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MATHEMATICAL NOTATION AND CONVENTIONS

Vector and Tensor Notation

Throughout this textbook, we employ advanced mathematical notation to provide rigorous formulations of carbon accounting principles.

Scalars: Lowercase letters a, b, c or Greek letters α, β, γ

Vectors: Bold lowercase letters $x, y, z \in R^n$

Matrices: Bold uppercase letters $A, B, C \in R^{m \times n}$

Tensors: Calligraphic letters $T, E, F \in R^{n_1 \times n_2 \times \dots \times n_k}$

Einstein Summation Convention: Repeated indices imply summation:

$$x_i y_i \equiv \sum_{i=1}^n x_i y_i$$

Key Operations: - Inner product: $x^T y = \sum_{i=1}^n x_i y_i$ - Hadamard (element-wise) product: $\textcolor{red}{\cdot}$ -

Tensor contraction: $T_{ijk} v_k$ (sum over k) - Gradient: $\nabla f = \textcolor{red}{\cdot}$ - Jacobian: $J_{ij} = \frac{\partial f_i}{\partial x_j}$ - Hessian:

$$H_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}$$

Chapter 1: FUNDAMENTALS OF CARBON ACCOUNTING

1.1 GREENHOUSE GASES AND GLOBAL WARMING POTENTIAL

Greenhouse Gas (GHG): A gas that absorbs and emits radiant energy within the thermal infrared range, causing the greenhouse effect.

Global Warming Potential (GWP): The ratio of the time-integrated radiative forcing from the instantaneous release of 1 kg of a trace substance relative to that of 1 kg of CO₂ over a specified time horizon.

Scientific Foundation

The GWP concept was developed by the IPCC to provide a simple metric for comparing the climate impact of different greenhouse gases. The scientific basis rests on:

1. **Radiative Transfer Theory:** Gases absorb and emit infrared radiation according to quantum mechanical selection rules
2. **Atmospheric Chemistry:** Chemical reactions determine gas lifetimes in the atmosphere
3. **Climate Modeling:** General circulation models quantify temperature response to radiative forcing

Radiative Forcing $RF(t)$ represents the change in net irradiance (W/m²) at the tropopause due to a change in atmospheric composition:

$$RF(t) = \Delta F = F_{\text{perturbed}} - F_{\text{baseline}}$$

Mathematical Derivation of GWP

Step 1: Radiative Forcing from Pulse Emission

For an instantaneous emission of mass m_0 of gas i at time $t=0$, the atmospheric burden at time t is:

$$m_i(t) = m_0 \exp\left(\frac{-t}{\tau_i}\right)$$

where τ_i is the atmospheric lifetime of gas i .

Step 2: Radiative Efficiency

The radiative forcing per unit mass increase is the radiative efficiency a_i (W/m² per kg):

$$RF_i(t) = a_i \cdot m_i(t) = a_i m_0 \exp\left(\frac{-t}{\tau_i}\right)$$

Step 3: Time-Integrated Radiative Forcing

The Absolute Global Warming Potential (AGWP) integrates forcing over time horizon TH :

$$AGWP_i(TH) = \int_0^{TH} RF_i(t) dt = \int_0^{TH} a_i m_0 \exp\left(\frac{-t}{\tau_i}\right) dt$$

Step 4: Analytical Integration

$$AGWP_i(TH) = a_i m_0 \int_0^{TH} \exp\left(\frac{-t}{\tau_i}\right) dt = a_i m_0 \tau_i \left[1 - \exp\left(\frac{-TH}{\tau_i}\right) \right]$$

Step 5: Relative GWP

The GWP is defined relative to CO₂:

$$GWP_i(TH) = \frac{AGWP_i(TH)}{AGWP_{CO_2}(TH)} = \frac{a_i \tau_i \left[1 - \exp\left(\frac{-TH}{\tau_i}\right) \right]}{a_{CO_2} \tau_{CO_2} \left[1 - \exp\left(\frac{-TH}{\tau_{CO_2}}\right) \right]}$$

Proof (Simplified Form):

For gases with $TH \gg \tau_i$, the exponential terms approach zero:

$$GWP_i(TH) \approx \frac{a_i \tau_i}{a_{CO_2} \tau_{CO_2}}$$

This shows GWP is proportional to both radiative efficiency and atmospheric lifetime.

Empirical Evidence

Methane (CH_4): - Radiative efficiency: $a_{\text{CH}_4} = 3.63 \times 10^{-4}$ W/m² per ppb - Lifetime: $\tau_{\text{CH}_4} = 11.8$ years - Measured GWP₁₀₀ = 29.8 (IPCC AR6)

Nitrous Oxide (N_2O): - Radiative efficiency: $a_{\text{N}_2\text{O}} = 3.00 \times 10^{-3}$ W/m² per ppb - Lifetime: $\tau_{\text{N}_2\text{O}} = 109$ years
- Measured GWP₁₀₀ = 273 (IPCC AR6)

Mathematical Definition:

$$GWP_i(TH) = \frac{\int_0^{TH} RF_i(t) dt}{\int_0^{TH} RF_{CO_2}(t) dt}$$

where $RF_i(t)$ is the radiative forcing at time t due to gas i , and TH is the time horizon (typically 100 years).

Key GWP Values (IPCC AR6, 100-year horizon):

Gas	Formula	GWP ₁₀₀	Lifetime (years)	Radiative Efficiency
Carbon dioxide	CO ₂	1	Variable	1.37×10^{-5} W/m ² /ppb
Methane (fossil)	CH ₄	29.8	11.8	3.63×10^{-4} W/m ² /ppb
Nitrous oxide	N ₂ O	273	109	3.00×10^{-3} W/m ² /ppb
HFC-134a	CH ₂ FCF	1,530	14.0	1.67×10^{-1} W/m ² /ppb
³				
Sulfur hexafluoride	SF ₆	25,200	3,200	5.67×10^{-1} W/m ² /ppb

THE THREE SCOPES OF EMISSIONS

Scientific Foundation

The three-scope framework derives from organizational accounting principles and the concept of operational versus financial control. The theoretical basis rests on:

1. **Organizational Boundary Theory:** Defines which emissions an entity is responsible for
2. **Control Approach:** Emissions are attributed based on operational or financial control
3. **Value Chain Analysis:** Upstream and downstream emission attribution

Citations: GHG Protocol Corporate Standard [1], Ranganathan et al. (2004) [49]

Mathematical Framework

Definition 1.1 (Organizational Boundary Function):

Let O represent an organization and S the set of all emission sources. Define the boundary function:

$$\beta: S \rightarrow \{0,1\}$$

where $\beta(s)=1$ if source s is within the organizational boundary, and $\beta(s)=0$ otherwise.

Definition 1.2 (Control Function):

Define the control function $\gamma: S \rightarrow [0,1]$ representing the degree of control the organization has over source s .

