

CHAPTER ONE – THE GENERAL BALANCE EQUATION

Example 1.03

An automobile driven by an internal combustion engine burns 10 kmol of gasoline² consisting of 100% octane (C₈H₁₈) and converts it completely to carbon dioxide and water vapour by a combustion reaction, whose stoichiometric equation is:



All CO₂ and H₂O produced in the reaction is discharged to the atmosphere via the engine's exhaust pipe (i.e. zero accumulation).

Assume CO₂ content of input combustion air = zero.

Problem.

What is the amount of carbon dioxide discharged to the atmosphere from 10 kmol octane? [Answer in kg of CO₂]

Solution

First note that the amount (mass or moles) of CO₂ is not a conserved quantity. Chemical reactions involve the consumption of reactant species and the generation of product species, so that no species appearing in the stoichiometric equation is conserved when a reaction occurs.

Define the system = automobile internal combustion engine

Specify the quantity = mol (kmol) of CO₂. [mole quantities give the simplest calculations for chemical reactions]

Write the balance equation

$$\text{ACC of CO}_2 \text{ in system} = \text{IN of CO}_2 \text{ to system} - \text{OUT of CO}_2 \text{ from system} + \text{GEN of CO}_2 \text{ in system} - \text{CON of CO}_2 \text{ in system}$$



Interpret the Terms

Accumulation of CO ₂ in system	= 0 kmol	(all CO ₂ is discharged)
Input of CO ₂ to system	= 0 kmol	(zero CO ₂ enters engine)
Output of CO ₂ from system	= unknown = X kmol	
Generation of CO ₂ in system	= (16/2) (consumption of C ₈ H ₁₈ in system)	
	= (16/2) (10 kmol) = 80 kmol	(from stoichiometry of reaction 1.01)
Consumption of CO ₂ in system	= 0 kmol	(CO ₂ is a product, not a reactant)

Substitute values for each term into the general balance equation.

$$0 = 0 - X + 80 - 0$$

Solve the balance equation for the unknown "X".

$$X = 80 \text{ kmol CO}_2 \text{ discharged to atmosphere.}$$

$$= (80 \text{ kmol})((1)(12.01) + (2)(16.00)) \text{ kg/kmol} = \underline{\underline{3521 \text{ kg CO}_2}}$$

² kmol ≡ kilomole ≡ molar mass (molecular weight) expressed as kilograms.

1 kmol C₈H₁₈ = [(12.01)(8) + (1.008)(18)] = 144.22 kg ≡ 162 litres ≡ 43 US gallons. i.e. 1 kmol is about 3 tanks of gasoline (a.k.a. petrol) for a family car.