

**METHOD OF CALCULATION OF THEORETICAL SO₂ CONTENT IN
THE EXHAUST GASES FROM COMBUSTION OF *DIESEL OIL***

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DATA REQUIRED :

1 – Analysis of Diesel oil : % C y % H₂

If the analysis is unknown, the following typical ratio may be used:

$$\% C = 87.0 \%$$

$$\% H_2 = 12.4 \%$$

2 – Analysis of Sulphur content of Diesel oil : % S

3 – Excess of air in the exhaust gases: % Excess

4 – Average analysis of Oxygen in exhaust gases: % O₂

5 – Reference level of Oxygen for presentation of emissions data : % O₂ Ref.

CALCULATION 1 :

Calculation of stoichiometric air necessary for combustion of 1 Kg of Diesel oil ,
in accordance with analysis (% C , % H₂ , % S):

$$(a) \text{ Oxygen for C} = (\%C/100) \times 22.4 / 12 \quad \text{m}^3$$

$$(b) \text{ Oxygen for H}_2 = (\%H_2/100) \times 22.4 / 4 \quad \text{m}^3$$

$$(c) \text{ Oxygen for S} = (\%S/100) \times 22.4 / 32 \quad \text{m}^3$$

$$(d) \text{ Total Oxygen} = (a) + (b) + (c) = O_2$$

$$\text{Dry stoichiometric air required} = (d) O_2 / 0.21 = \text{Air Nm}^3 / \text{Kg Diesel oil}$$

CALCULATION 2 : Exhaust Gases from combustion

Volume of gases formed in combustion:

$$(a') \quad CO_2 = (\%C/100) \times 22.4 / 12 \quad \text{N m}^3$$

$$(b') \quad H_2O = (\%H_2/100) \times 22.4 / 2 \quad \text{N m}^3$$

$$(c') \quad SO_2 = (\%S/100) \times 22.4 / 32 \quad \text{N m}^3$$

$$(d') \quad N_2 = \text{stoichiometric Air} \times 0.79 \quad \text{N m}^3$$

$$\text{GHE} = \text{Wet Gases stoich.} = (a') + (b') + (c') + (d') \text{ Nm}^3 / \text{Kg Diesel oil}$$

$$\text{GSE} = \text{Dry Gases stoich.} = (a') + (c') + (d') \text{ Nm}^3 / \text{Kg Diesel oil}$$

Excess Air:

$$\text{Excess Air} = \text{stoichiometric Air} \times \% \text{ Excess} / 100$$

Total exhaust gases from combustion :

$$\text{GHT} = \text{Total wet exhaust gases} = \text{Excess air} + \text{GHE}$$

$$\text{GST} = \text{Total dry exhaust gases} = \text{Excess air} + \text{GSE}$$

CALCULATION 3 : Theoretical emission of SO₂ with exhaust gases

ST = maximum emission of SO₂ =

$$\% \text{ S} \times 10,000 \times 64 / 32 = \% \text{ S} \times 20,000 = \text{mg S} / \text{Kg Diesel oil}$$

Concentration of maximum theoretical SO₂ in gases, relative to % O₂ measured :

$$\text{A) Based on wet gases: SO}_2 \text{ (mg/Nm}^3\text{)} = \text{ST} / \text{GHT}$$

$$\text{B) Based on dry gases: SO}_2 \text{ (mg/Nm}^3\text{)} = \text{ST} / \text{GST}$$

Concentration of maximum theoretical SO₂ in gases, relative to Reference % O₂:

C) Based on wet gases:

$$\text{SO}_2 \text{ (mg/Nm}^3\text{)} = (\text{A}) \times (21 - \% \text{O}_2 \text{ Ref.}) / (21 - \% \text{O}_2 \text{ measured})$$

D) Based on dry gases:

$$\text{SO}_2 \text{ (mg/Nm}^3\text{)} = (\text{B}) \times (21 - \% \text{O}_2 \text{ Ref.}) / (21 - \% \text{O}_2 \text{ measured})$$

NOTES :

1. The emissions of SO₂ calculated must be normally refer to dry gases.
2. The emissions calculated are the maximum theoretically possible with the data of % S and % Excess air applied . In practice, the actual emissions are somewhat lower due to the fact that part of the SO₂ is converted into Sulphates (basically of calcium) and part into SO₃ . The calculation thus represents the maximum emission of Sulphur in the form of SO₂ .
3. The emissions data refer to the Reference % O₂, in accordance with the legislation in force in each Autonomous Community, for the type of combustion plant utilised.