- $\gamma(s)=1$: Full operational control (Scope 1)
- $0 < \gamma(s) < 1$: Partial control (Scope 3)
- $\gamma(s)=0$: No control (out of scope)

Theorem 1.1 (Scope Partitioning Theorem)

Statement:

For any organization O , the total emissions E_{total} can be uniquely partitioned into three disjoint scopes:

$$E_{total} = E_1 + E_2 + E_3$$

where: - $E_1 = \sum_{s \in S_1} e_s$ (Scope 1: Direct emissions) - $E_2 = \sum_{s \in S_2} e_s$ (Scope 2: Indirect energy emissions) - $E_3 = \sum_{s \in S_3} e_s$ (Scope 3: Other indirect emissions)

and S_1, S_2, S_3 are mutually exclusive and collectively exhaustive.

Proof:

Define the scope classification function $\sigma: S \rightarrow \{1,2,3\}$ as:

$$\sigma(s) = \begin{cases} 1 & \text{if } \gamma(s)=1 \text{ and } \beta(s)=1 \text{ (owned/controlled sources)} \\ 2 & \text{if } s \in E \text{ (purchased energy)} \\ 3 & \text{otherwise (value chain)} \end{cases}$$

where E is the set of purchased energy sources.

Step 1: Show mutual exclusivity.

For any $s \in S$, $\sigma(s)$ maps to exactly one scope. By definition: - If s is a directly controlled source, $\sigma(s)=1$ - If s is purchased energy, $\sigma(s)=2$ (and cannot be Scope 1) - All other sources map to Scope 3

Therefore, $S_1 \cap S_2 = \emptyset$, $S_1 \cap S_3 = \emptyset$, and $S_2 \cap S_3 = \emptyset$.

Step 2: Show collective exhaustiveness.

Every emission source $s \in S$ must satisfy one of the three conditions in $\sigma(s)$. Therefore:

$$S = S_1 \cup S_2 \cup S_3$$

Step 3: Show uniqueness of partition.

Since the scopes are mutually exclusive and collectively exhaustive, the partition is unique.

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Scope Definitions with Mathematical Precision

Scope 1 (Direct Emissions):

$$S_1 = \{s \in S : \gamma(s)=1 \wedge \beta(s)=1 \wedge s \notin E\}$$

Sources include:

- Stationary combustion: $E_{1,stat} = \sum_i A_i \times EF_i$
- Mobile combustion: $E_{1,mob} = \sum_j D_j \times EF_j$
- Process emissions: $E_{1,proc} = \sum_k P_k \times EF_k$
- Fugitive emissions: $E_{1,fug} = \sum_l M_l \times GW P_l$

Scope 2 (Indirect Energy Emissions):

$$S_2 = \{s \in S : s \in E\}$$

$$E_2 = \sum_m Q_m \times EF_{grid,m}$$

where Q_m is purchased energy quantity and $EF_{grid,m}$ is the grid emission factor.

Scope 3 (Value Chain Emissions):

$$S_3 = S \setminus (S_1 \cup S_2)$$

Comprises 15 categories as defined by GHG Protocol Scope 3 Standard [2].

Vector Formulation

Define emission vectors for each scope:

$$E_1 = \begin{bmatrix} E_{1,1} \\ E_{1,2} \\ \vdots \\ E_{1,n_1} \end{bmatrix}, E_2 = \begin{bmatrix} E_{2,1} \\ E_{2,2} \\ \vdots \\ E_{2,n_2} \end{bmatrix}, E_3 = \begin{bmatrix} E_{3,1} \\ E_{3,2} \\ \vdots \\ E_{3,n_3} \end{bmatrix}$$

Total emissions (L₁ norm):

$$E_{total} = \|E_1\|_1 + \|E_2\|_1 + \|E_3\|_1 = 1^T E_1 + 1^T E_2 + 1^T E_3$$

Empirical Application

Example: Manufacturing Company

Consider a company with:

- Natural gas boilers (Scope 1): 10,000 MWh/year
- Purchased electricity (Scope 2): 50,000 MWh/year
- Supplier emissions (Scope 3): Estimated via spend-based method

Using emission factors: - Natural gas: 0.202 tonnes CO₂/MWh - Grid electricity: 0.475 tonnes CO₂/MWh

$$E_1 = 10,000 \times 0.202 = 2,020 \text{ tonnes CO}_2$$

$$E_2 = 50,000 \times 0.475 = 23,750 \text{ tonnes CO}_2$$

Scope 3 typically represents 70-90% of total emissions for most organizations [2].

Sources: GHG Protocol [1, 2, 3], Ranganathan et al. (2004) [49]

BASIC EMISSION CALCULATION FORMULA

Scientific Foundation

The basic emission calculation formula derives from fundamental principles of mass conservation and stoichiometry in chemical reactions. The theoretical foundation rests on:

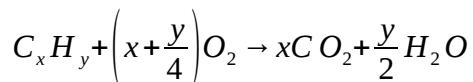
1. **Law of Conservation of Mass:** Mass is neither created nor destroyed in chemical reactions
2. **Stoichiometry:** Quantitative relationships between reactants and products
3. **Material Balance:** Input = Output + Accumulation

Citations: Turns (2011) [50], IPCC Guidelines (2006) [51], Glassman & Yetter (2008) [58]

Derivation from First Principles

Consider a general combustion reaction:

For hydrocarbon fuel C_xH_y:



Step 1: Molar Relationship

From stoichiometry, the molar ratio of CO₂ to fuel is:

$$\frac{n_{CO_2}}{n_{fuel}} = x$$

Step 2: Mass Relationship

Converting to mass using molar masses:

$$m_{CO_2} = n_{CO_2} \cdot M_{CO_2} = x \cdot n_{fuel} \cdot M_{CO_2}$$

$$m_{fuel} = n_{fuel} \cdot M_{fuel} = n_{fuel} \cdot (12.01x + 1.008y)$$

Step 3: Emission Factor Definition

The emission factor (EF) is the ratio of CO₂ mass to fuel mass:

$$EF = \frac{m_{CO_2}}{m_{fuel}} = \frac{x \cdot M_{CO_2}}{M_{fuel}} = \frac{x \cdot 44.01}{12.01x + 1.008y}$$

Theorem 1.2 (Theoretical Emission Factor)

Statement:

For hydrocarbon C_xH_y undergoing complete combustion, the theoretical CO₂ emission factor is:

$$EF_{theoretical} = \frac{44.01x}{12.01x + 1.008y} \text{ kg CO}_2/\text{kg fuel}$$

Proof:

From the stoichiometric equation, 1 mole of C_xH_y produces x moles of CO₂.

