertgas_{fuel} and to mol-inertgas.

OUTPUT:

- 1. SO₂ concentration on a dry basis for the combustion of a fuel gas
- <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. H₂Sconcentration
- 2.vol%H₂O_{fuel}
- 3.vol%HC_{fuel}
- 4. vol%inertgas_{fuel}
- 5. MW_{HC}
- 6.wt%C_{HC}
- 7.wt%H_{HC}
- 8. vol% dryO_{2,exhaust}
- Note 4:The sum of the following four terms must total 100%: 1) H_2 Sconcentration converted to a percent by dividing by 10,000(i.e. vol%H₂S_{fuel} by analogy); 2) vol%inertgas_{fuel}; 3) vol%HC_{fuel};and 4) vol%H₂O_{fuel}. wt%C_{HC} and wt%H_{HC} must total 100% by thedefinition of hydrocarbon. The sum of wt%C_{HC} and wt%H_{HC} musttotal 100%. For example, a fuel gas on a dry basis is 50-ppm H₂S,2% CO₂, 3% N₂, and 95% methane: 1) vol%H₂S_{fuel} = 50 / 10,000 =0.0%; 2) vol%inertgas_{fuel} = 2 + 3 = 5%; 3) vol%HC_{fuel} = 95%; 4)vol%H₂O_{fuel} = 0%; 5) wt%C_{HC} = 75%; and 6) wt%H_{HC} = 25%.

ASSUMPTIONS:

- **1.** Any and all water in the fuel gas and/or in the ambient air is inert during combustion of the fuel gas.
- 2. All fuel gas consists of inert gas (e.g. N₂ and CO₂), gaseous hydrocarbons, hydrogen sulfide, and water vapor. Note 4 is the only reason why the water vapor in the fuel may not be negligible.
- **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 vapor 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 part-inertgas, all N₂,and all excess O₂ is inert in the combustion process.
- **6.** For regulatory purposes (i.e. the purpose of developing this output), all of the sulfur in the fuel gas forms SO₂ in the exhaust gas and none of the sulfur is removed by from the exhaust gas.
- <u>Note 5</u>: **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:

- <u>Note 6</u>: **Eqs. (1-1) (1-6)** are definitions of variables as functions of inputs, constants, and other variables on a computational basis of 1 *gmole* hydrocarbon fuel gas (including hydrogen sulfide and inert gas).
- Eq. (1-1) part- $H_2S = H_2Sconcentration / 10^6$
- Eq. (1-2) part-inertgas = $vol_{dry}^{\delta} inertgas_{fuel} / 100\%$
- Eq. (1-3) part-HC = $= vol\%_{dry}HC_{fuel} / 100\%$
- Eq. (1-4) $S_{fuel} = part-H_2S$
- Eq. (1-5) $C_{fuel} = part-HC \times (wt%C_{HC} / 100\%) \times (MW_{HC} / 12.01)$
- Eq. (1-6) $H_{2,fuel} = part-H_2S + (part-HC \times (wt%H_{2,HC} / 100\%) \times (MW_{HC} / 2.016))$