EXAMPLE :

DATA :

Analysis of diesel oil :

$$\begin{aligned} \% \text{ C} &= 87.0 \% \\ \% \text{ H}_2 &= 12.4 \% \\ \% \text{ S} &= 0.3 \% \end{aligned}$$

Analysis of the exhaust gases:

$$\begin{aligned} \% \text{ O}_2 &= 12.3 \% \\ \text{Excess of air} &= 145 \% \end{aligned}$$

Required Reference oxygen for the emission data: 5 %

CALCULATION 1 : Theoretical air required

$$\begin{aligned} \text{Oxygen for C} &= (87.0/100) \times 22.4 / 12 &= 1.6240 \text{ Nm}^3 \\ \text{Oxygen for H}_2 &= (12.4/100) \times 22.4 / 4 &= 0.6944 \text{ Nm}^3 \\ \text{Oxygen for S} &= (0.3/100) \times 22.4 / 32 &= 0.0021 \text{ Nm}^3 \\ \text{Total Oxygen} &= 1.624 + 0.6944 + 0.0021 &= 2.3205 \text{ Nm}^3 \end{aligned}$$

$$\text{Stoichiometric air required} = 2.3205 / 0.21 = 11.050 \text{ Nm}^3 / \text{Kg of Diesel oil}$$

CALCULATION 2 : Exhaust Gases from combustion

$$\begin{aligned} \text{CO}_2 &= (87.0/100) \times 22.4 / 12 &= 1.6240 \text{ Nm}^3 \\ \text{H}_2\text{O} &= (12.4/100) \times 22.4 / 2 &= 1.3888 \text{ Nm}^3 \\ \text{SO}_2 &= (0.3/100) \times 22.4 / 32 &= 0.0021 \text{ Nm}^3 \\ \text{N}_2 &= 11.050 \times 0.79 &= 8.7295 \text{ Nm}^3 \end{aligned}$$

Stoichiometric Wet Gases =

$$1.6240 + 1.3888 + 0.0021 + 8.7295 = 11.7444 \text{ Nm}^3 / \text{Kg Diesel oil}$$

Stoichiometric Dry Gases =

$$1.6240 + 0.0021 + 8.7295 = 10.3556 \text{ Nm}^3 / \text{Kg Diesel oil}$$

$$\text{Excess Air} = 11.050 \times 145 / 100 = 16.0225 \text{ Nm}^3 / \text{Kg Diesel oil}$$

Total exhaust gases from combustion:

GHT = Total damp exhaust gases =

$$16.0225 + 11.7444 = 27.7669 \text{ Nm}^3 / \text{Kg Diesel oil}$$

GST = Total dry exhaust gases =

$$16.0225 + 10.3556 = 26.3781 \text{ Nm}^3 / \text{Kg Diesel oil}$$

CALCULATION 3 : Theoretical SO₂ Emissions

ST = total maximum SO₂ emitted = $0.3 \times 20,000 = 6,000 \text{ mg} / \text{Kg Diesel oil}$

Concentration of SO₂ relative to actual measure % O₂ (12.3 %) :

$$\text{A) Based on wet gases} = 6,000 / 27.7669 = 216 \text{ mg} / \text{Nm}^3$$

$$\text{B) Based on dry gases} = 6,000 / 26.3781 = 227 \text{ mg} / \text{Nm}^3$$

Concentration of SO₂ relative to Reference % O₂ for data (5 %) :

$$\text{C) Based on wet gases} = 216 \times (21-5) / (21-12.3) = 397 \text{ mg} / \text{Nm}^3$$

$$\text{D) Based on dry gases} = 227 \times (21-5) / (21-12.3) = 417 \text{ mg} / \text{Nm}^3$$