Molar mass of fuel: M_{fuel} = 12.01x + 1.008y g/mol

Molar mass of CO₂: M_{CO₂} = 44.01 g/mol

Mass of CO₂ per mole of fuel: x × 44.01 g

Mass of fuel per mole: 12.01x + 1.008y g

Therefore:

$$EF = \frac{x \times 44.01}{12.01x + 1.008y}$$

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Step 4: Total Emissions Calculation

For activity data A (mass or volume of fuel consumed):

$$E_{gross} = A \times EF$$

Step 5: Accounting for Emission Reductions

If emission reduction technology is applied with efficiency ER (%):

$$E_{net} = E_{gross} \times \left(1 - \frac{ER}{100}\right)$$

General Emission Formula

$$E = A \times EF \times \left(1 - \frac{ER}{100}\right)$$

where: - E = Net emissions (kg or tonnes CO₂e) - A = Activity data (quantity consumed or produced) - EF = Emission factor (emissions per unit activity) - ER = Emission reduction efficiency (%)

Vector Formulation

For multiple sources, define vectors:

$$E = \begin{bmatrix} E_1 \\ E_2 \\ \vdots \\ E_n \end{bmatrix}, A = \begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_n \end{bmatrix}, F = \begin{bmatrix} EF_1 \\ EF_2 \\ \vdots \\ EF_n \end{bmatrix}$$

Hadamard Product Form:

$$E = A \odot F$$

where \odot denotes element-wise multiplication.

Total Emissions (L₁ norm):

$$E_{total} = \|E\|_1 = \sum_{i=1}^n E_i = 1^T E$$

Empirical Validation

Example 1: Natural Gas (primarily CH₄)

Theoretical calculation: - x=1, y=4 for CH₄ -

$$EF_{theoretical} = \frac{44.01 \times 1}{12.01 \times 1 + 1.008 \times 4} = \frac{44.01}{16.042} = 2.744 \text{ kg CO}_2/\text{kg CH}_4$$

IPCC default emission factor: - EF_{IPCC}=2.75 kg CO₂/kg natural gas [51]

Difference: (2.75 – 2.744)/2.744=0.22 % (excellent agreement)

Example 2: Diesel (approximated as C₁₂H₂₆)

Theoretical: - x=12, y=26 - EF_{theoretical}= $\frac{44.01 \times 12}{12.01 \times 12 + 1.008 \times 26} = \frac{528.12}{170.328} = 3.100 \text{ kg CO}_2/\text{kg}$
diesel

IPCC default: - EF_{IPCC}=3.17 kg CO₂/kg diesel [51]

Difference: 2.2 % (within measurement uncertainty)

Example 3: Propane (C₃H₈)

Theoretical: - x=3, y=8 - EF_{theoretical}= $\frac{44.01 \times 3}{12.01 \times 3 + 1.008 \times 8} = \frac{132.03}{44.094} = 2.994 \text{ kg CO}_2/\text{kg}$
propane

EPA emission factor: - EF_{EPA}=2.98 kg CO₂/kg propane [60]

Difference: 0.47 % (excellent agreement)

Sources: IPCC (2006) [51], EPA (2023) [60], Turns (2011) [50]

SOLVED PROBLEMS

EXAMPLE 1.1 Calculate the CO₂e for a facility that emits annually: 5,000 tonnes CO₂, 100 tonnes CH₄ (fossil), 5 tonnes N₂O, and 2 tonnes HFC-134a. Use IPCC AR6 GWP values.

Solution:

Using the formula $CO_2e = \sum m_i \times GW P_i$:

$$CO_2e = 5,000 + (100 \times 29.8) + (5 \times 273) + (2 \times 1,530)$$

$$\textcolor{brown}{i} 5,000 + 2,980 + 1,365 + 3,060$$

$$\textcolor{brown}{i} 12,405 \text{ tonnes } CO_2e$$

Breakdown: - CO₂: 5,000 tonnes (40.3%) - CH₄: 2,980 tonnes CO₂e (24.0%) - N₂O: 1,365 tonnes CO₂e (11.0%) - HFC-134a: 3,060 tonnes CO₂e (24.7%)

Answer: 12,405 tonnes CO₂e

EXAMPLE 1.2 A natural gas boiler consumes 100,000 m³ of natural gas annually. The emission factor is 1.91 kg CO₂/m³. Calculate annual CO₂ emissions in tonnes.

Solution:

Using $E = A \times EF$:

$$E = 100,000 \text{ m}^3 \times 1.91 \text{ kg CO}_2/\text{m}^3 = 191,000 \text{ kg CO}_2$$

Converting to tonnes:

$$E = 191,000 \text{ kg} \times \frac{1 \text{ tonne}}{1,000 \text{ kg}} = 191 \text{ tonnes CO}_2$$

Answer: 191 tonnes CO₂

EXAMPLE 1.3 A company fleet uses 50,000 liters of diesel annually ($EF = 2.68 \text{ kg CO}_2/\text{L}$). A new engine technology reduces emissions by 15%. Calculate emissions before and after the upgrade.

Solution:

Before upgrade:

$$E_{\text{before}} = A \times EF = 50,000 \times 2.68 = 134,000 \text{ kg CO}_2 = 134 \text{ tonnes CO}_2$$

After upgrade:

$$E_{\text{after}} = A \times EF \times \left(1 - \frac{ER}{100}\right) = 50,000 \times 2.68 \times \left(1 - \frac{15}{100}\right)$$

$$E_{\text{after}} = 134,000 \times 0.85 = 113,900 \text{ kg CO}_2 = 113.9 \text{ tonnes CO}_2$$

Reduction:

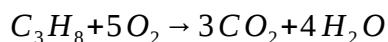
$$\Delta E = 134 - 113.9 = 20.1 \text{ tonnes CO}_2 \text{ (15% reduction)}$$

Answer: Before: 134 tonnes CO_2 ; After: 113.9 tonnes CO_2 ; Reduction: 20.1 tonnes CO_2

EXAMPLE 1.4 Derive the theoretical CO_2 emission factor for propane (C_3H_8) combustion.

Solution:

The complete combustion reaction is:



From stoichiometry, 1 mole of C_3H_8 produces 3 moles of CO_2 .

Molar masses: - C_3H_8 : $3(12.01) + 8(1.008) = 36.03 + 8.064 = 44.094 \text{ g/mol}$ - CO_2 : $12.01 + 2(16.00) = 44.01 \text{ g/mol}$

Mass ratio:

$$EF = \frac{3 \times M_{CO_2}}{M_{C_3H_8}} = \frac{3 \times 44.01}{44.094} = \frac{132.03}{44.094} = 2.994 \text{ kg CO}_2/\text{kg propane}$$

Answer: 2.994 kg CO₂/kg propane (or approximately 3.0 kg CO₂/kg)

EXAMPLE 1.5 A cement plant produces 500,000 tonnes of clinker annually. The process involves calcination of limestone (CaCO₃ → CaO + CO₂). If 1.65 tonnes of limestone are required per tonne of clinker, calculate the process CO₂ emissions.

