Innovating Green Energy Generation: On the Development of a Filter for Fossil Fuel Power Plants' Chimneys to Minimize Emissions of Exhaust Gases and Produce Methanol

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SUPPORTING INFORMATION.

Calculation of Emission Rates of Exhaust Gases.

⇨ *Relation between annual kWh production and total emissions of gases*

- For the production of **485,807,700 kWh**, **311,861 metric tons of CO_2** have been emitted.
- For the production of **433,625,883 kWh**, **179 metric tons of SO_2** have been emitted.
- For the production of **433,625,883 kWh**, **204 metric tons of NO_X** have been emitted.

Let us now assume that the fossil fuel power plants worked every single day of 2022 (365 days).

⇨ *Relation between daily kWh production and daily emissions of gases*

- For the production of $\frac{485,807,700}{365} = \mathbf{1,330,980\ kWh}$, $\frac{311,861\times10^3}{365}$ =**854,413.698630137 kg of CO_2** have been emitted.
- For the production of $\frac{433,625,883}{365} = \mathbf{1,188,016.117808219\ kWh}$, $\frac{179\times10^3}{365}$ = **490.4109589041096 kg of SO_2** have been emitted.
- For the production of $\frac{433,625,883}{365} = \mathbf{1,188,016.117808219\ kWh}$, $\frac{204\times10^3}{365}$ = **558.9041095890411 kg of NO_X** have been emitted.

Given that 1day=86,400sec, the emission rates at grams per second (gs^{-1}) can now be calculated.

⇨ *Emission Rates at g/s*

- For the production of $\frac{1{,}330{,}980}{86{,}400} = 15.40486111111111 \text{ kWh kWh},$

$\frac{854{,}413.698630137 \times 10^3}{86{,}400}$ = **9,889.047437848808 g of CO_2** have been emitted.

- For the production of $\frac{1{,}188{,}016.117808219}{86{,}400} = 13.75018654870624 \text{ kWh},$

$\frac{490.4109589041096 \times 10^3}{86{,}400}$ **= 5.676052765093861 g of SO_2** have been emitted.

- For the production of $\frac{1{,}188{,}016.117808219}{86{,}400} = 13.75018654870624 \text{ kWh},$

$\frac{558.9041095890411 \times 10^3}{86{,}400}$ **= 6.468797564687976 g of NO_X** have been emitted.

As a general note regarding NO_X, it must be acknowledged that while it comprises all oxygenated nitrogen species, NO is the most dominant species in combustion gases and accounts for anywhere between 95-99% of the total NOx in the gas stream. Thus:

$6.468797564687976 \times \frac{95}{100} = \mathbf{6.145357686453577}$ **g of NO** have been emitted.

Stoichiometric Calculations for Methanol Synthesis.

$n = \frac{m}{M} = \frac{8{,}900.143\ g}{44.01\ gmol^{-1}} = 202.308\ mol$ CO_2

Given that 70% of CO_2 will convert into CH_3OH, 30% of CO_2 will convert into CO and theorizing 0 moles of initial CO amount:

$n = 0.7 \times 202.308\ mol = 141.6156\ mol$ CO_2 in Reaction 1

$n = 0.3 \times 202.308\ mol = 60.6924\ mol$ CO_2 in Reaction 3

Now the required H_2 (for the reactions to be fully realized) will be calculated.

Reaction (1): $CO_2(g) + 3H_2(g) \rightleftharpoons CH_3OH(g) + H_2O(g)$

$\frac{n(CO2)}{n(H2)} = \frac{1}{3} \Leftrightarrow n(H2) = 3 \times n(CO2) = 3 \times 141.6156 \Leftrightarrow n = 424.8468\ mol$ H_2 required

Reaction (3): $CO_2(g) + H_2(g) \rightleftharpoons CO(g) + H_2O(g)$

$\frac{n(CO2)}{n(H2)} = \frac{1}{1} \Leftrightarrow n(H2) = n(CO2) \Rightarrow n = 60.6924\ mol$ H_2 required

Thus, in Reaction (3), the amount of CO produced will now be calculated:

$\frac{n(CO2)}{n(CO)} = \frac{1}{1} \Leftrightarrow n(CO) = n(CO2) \Rightarrow n = 60.6924\ mol$ CO produced

Additionally, Reaction (2), H_2 reacts with all CO to form CH_3OH methanol.