- 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. The inert water vapor from the fuel gas and from the ambient air was not shown in eq. (2-3); see assumptions 2 3. 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). Eq. (2-6) shows that like the N_2 , the inert gas in the fuel is the same in the exhaust gas. The double arrows in eqs. (2-4) (2-6) show no chemical reactions (i.e. inert from assumption 5).
- Eq. (2-1) $S_{fuel} + O_{2,S} + N_{2,S} \implies mol-SO_2 + N_{2,S}$
- Eq. (2-2) $C_{fuel} + O_{2,C} + N_{2,C} \implies mol-CO_2 + N_{2,C}$
- Eq. (2-3) $H_{2,fuel} + O_{2,H2} + N_{2,H2} \implies mol-H_2O + N_{2,H2}$
- Eq. (2-4) total-O₂ O_{2,S} O_{2,C} O_{2,H2} \iff mol-O₂
- Eq. (2-5) total-N₂ \iff mol-N₂
- Eq. (2-6) part-inertgas 🖙 part-inertgas
- <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) $mol-SO_2 = S_{fuel} = O_{2,S}$
- Eq. (3-2) $mol-CO_2 = C_{fuel} = O_{2,C}$
- Eq. (3-3) mol-H₂O = $H_{2,fuel} = 2 \times O_{2,H2}$
- Eq. (3-4) $mol-O_2 = total-O_2 O_{2,S} O_{2,C} O_{2,H2} = total-O_2 mol-SO_2 mol CO_2 - (0.5 × mol-H_2O)$
- Eq. (3-5) $mol-N_2 = total-N_2 = 3.76 \times total-O_2 = 3.76 \times (mol-SO_2 + mol-CO_2 + (0.5 \times mol-H_2O) + mol-O_2) = (3.76 \times mol-SO_2) + (3.76 \times mol-CO_2) + (1.88 \times mol-H_2O) + (3.76 \times mol-O_2)$
- 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-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-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) $vol_{dry}O_{2,exhaust} = 100\% \times mol-O_2 / (part-inertgas + mol-SO_2 + mol-CO_2 + mol-O_2 + mol-N_2)$
- Eq. (4-2) $mol-O_2 = vol\%_{dry}O_{2,exhaust} \times (part-inertgas + mol-SO_2 + mol-CO_2 + mol-N_2) / (100\% vol\%_{dry}O_{2,exhaust})$
- Eq. (4-3) $mol-O_2 = vol_{dry}O_{2,exhaust} \times (part-inertgas + mol-SO_2 + mol-CO_2 + ((3.76 \times mol-SO_2) + (3.76 \times mol-CO_2) + (1.88 \times mol-H_2O) + (3.76 \times mol-O_2))) / (100\% vol_{dry}O_{2,exhaust})$
- Eq. (4-4) $mol-O_2 = vol\%_{dry}O_{2,exhaust} \times (part-inertgas + (4.76 \times mol-SO_2) + (4.76 \times mol-CO_2) + (1.88 \times mol-H_2O) + (3.76 \times mol-O_2)) / (100\% vol\%_{dry}O_{2,exhaust})$
- Eq. (4-5) $mol-O_2 \times (1 (3.76 \times vol\%_{dry}O_{2,exhaust} / (100\% vol\%_{dry}O_{2,exhaust}))) = vol\%_{dry}O_{2,exhaust} \times (part-inertgas + (4.76 \times mol-SO_2) + (4.76 \times mol-CO_2) + (1.88 \times mol-H_2O)) / (100\% vol\%_{dry}O_{2,exhaust})$
- Eq. (4-6) $mol-O_2 \times ((100\% vol\%_{dry}O_{2,exhaust}) (3.76 \times vol\%_{dry}O_{2,exhaust})) = vol\%_{dry}O_{2,exhaust} \times (part-inertgas + (4.76 \times mol-SO_2) + (4.76 \times mol-CO_2) + (1.88 \times mol-H_2O))$
- Eq. (4-7) $mol-O_2 = vol_{dry}O_{2,exhaust} \times (part-inertgas + (4.76 \times mol-SO_2) + (4.76 \times mol-CO_2) + (1.88 \times mol-H_2O)) / (100\% (4.76 \times vol_{dry}O_{2,exhaust}))$
- Eq. (4-8) $mol-O_2 = vol_{dry}O_{2,exhaust} \times (part-inertgas + (4.76 \times mol-SO_2) + (4.76 \times mol-CO_2) + (1.88 \times mol-H_2O)) / (4.76 \times (21\% vol_{dry}O_{2,exhaust}))$
- <u>Note 10</u>: Eq. (5-1) is the definition of SO_2 concentration. 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 = $10^6 \times \text{mol-SO}_2 / (\text{part-inertgas} + \text{mol-SO}_2 + \text{mol-CO}_2 + \text{mol-O}_2 + \text{mol-N}_2)$

- **<u>Eq. (5-2)</u>** SO₂concentration = $10^6 \times \text{mol-SO}_2 / (\text{part-inertgas} + \text{mol-SO}_2 + \text{mol-CO}_2 + \text{mol-O}_2 + (3.76 \times \text{mol-SO}_2) + (3.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) + (3.76 \times \text{mol-O}_2))$
- **Eq. (5-3)** SO₂concentration = $10^6 \times \text{mol-SO}_2 / (\text{part-inertgas} + (4.76 \times \text{mol-SO}_2) + (4.76 \times \text{mol-CO}_2) + (1.88 \times \text{mol-H}_2\text{O}) + (4.76 \times \text{mol-O}_2) + (2.76 \times \text{mol-O}_2) + (2.76$
- **<u>Eq. (5-5)</u>** SO₂concentration = $10^6 \times \text{mol-SO}_2 / ((1 + (vol\%_{dry}O_{2,exhaust} / (21\% vol\%_{dry}O_{2,exhaust}))) \times (part-inertgas + (4.76 \times mol-SO_2) + (4.76 \times mol-CO_2) + (1.88 \times mol-H_2O)))$
- Note 11: Eqs. (6-1) (6-4) were derived such that the eq. (6-4) depends on only constants and inputs. Eq. (6-1) is the result of substituting mol-SO₂, mol-CO₂, and mol-H₂O from eq. (5-5) into eqs. (3-1) (3-3) and then substituting S_{fuel} , C_{fuel} , and $H_{2,fuel}$ into eqs. (1-4) (1-6). Eq. (6-2) is the result of combining the two part-H₂S terms in the denominator and combining the two part-HC terms in eq. (6-1). Eq. (6-3) is the result of combining the two MW_{CH} terms, moving part-inertgas, and combining some constants in eq. (6-2). Eq. (6-4) is the result of substituting part-H₂S, part-inertgas, and part-HC from eq. (6-3) into eqs. (1-1) (1-3), respectively.

- <u>Eq. (6-4)</u> SO₂concentration = H₂Sconcentration / ((1 + (vol%_{dry}O_{2,exhaust} / $(21\% - vol%_{dry}O_{2,exhaust}))) X ((6.64 X H₂Sconcentration / <math>10^6$) +

 $(vol\%_{dry}inertgas_{fuel} / 100\%) + (MW_{HC} \times (vol\%_{dry}HC_{fuel} / 100\%) \times ((0.396 \times wt\%C_{HC} / 100\%) + (0.933 \times wt\%H_{HC} / 100\%)))))$

Note 12: **Eq. (6-4)** is relatively long and could confuse some people needing to use this equation. To resolve this potential problem, **eq. (6-4)** was simplified in the permit by breaking it into sixteen simple steps.