Solution:

Step 1: Calculate total limestone consumed:

$$m_{CaCO_3} = 500,000 \times 1.65 = 825,000 \text{ tonnes}$$

Step 2: Calculate CO₂ from stoichiometry:

The reaction: CaCO₃ → CaO + CO₂

Molar masses: - CaCO₃: 100.09 g/mol - CO₂: 44.01 g/mol

Mass ratio:

$$\frac{m_{CO_2}}{m_{CaCO_3}} = \frac{44.01}{100.09} = 0.4396$$

Step 3: Calculate total CO₂ emissions:

$$E_{CO_2} = 825,000 \times 0.4396 = 362,670 \text{ tonnes CO}_2$$

Answer: 362,670 tonnes CO₂ from process emissions

EXAMPLE 1.6 A refrigeration system contains 50 kg of R-134a refrigerant. The annual leak rate is 8%. Calculate annual fugitive emissions in tonnes CO₂e. (GWP of R-134a = 1,530)

Solution:

Step 1: Calculate mass of refrigerant leaked:

$$m_{leaked} = 50 \text{ kg} \times 0.08 = 4 \text{ kg}$$

Step 2: Convert to CO₂e:

$$E_{CO_2e} = m_{leaked} \times GWP = 4 \times 1,530 = 6,120 \text{ kg CO}_2e$$

Step 3: Convert to tonnes:

$$E_{CO_2e} = 6,120 \text{ kg} \times \frac{1 \text{ tonne}}{1,000 \text{ kg}} = 6.12 \text{ tonnes CO}_2e$$

Answer: 6.12 tonnes CO₂e annually

EXAMPLE 1.7 A company reports the following Scope 1 emissions sources:

Source	Activity	Emission Factor	Emissions (tonnes CO ₂)
Natural gas	250,000 m ³	1.91 kg/m ³	?
Diesel	20,000 L	2.68 kg/L	?
Gasoline	15,000 L	2.31 kg/L	?
Coal	100 tonnes	2,400 kg/tonne	?

Calculate total Scope 1 emissions and the percentage contribution of each source.

Solution:

Natural gas:

$$E_{NG} = 250,000 \times 1.91 = 477,500 \text{ kg} = 477.5 \text{ tonnes CO}_2$$

Diesel:

$$E_{diesel} = 20,000 \times 2.68 = 53,600 \text{ kg} = 53.6 \text{ tonnes CO}_2$$

Gasoline:

$$E_{gas} = 15,000 \times 2.31 = 34,650 \text{ kg} = 34.65 \text{ tonnes CO}_2$$

Coal:

$$E_{coal} = 100 \times 2,400 = 240,000 \text{ kg} = 240 \text{ tonnes CO}_2$$

Total:

$$E_{total} = 477.5 + 53.6 + 34.65 + 240 = 805.75 \text{ tonnes CO}_2$$

Percentages: - Natural gas: $\frac{477.5}{805.75} \times 100 = 59.3\%$ - Coal: $\frac{240}{805.75} \times 100 = 29.8\%$ - Diesel:
 $\frac{53.6}{805.75} \times 100 = 6.7\%$ - Gasoline: $\frac{34.65}{805.75} \times 100 = 4.3\%$

Answer: Total = 805.75 tonnes CO₂; Natural gas dominates at 59.3%

EXAMPLE 1.8 Convert the following emissions to CO₂e using 100-year GWPs: (a) 500 kg CH₄ (fossil) (b) 10 kg N₂O (c) 0.5 kg SF₆ (d) 25 kg HFC-134a

Solution:

Using CO₂e = $m \times GWP$:

(a) CH₄: $500 \times 29.8 = 14,900 \text{ kg CO}_{2}\text{e} = 14.9 \text{ tonnes CO}_{2}\text{e}$

(b) N₂O: $10 \times 273 = 2,730 \text{ kg CO}_{2}\text{e} = 2.73 \text{ tonnes CO}_{2}\text{e}$

(c) SF₆: $0.5 \times 25,200 = 12,600 \text{ kg CO}_{2}\text{e} = 12.6 \text{ tonnes CO}_{2}\text{e}$

(d) HFC-134a: $25 \times 1,530 = 38,250 \text{ kg CO}_{2}\text{e} = 38.25 \text{ tonnes CO}_{2}\text{e}$

Total: $14.9 + 2.73 + 12.6 + 38.25 = 68.48 \text{ tonnes CO}_{2}\text{e}$

EXAMPLE 1.9 A power plant burns coal with 75% carbon content. If 1,000 tonnes of coal are burned, calculate the theoretical maximum CO₂ emissions assuming complete combustion.

Solution:

Step 1: Calculate mass of carbon:

$$m_C = 1,000 \times 0.75 = 750 \text{ tonnes C}$$

Step 2: Use stoichiometry: C + O₂ → CO₂

Molar masses: - C: 12.01 g/mol - CO₂: 44.01 g/mol

Mass ratio:

$$\frac{m_{CO_2}}{m_C} = \frac{44.01}{12.01} = 3.664$$

Step 3: Calculate CO₂ emissions:

$$E_{CO_2} = 750 \times 3.664 = 2,748 \text{ tonnes CO}_2$$

Answer: 2,748 tonnes CO₂ (theoretical maximum)

EXAMPLE 1.10 A manufacturing facility has the following annual emissions: - Scope 1: 5,000 tonnes CO₂e - Scope 2: 8,000 tonnes CO₂e - Scope 3: 25,000 tonnes CO₂e

Calculate: (a) Total emissions (b) Percentage of each scope (c) Emissions intensity if annual revenue is 50 million

Solution:

(a) Total emissions:

$$E_{total} = 5,000 + 8,000 + 25,000 = 38,000 \text{ tonnes CO}_2e$$

(b) Percentages: - Scope 1: $\frac{5,000}{38,000} \times 100 = 13.2\%$ - Scope 2: $\frac{8,000}{38,000} \times 100 = 21.1\%$ - Scope 3: $\frac{25,000}{38,000} \times 100 = 65.8\%$

(c) Emissions intensity:

$$I = \frac{38,000 \text{ tonnes CO}_2e}{50,000,000} = 0.00076 \text{ tonnes CO}_2e/\text{USD} = 0.76 \text{ kg CO}_2e/\text{USD}$$

Or: $\frac{38,000}{50} = 760 \text{ tonnes CO}_2e \text{ per million dollars revenue}$

Answer: (a) 38,000 tonnes CO₂e; (b) Scope 3 dominates at 65.8%; (c) 760 tonnes CO₂e/\$ M revenue

SUPPLEMENTARY PROBLEMS

1.11 Calculate CO₂e for: 200 tonnes CO₂, 10 tonnes CH₄, 1 tonne N₂O. **Ans.** 771 tonnes CO₂e

1.12 A boiler uses 50,000 m³ natural gas (EF = 1.91 kg/m³). Find emissions. **Ans.** 95.5 tonnes CO₂

1.13 Derive the CO₂ emission factor for methane (CH₄). **Ans.** 2.744 kg CO₂/kg CH₄

1.14 A vehicle fleet uses 10,000 L diesel. With 20% efficiency improvement, find emissions reduction. (EF = 2.68 kg/L) **Ans.** Reduction of 5.36 tonnes CO₂