Reaction (2): $CO(g) + 2H_2(g) \rightleftharpoons CH_3OH(g)$

$\frac{n(CO)}{n(H2)} = \frac{1}{2} \Leftrightarrow n(H2) = 2 \times n(CO) = 2 \times 60.6924 \Leftrightarrow n = 121.3848\ mol$ H_2 required

In total, the amount of H_2 required per methanol-synthesis-process is:

$n = (424.8468 + 60.6924 + 121.3848)mol = 606.924\ mol$ H_2 requited in total per second.

The products of the reactions must now be calculated.

It has already been stated that $202.308\ mol$ CO_2 are used as reactants and become fully consumed.

Similarly, $60.6924\ mols$ CO are produced and then fully react with H_2 to form methanol.

The total methanol produced will now be calculated.

From Reaction (1): $CO_2(g) + 3H_2(g) \rightleftharpoons CH_3OH(g) + H_2O(g)$

$\frac{n(CO2)}{n(CH3OH)} = \frac{1}{1} \Leftrightarrow n(CH3OH) = n(CO2) \Rightarrow n = 141.6156\ mol$ CH_3OH produced.

From Reaction (2): $CO(g) + 2H_2(g) \rightleftharpoons CH_3OH(g)$

$\frac{n(CO)}{n(CH3OH)} = \frac{1}{1} \Leftrightarrow n(CH3OH) = n(CO) \Rightarrow n = 60.6924\ mol$ CH_3OH produced.

Therefore, the total amount of CH_3OH produced from this process is:

$n = (141.6156 + 60.6924)mol = 202.308\ mol$ CH_3OH produced per process.

Finally, the total water (H_2O) produced from this process will now be calculated.

From Reaction (1): $CO_2(g) + 3H_2(g) \rightleftharpoons CH_3OH(g) + H_2O(g)$

$\frac{n(CO2)}{n(H2O)} = \frac{1}{1} \Leftrightarrow n(H2O) = n(CO2) \Rightarrow n = 141.6156\ mol$ H_2O produced.

In Reaction (2): $CO(g) + 2H_2(g) \rightleftharpoons CH_3OH(g)$, no water is produced, so n=0 mol H_2O produced.

From Reaction (3): $CO_2(g) + H_2(g) \rightleftharpoons CO(g) + H_2O(g)$

$\frac{n(CO)}{n(H2O)} = \frac{1}{1} \Leftrightarrow n(H2O) = n(CO) \Rightarrow n = 60.6924\ mol$ H_2O produced.

Therefore, the total amount of H_2O produced from this process is:

$n = (141.6156 + 60.6924)mol = 202.308\ mol$ H_2O produced per process.

Assuming 64% total catalytic efficiency: $202.308 \times \frac{80}{100}$ =129.47712.

So, 129.47712 mol H_2O and 129.47712 mol CH_3OH will be finally produced.

But 95% of methanol and 40% of water is received from the distillation process:

So: $129.47712 \times \frac{64}{100}$ =123.003264 mol CH_3OH will be finally received.

So: $129.47712 \times \frac{40}{100}$ =51.790848 mol H_2O will be finally received.

Stoichiometric Calculations for Water Electrolysis.

$(51.790848\ - 0.157) \times \frac{80}{100} = 41.3070784\ mol$ H_2O will contribute to the H_2 molecules production.

Thus, from Reaction (6): $2H_2O(g) \rightarrow O_2(g) + 2H_2(g)$

$\frac{n(H2O)}{n(H2)} = \frac{2}{2} \Leftrightarrow n(H2) = n(H2O) \Rightarrow n = 46.4704632\ mol$ H_2 will be finally produced per reaction.

Thus: $(606.924 - 41.3070784)mol$= 565.6816536 moles H_2 still must be provided for CH_3OH synthesis.

Stoichiometric Calculations for Anions Production.

$$n = \frac{m}{M} = \frac{5.676052765093861\ \mathrm{g}}{64.06\ \mathrm{gmol^{-1}}} = 0.0886\ \mathrm{mol\ SO_2}.$$

From Reaction (7): $2SO_2(g) + O_2(g) \rightleftharpoons 2SO_3(g)$

$\frac{n(SO2)}{n(SO3)} = \frac{2}{2} \Leftrightarrow n(SO3) = n(SO2) \Rightarrow n = 0.0886$ mol SO_3 produced.