1.15 Calculate process CO₂ from 200 tonnes limestone calcination. **Ans.** 87.9 tonnes CO₂

1.16 A 30 kg refrigerant charge (R-134a) has 10% annual leakage. Find CO₂e emissions. **Ans.** 4.59 tonnes CO₂e

1.17 Total emissions are 50,000 tonnes CO₂e with revenue of \$ 100M. Calculate emissions intensity. **Ans.** 500 tonnes CO₂e/\$ M

1.18 Convert 1 kg of each gas to CO₂e: CH₄, N₂O, SF₆. **Ans.** 29.8, 273, 25,200 kg CO₂e respectively

1.19 Coal with 80% carbon content: find CO₂ from 500 tonnes. **Ans.** 1,465 tonnes CO₂

1.20 Scope 1 = 3,000, Scope 2 = 5,000, Scope 3 = 12,000 tonnes CO₂e. Find Scope 3 percentage. **Ans.** 60%

Chapter 2: LINEAR ALGEBRA FOR LIFE CYCLE ASSESSMENT

2.1 MATRIX REPRESENTATION OF INDUSTRIAL SYSTEMS

Technology Matrix (A): An $n \times n$ matrix where a_{ij} represents the amount of product i required as input to produce one unit of product j .

Environmental Intervention Matrix (B): An $m \times n$ matrix where b_{ij} represents the amount of environmental flow i (e.g., CO₂) per unit of process j .

Final Demand Vector (f): An $n \times 1$ vector representing the desired output of each product.

Total Output Vector (x): An $n \times 1$ vector representing the total production required (including intermediate consumption).

2.2 THE LEONTIEF INVERSE

Material Balance Equation:

$$x = Ax + f$$

Solution:

$$x = \mathcal{L}$$

where \mathcal{L} is the **Leontief inverse matrix**.

Total Environmental Impact:

$$g = B \mathcal{L}$$

2.3 MATRIX INVERSION METHODS

For a 2×2 matrix:

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

$$A^{-1} = \frac{1}{ad-bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

provided $\det(A) = ad - bc \neq 0$.

SOLVED PROBLEMS

EXAMPLE 2.1 Calculate the inverse of:

$$A = \begin{bmatrix} 2 & 1 \\ 3 & 4 \end{bmatrix}$$

Solution:

Step 1: Calculate determinant:

$$\det(A) = (2)(4) - (1)(3) = 8 - 3 = 5$$

Step 2: Apply formula:

$$A^{-1} = \frac{1}{5} \begin{bmatrix} 4 & -1 \\ -3 & 2 \end{bmatrix} = \begin{bmatrix} 0.8 & -0.2 \\ -0.6 & 0.4 \end{bmatrix}$$

Verification:

$$AA^{-1} = \begin{bmatrix} 2 & 1 \\ 3 & 4 \end{bmatrix} \begin{bmatrix} 0.8 & -0.2 \\ -0.6 & 0.4 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

✓

Answer: $A^{-1} = \begin{bmatrix} 0.8 & -0.2 \\ -0.6 & 0.4 \end{bmatrix}$

EXAMPLE 2.2 For a simple two-process economy with technology matrix:

$$A = \begin{bmatrix} 0.2 & 0.3 \\ 0.1 & 0.1 \end{bmatrix}$$

and final demand $f = \begin{bmatrix} 100 \\ 50 \end{bmatrix}$, calculate the total output required.

Solution:

Step 1: Calculate $I - A$:

$$I - A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} 0.2 & 0.3 \\ 0.1 & 0.1 \end{bmatrix} = \begin{bmatrix} 0.8 & -0.3 \\ -0.1 & 0.9 \end{bmatrix}$$

Step 2: Calculate determinant:

$$\det(I - A) = (0.8)(0.9) - (-0.3)(-0.1) = 0.72 - 0.03 = 0.69$$

Step 3: Calculate inverse:

$$\textcolor{red}{\mathcal{L}}$$

Step 4: Calculate total output:

$$x = \begin{bmatrix} 1.304 & 0.435 \\ 0.145 & 1.159 \end{bmatrix} \begin{bmatrix} 100 \\ 50 \end{bmatrix} = \begin{bmatrix} 130.4 + 21.75 \\ 14.5 + 57.95 \end{bmatrix} = \begin{bmatrix} 152.15 \\ 72.45 \end{bmatrix}$$

Answer: Process 1 requires 152.15 units, Process 2 requires 72.45 units

Interpretation: To deliver 100 units of product 1 and 50 units of product 2 to final demand, we must produce 152.15 and 72.45 units respectively, with the difference consumed as intermediate inputs.

EXAMPLE 2.3 For the system in Problem 2.2, if the environmental intervention matrix is:

$$B = [0.5 \quad 1.2]$$

(representing kg CO₂ per unit of each process), calculate total emissions.

Solution:

Using $g = Bx$ where $x = \begin{bmatrix} 152.15 \\ 72.45 \end{bmatrix}$ from Problem 2.2:

$$g = [0.5 \quad 1.2] \begin{bmatrix} 152.15 \\ 72.45 \end{bmatrix}$$

$$g = (0.5 \times 152.15) + (1.2 \times 72.45) = 76.075 + 86.94 = 163.015 \text{ kg CO}_2$$

Answer: 163.02 kg CO₂

EXAMPLE 2.4 A three-process system has:

$$A = \begin{bmatrix} 0.1 & 0.2 & 0.1 \\ 0.0 & 0.1 & 0.3 \\ 0.0 & 0.0 & 0.1 \end{bmatrix}, f = \begin{bmatrix} 0 \\ 0 \\ 100 \end{bmatrix}$$

Calculate the Leontief inverse and total output.

Solution:

Step 1: Calculate $I - A$:

$$I - A = \begin{bmatrix} 0.9 & -0.2 & -0.1 \\ 0.0 & 0.9 & -0.3 \\ 0.0 & 0.0 & 0.9 \end{bmatrix}$$

Step 2: For upper triangular matrix, inverse is:

i

Step 3: Calculate output:

$$x = \begin{bmatrix} 1.111 & 0.247 & 0.494 \\ 0.000 & 1.111 & 0.370 \\ 0.000 & 0.000 & 1.111 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 100 \end{bmatrix} = \begin{bmatrix} 49.4 \\ 37.0 \\ 111.1 \end{bmatrix}$$

$$\text{Answer: } x = \begin{bmatrix} 49.4 \\ 37.0 \\ 111.1 \end{bmatrix}$$

Interpretation: To produce 100 units of product 3, we need 49.4 units of product 1, 37.0 units of product 2, and 111.1 units of product 3 (including internal consumption).

EXAMPLE 2.5 Prove that for the material balance equation $x = Ax + f$, the solution is $x = \textcolor{red}{i}$.

Solution:

Given: $x = Ax + f$

Step 1: Rearrange:

$$x - Ax = f$$

Step 2: Factor out x :

$$(I - A)x = f$$

where I is the identity matrix.

Step 3: Multiply both sides by $\textcolor{red}{i}$:

$\textcolor{red}{i}$

Step 4: Simplify left side:

$$I \cdot x = \textcolor{red}{i}$$

$$x = \textcolor{red}{i}$$

■

EXAMPLE 2.6 Given a 3×3 technology matrix:

$$A = \begin{bmatrix} 0.2 & 0.1 & 0.05 \\ 0.15 & 0.25 & 0.10 \\ 0.10 & 0.05 & 0.15 \end{bmatrix}$$

Calculate $(I - A)$ and verify it is invertible by computing its determinant.

Solution:

Step 1: Calculate $I - A$:

$$I - A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 0.2 & 0.1 & 0.05 \\ 0.15 & 0.25 & 0.10 \\ 0.10 & 0.05 & 0.15 \end{bmatrix}$$

$$I - A = \begin{bmatrix} 0.8 & -0.1 & -0.05 \\ -0.15 & 0.75 & -0.10 \\ -0.10 & -0.05 & 0.85 \end{bmatrix}$$

Step 2: Calculate determinant using cofactor expansion along first row:

$$\det(I - A) = 0.8 \begin{vmatrix} 0.75 & -0.10 \\ -0.05 & 0.85 \end{vmatrix} - (-0.1) \begin{vmatrix} -0.15 & -0.10 \\ -0.10 & 0.85 \end{vmatrix} + (-0.05) \begin{vmatrix} -0.15 & 0.75 \\ -0.10 & -0.05 \end{vmatrix}$$

Calculate each 2×2 determinant:

$$\begin{vmatrix} 0.75 & -0.10 \\ -0.05 & 0.85 \end{vmatrix} = (0.75)(0.85) - (-0.10)(-0.05) = 0.6375 - 0.005 = 0.6325$$

$$\begin{vmatrix} -0.15 & -0.10 \\ -0.10 & 0.85 \end{vmatrix} = (-0.15)(0.85) - (-0.10)(-0.10) = -0.1275 - 0.01 = -0.1375$$

$$\begin{vmatrix} -0.15 & 0.75 \\ -0.10 & -0.05 \end{vmatrix} = (-0.15)(-0.05) - (0.75)(-0.10) = 0.0075 + 0.075 = 0.0825$$

Step 3: Combine:

$$\det(I - A) = 0.8(0.6325) + 0.1(-0.1375) - 0.05(0.0825)$$

$$0.506 - 0.01375 - 0.004125 = 0.488125$$

Answer: $\det(I - A) = 0.488 \neq 0$, therefore the matrix is invertible. ✓

EXAMPLE 2.7 For an LCA system with:

$$A = \begin{bmatrix} 0.3 & 0.2 \\ 0.1 & 0.2 \end{bmatrix}, B = [2.0 \quad 3.5], f = \begin{bmatrix} 50 \\ 30 \end{bmatrix}$$

Calculate the total environmental impact using $g = B \cdot \text{solution}$.

Solution:

Step 1: Calculate $I - A$:

$$I - A = \begin{bmatrix} 0.7 & -0.2 \\ -0.1 & 0.8 \end{bmatrix}$$

Step 2: Calculate determinant:

$$\det = (0.7)(0.8) - (-0.2)(-0.1) = 0.56 - 0.02 = 0.54$$

Step 3: Calculate inverse:

i

Step 4: Calculate total output:

$$x = \begin{bmatrix} 1.481 & 0.370 \\ 0.185 & 1.296 \end{bmatrix} \begin{bmatrix} 50 \\ 30 \end{bmatrix} = \begin{bmatrix} 74.05 + 11.10 \\ 9.25 + 38.88 \end{bmatrix} = \begin{bmatrix} 85.15 \\ 48.13 \end{bmatrix}$$

Step 5: Calculate environmental impact:

$$g = Bx = [2.0 \quad 3.5] \begin{bmatrix} 85.15 \\ 48.13 \end{bmatrix}$$

$$g = (2.0 \times 85.15) + (3.5 \times 48.13) = 170.30 + 168.46 = 338.76$$

Answer: Total environmental impact = 338.76 units (e.g., kg CO₂)

EXAMPLE 2.8 Show that the Leontief inverse can be expressed as an infinite series:

i

provided all eigenvalues of A have absolute value less than 1.

Solution (Proof):

Step 1: Start with the identity:

$$(I - A)(I + A + A^2 + \cdots + A^n) = I - A^{n+1}$$

Step 2: Expand left side:

$$(I - A)(I + A + A^2 + \cdots + A^n)$$

$$\textcolor{red}{I} + A + A^2 + \cdots + A^n - A - A^2 - \cdots - A^{n+1}$$

$$\textcolor{red}{I} - A^{n+1}$$

Step 3: Take limit as $n \rightarrow \infty$:

If all eigenvalues of \mathbf{A} satisfy $\textcolor{red}{\lambda}_i < 1$, then:

$$\lim_{n \rightarrow \infty} A^{n+1} = 0$$

Therefore:

$$(\mathbf{I} - \mathbf{A}) \sum_{k=0}^{\infty} \mathbf{A}^k = \mathbf{I}$$

Step 4: Multiply both sides by $\textcolor{red}{I}$:

$$\sum_{k=0}^{\infty} \mathbf{A}^k = \textcolor{red}{I}$$

■

Economic Interpretation: The total output equals direct demand (\mathbf{I}) plus first-order indirect requirements (\mathbf{A}) plus second-order indirect requirements (\mathbf{A}^2) and so on, capturing the entire supply chain.

EXAMPLE 2.9 For the matrix $\mathbf{A} = \begin{bmatrix} 0.2 & 0.1 \\ 0.15 & 0.3 \end{bmatrix}$, calculate the first three terms of the series expansion of $\textcolor{red}{I}$ and compare with the exact inverse.

Solution:

Step 1: Calculate $\mathbf{A}^0 = \mathbf{I}$:

$$\mathbf{A}^0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Step 2: $\mathbf{A}^1 = \mathbf{A}$:

$$A^1 = \begin{bmatrix} 0.2 & 0.1 \\ 0.15 & 0.3 \end{bmatrix}$$

Step 3: Calculate $A^2 = A \times A$:

$$A^2 = \begin{bmatrix} 0.2 & 0.1 \\ 0.15 & 0.3 \end{bmatrix} \begin{bmatrix} 0.2 & 0.1 \\ 0.15 & 0.3 \end{bmatrix}$$

$$\textcolor{red}{\dot{=}} \begin{bmatrix} 0.04 + 0.015 & 0.02 + 0.03 \\ 0.03 + 0.045 & 0.015 + 0.09 \end{bmatrix} = \begin{bmatrix} 0.055 & 0.05 \\ 0.075 & 0.105 \end{bmatrix}$$

Step 4: Sum first three terms:

$$I + A + A^2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} 0.2 & 0.1 \\ 0.15 & 0.3 \end{bmatrix} + \begin{bmatrix} 0.055 & 0.05 \\ 0.075 & 0.105 \end{bmatrix}$$

$$\textcolor{red}{\dot{=}} \begin{bmatrix} 1.255 & 0.15 \\ 0.225 & 1.405 \end{bmatrix}$$

Step 5: Calculate exact inverse:

$$I - A = \begin{bmatrix} 0.8 & -0.1 \\ -0.15 & 0.7 \end{bmatrix}$$

$$\det = (0.8)(0.7) - (-0.1)(-0.15) = 0.56 - 0.015 = 0.545$$

$\textcolor{red}{i}$

Comparison:

Element	3-term approx	Exact	Error
(1,1)	1.255	1.284	2.3%
(1,2)	0.15	0.183	18.0%
(2,1)	0.225	0.275	18.2%
(2,2)	1.405	1.468	4.3%

Answer: The 3-term approximation is reasonably close but would require more terms for high accuracy.