Similarly, for nitrogen monoxide:

$$n = \frac{m}{M} = \frac{6.145357686453577\ \mathrm{g}}{30.01\ \mathrm{gmol^{-1}}} = 0.2048\ \mathrm{mol\ NO}.$$

From Reaction (10): $2NO(g) + O_2(g) \rightarrow 2NO_2(g)$

$\frac{n(NO)}{n(NO2)} = \frac{2}{2} \Leftrightarrow n(NO2) = n(NO) \Rightarrow n = 0.2048$ mol NO_2 produced.

Now the amounts of H_2SO_4, HNO_3, NO, and H_2O must be calculated.

From Reaction (11): $SO_3(g) + H_2O(l) \rightarrow H_2SO_4(aq)$

$\frac{n(SO3)}{n(H2SO4)} = \frac{1}{1} \Leftrightarrow n(H2SO4) = n(SO3) \Rightarrow n = 0.0886 \text{ mol}$ H_2SO_4 produced.

$\frac{n(SO3)}{n(H2O)} = \frac{1}{1} \Leftrightarrow n(H2O) = n(SO3) \Rightarrow n = 0.0886 \text{ mol}$ H_2O must be provided.

From Reaction (12): $3NO_2(g) + H_2O(l) \rightarrow 2HNO_3(aq) + NO(aq)$

$\frac{n(NO2)}{n(HNO3)} = \frac{3}{2} \Leftrightarrow n(HNO3) = \frac{2}{3}n(NO2) \Rightarrow n = \frac{2}{3} \times 0.2048 = 0.13653 \text{ mol}$ HNO_3 produced.

$\frac{n(NO2)}{n(NO)} = \frac{3}{1} \Leftrightarrow n(NO) = \frac{1}{3}n(NO2) \Rightarrow n = \frac{1}{3} \times 0.2048 = 0.068267 \text{ mol NO}$ produced.

$\frac{n(NO2)}{n(H2O)} = \frac{3}{1} \Leftrightarrow n(H2O) = \frac{1}{3}n(NO2) \Rightarrow n = \frac{1}{3} \times 0.2048 = 0.068267 \text{ mol}$ H_2O must be provided.

Thus, ultimately: $n = (0.0886 + 0.068267)\text{mol} = 0.156867 \text{ mol/sec}$ H_2O should be provided.

Based on these data, the decomposition of the acids into their respective ions will be analyzed.

From Reaction (13): $H_2SO_4(aq) \rightarrow 2H^+(aq) + SO_4^{2-}(aq)$

$\frac{n(H\{+\})}{n(H2SO4)} = \frac{2}{1} \Leftrightarrow n(H\{+\}) = 2n(HSO4) \Rightarrow n = 0.0886 \times 2 = 0.1772 \text{ mol}$ H^+ produced.

$\frac{n(SO4\{2-\})}{n(H2SO4)} = \frac{1}{1} \Leftrightarrow n(SO4\{2-\}) = n(H2SO4) \Rightarrow n = 0.0886 \text{ mol}$ SO_4^{2-} produced.

From Reaction (14): $HNO_3(aq) \rightarrow H^+(aq) + NO_3^-(aq)$

$\frac{n(NO3\{-\})}{n(HNO3\})} = \frac{1}{1} \Leftrightarrow n(NO3\{-\}) = n(HNO3) \Rightarrow n = 0.13653 \text{ mol}$ NO_3^- produced.

$\frac{n(H\{+\})}{n(HNO3\})} = \frac{1}{1} \Leftrightarrow n(H\{+\}) = n(HNO3) \Rightarrow n = 0.13653 \text{ mol}$ H^+ produced.

So, in total, the amount of H^+ cations produced per second is:

$n = (0.13653 + 0.1772\ )mol = 0.3137\ mol$ H^+ produced per process.

Therefore, based on HER Reaction (5): $2H^+(aq) + 2e^- \rightarrow H_2(g)$

$\frac{n(H\{+\})}{n(H2)} = \frac{2}{1} \Leftrightarrow n(H\{+\}) = 2n(H2) \Rightarrow n = 0.3137 \times 2 = 1.25486 \text{ mol}$ H_2 produced.