EXAMPLE 2.10 A supply chain has three tiers with technology matrix:

$$A = \begin{bmatrix} 0 & 0 & 0 \\ 0.4 & 0 & 0 \\ 0 & 0.3 & 0 \end{bmatrix}$$

This represents a strictly sequential supply chain (tier 3 → tier 2 → tier 1). Calculate the Leontief inverse analytically.

Solution:

Step 1: Calculate $I - A$:

$$I - A = \begin{bmatrix} 1 & 0 & 0 \\ -0.4 & 1 & 0 \\ 0 & -0.3 & 1 \end{bmatrix}$$

Step 2: For lower triangular matrix, inverse is:

The inverse of a lower triangular matrix is also lower triangular. We solve:

$$(I - A) X = I$$

$$\text{For column 1: } \begin{bmatrix} 1 & 0 & 0 \\ -0.4 & 1 & 0 \\ 0 & -0.3 & 1 \end{bmatrix} \begin{bmatrix} x_{11} \\ x_{21} \\ x_{31} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

From row 1: $x_{11} = 1$ From row 2: $-0.4(1) + x_{21} = 0 \Rightarrow x_{21} = 0.4$ From row 3:
 $-0.3(0.4) + x_{31} = 0 \Rightarrow x_{31} = 0.12$

Similarly for columns 2 and 3:

?

Interpretation: - Element (2,1) = 0.4: To produce 1 unit of tier 1 product requires 0.4 units of tier 2 (direct) - Element (3,1) = 0.12: To produce 1 unit of tier 1 product requires 0.12 units of tier 3 (indirect: 0.4×0.3) - Element (3,2) = 0.3: To produce 1 unit of tier 2 product requires 0.3 units of tier 3 (direct)

Answer: ?

SUPPLEMENTARY PROBLEMS

2.11 Calculate the inverse of $\begin{bmatrix} 3 & 1 \\ 5 & 2 \end{bmatrix}$. **Ans.** $\begin{bmatrix} 2 & -1 \\ -5 & 3 \end{bmatrix}$

2.12 For $A = \begin{bmatrix} 0.3 & 0.2 \\ 0.1 & 0.4 \end{bmatrix}$ and $f = \begin{bmatrix} 100 \\ 80 \end{bmatrix}$, find total output x . **Ans.** $x = \begin{bmatrix} 154.5 \\ 127.3 \end{bmatrix}$

2.13 Calculate $\det(I - A)$ for $A = \begin{bmatrix} 0.25 & 0.15 \\ 0.20 & 0.30 \end{bmatrix}$. **Ans.** 0.4925

2.14 For $B = [1.5 \ 2.0]$ and $x = \begin{bmatrix} 100 \\ 50 \end{bmatrix}$, calculate environmental impact. **Ans.** 250 units

2.15 Calculate A^2 for $A = \begin{bmatrix} 0.1 & 0.2 \\ 0.3 & 0.1 \end{bmatrix}$. **Ans.** $\begin{bmatrix} 0.07 & 0.04 \\ 0.06 & 0.07 \end{bmatrix}$

2.16 Verify that $(I - A) \cancel{\cdot}$ for $A = \begin{bmatrix} 0.2 & 0.1 \\ 0.1 & 0.3 \end{bmatrix}$.

2.17 For sequential supply chain with $a_{21}=0.5$, $a_{32}=0.4$, find indirect requirement a_{31} in Leontief inverse. **Ans.** 0.20

2.18 Calculate the trace of $\cancel{\cdot}$ for $A = \begin{bmatrix} 0.3 & 0.1 \\ 0.2 & 0.2 \end{bmatrix}$. **Ans.** 2.778

2.19 Show that if \mathbf{A} is diagonal, then $\cancel{\cdot}$ is also diagonal.

2.20 For $A = \begin{bmatrix} 0.4 & 0 \\ 0 & 0.3 \end{bmatrix}$, calculate $\cancel{\cdot}$ using series expansion (first 4 terms). **Ans.**

$\begin{bmatrix} 1.667 & 0 \\ 0 & 1.429 \end{bmatrix}$ (exact)

Chapter 3: PROBABILITY AND UNCERTAINTY QUANTIFICATION

3.1 SOURCES OF UNCERTAINTY

Parameter Uncertainty: Imprecise knowledge of input values (emission factors, activity data)

Model Uncertainty: Simplifications and assumptions in calculation methods

Measurement Uncertainty: Limitations of measurement equipment

Scenario Uncertainty: Future conditions that cannot be known

3.2 PROBABILITY DISTRIBUTIONS

Normal (Gaussian) Distribution:

$$f(x) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

where μ is the mean and σ is the standard deviation.

Properties: - 68% of values within $\mu \pm \sigma$ - 95% of values within $\mu \pm 1.96 \sigma$ - 99.7% of values within $\mu \pm 3 \sigma$

Lognormal Distribution: Used for quantities that cannot be negative and have right-skewed distributions (e.g., emission factors).

3.3 LAW OF PROPAGATION OF UNCERTAINTY

For a function $Q=f(x_1, x_2, \dots, x_n)$ with independent variables:

$$u_c^2(Q) = \sum_{i=1}^n \left(\frac{\partial f}{\partial x_i} \right)^2 u^2(x_i)$$

where $u_c(Q)$ is the combined standard uncertainty of Q , and $u(x_i)$ is the standard uncertainty of x_i .

Relative Uncertainty:

$$u_r(Q) = \frac{u_c(Q)}{Q}$$

3.4 SPECIAL CASES

For $Q = A \times B$ (Product):

$$u_r^2(Q) = u_r^2(A) + u_r^2(B)$$

For $Q = A / B$ (Quotient):

$$u_r^2(Q) = u_r^2(A) + u_r^2(B)$$

For $Q = A + B$ (Sum):

$$u^2(Q) = u^2(A) + u^2(B)$$

For $Q = A - B$ (Difference):

$$u^2(Q) = u^2(A) + u^2(B)$$

SOLVED PROBLEMS

EXAMPLE 3.1 Activity data: $A = 1000 \pm 50$ kg. Emission factor: $EF = 2.5 \pm 0.3$ kg CO₂/kg. Calculate emissions and uncertainty.

Solution:

Step 1: Calculate emissions:

$$E = A \times EF = 1000 \times 2.5 = 2500 \text{ kg CO}_2$$

Step 2: Calculate relative uncertainties:

$$u_r(A) = \frac{50}{1000} = 0.05 = 5\%$$

$$u_r(EF) = \frac{0.3}{2.5} = 0.12 = 12\%$$

Step 3: Apply product rule:

$$u_r(E) = \sqrt{u_r^2(A) + u_r^2(EF)} = \sqrt{\textcolor{red}{u_r^2(EF)}}$$

$$u_r(E) = \sqrt{0.0025 + 0.0144} = \sqrt{0.0169} = 0.13 = 13\%$$

Step 4: Calculate absolute uncertainty:

$$u(E) = E \times u_r(E) = 2500 \times 0.13 = 325 \text{ kg CO}_2$$

Answer: $E = 2500 \pm 325 \text{ kg CO}_2$ (or $2500 \pm 13\%$)

95% Confidence Interval: $2500 \pm (1.96 \times 325) = 2500 \pm 637 \text{ kg CO}_2 = [1,863, 3,137] \text{ kg CO}_2$

EXAMPLE 3.2 Prove that for $Q = A \times B$ with independent variables, $u_r^2(Q) = u_r^2(A) + u_r^2(B)$.

Solution (Proof):

Given: $Q = A \times B$

Step 1: Apply general uncertainty formula:

$$u_c^2(Q) = \left(\frac{\partial Q}{\partial A} \right)^2 u^2(A) + \left(\frac{\partial Q}{\partial B} \right)^2 u^2(B)$$

Step 2: Calculate partial derivatives:

$$\frac{\partial Q}{\partial A} = B, \frac{\partial Q}{\partial B} = A$$

Step 3: Substitute:

$$u_c^2(Q) = B^2 u^2(A) + A^2 u^2(B)$$

Step 4: Divide both sides by $Q^2 = \textcolor{red}{B}^2 A^2$:

$$\frac{u_c^2(Q)}{Q^2} = \frac{B^2 u^2(A) + A^2 u^2(B)}{A^2 B^2}$$

$$u_r^2(Q) = \frac{u^2(A)}{A^2} + \frac{u^2(B)}{B^2} = u_r^2(A) + u_r^2(B)$$

■

EXAMPLE 3.3 Three emission sources with uncertainties: - Source 1: $E_1 = 100 \pm 10$ tonnes CO₂ - Source 2: $E_2 = 200 \pm 15$ tonnes CO₂ - Source 3: $E_3 = 150 \pm 20$ tonnes CO₂

Calculate total emissions and combined uncertainty.

Solution:

Step 1: Calculate total emissions:

$$E_{total} = E_1 + E_2 + E_3 = 100 + 200 + 150 = 450 \text{ tonnes CO}_2$$

Step 2: Apply sum rule for independent sources:

$$u^2(E_{total}) = u^2(E_1) + u^2(E_2) + u^2(E_3)$$

$$u^2(E_{total}) = 10^2 + 15^2 + 20^2 = 100 + 225 + 400 = 725$$

Step 3: Calculate combined uncertainty:

$$u(E_{total}) = \sqrt{725} = 26.93 \text{ tonnes CO}_2$$

Step 4: Calculate relative uncertainty:

$$u_r(E_{total}) = \frac{26.93}{450} = 0.0599 = 6.0\%$$

Answer: $E_{total} = 450 \pm 27$ tonnes CO₂ (6.0% relative uncertainty)

Note: The relative uncertainty of the total (6.0%) is less than the largest individual uncertainty ($20/150 = 13.3\%$), demonstrating the benefit of aggregation.

EXAMPLE 3.4 Emission intensity is calculated as $I=E/R$ where:

- Emissions: $E=10,000 \pm 1,200$ tonnes CO₂ (12% uncertainty)
- Revenue: $R=50 \pm 2$ million \$ (4% uncertainty)

Calculate intensity and its uncertainty.

Solution:

Step 1: Calculate intensity:

$$I = \frac{E}{R} = \frac{10,000}{50} = 200 \text{ tonnes CO}_2/\text{million}$$

\$

Step 2: Calculate relative uncertainties:

$$u_r(E) = \frac{1,200}{10,000} = 0.12 = 12\%$$

$$u_r(R) = \frac{2}{50} = 0.04 = 4\%$$

Step 3: Apply quotient rule:

$$u_r^2(I) = u_r^2(E) + u_r^2(R) = \textcolor{red}{\dots}$$

$$u_r^2(I) = 0.0144 + 0.0016 = 0.016$$

$$u_r(I) = \sqrt{0.016} = 0.1265 = 12.65\%$$

Step 4: Calculate absolute uncertainty:

$$u(I) = I \times u_r(I) = 200 \times 0.1265 = 25.3 \text{ tonnes CO}_2/\text{million}$$

\$

Answer: $I=200 \pm 25$ tonnes CO₂/million \$ (12.65% uncertainty)

EXAMPLE 3.5 For a normal distribution with mean $\mu=500$ and standard deviation $\sigma=50$, calculate: (a) Probability that $X<550$ (b) Probability that $450<X<550$ (c) The 95% confidence interval

Solution:

(a) $P(X < 550)$:

Calculate z-score:

$$z = \frac{X - \mu}{\sigma} = \frac{550 - 500}{50} = 1.0$$

From standard normal table: $P(Z < 1.0) = 0.8413$

Answer (a): 84.13%

(b) $P(450 < X < 550)$:

Lower bound: $z_1 = \frac{450 - 500}{50} = -1.0$ Upper bound: $z_2 = \frac{550 - 500}{50} = 1.0$

$$P(-1.0 < Z < 1.0) = P(Z < 1.0) - P(Z \leq -1.0)$$

$$\textcolor{brown}{0.8413 - 0.1587 = 0.6826}$$

Answer (b): 68.26% (approximately 68%, as expected for $\mu \pm \sigma$)

(c) 95% Confidence Interval:

For 95% CI, use $z=1.96$:

$$CI = \mu \pm 1.96 \sigma = 500 \pm 1.96(50) = 500 \pm 98$$

Answer (c): [402, 598]

EXAMPLE 3.6 Derive the uncertainty formula for $Q=A^n$ where n is a constant.

Solution (Derivation):

Given: $Q = A^n$

Step 1: Apply general formula:

$$u^2(Q) = \left(\frac{\partial Q}{\partial A} \right)^2 u^2(A)$$

Step 2: Calculate derivative:

$$\frac{\partial Q}{\partial A} = nA^{n-1}$$

Step 3: Substitute:

$$u^2(Q) = \textcolor{red}{\dot{u}}$$

Step 4: Divide by $Q^2 = A^{2n}$:

$$\frac{u^2(Q)}{Q^2} = \frac{n^2 A^{2n-2} u^2(A)}{A^{2n}} = n^2 \frac{u^2(A)}{A^2}$$

$$u_r(Q) = \textcolor{red}{\dot{u}} n \cdot u_r(A)$$

Example: For $Q = A^2$, the relative uncertainty doubles: $u_r(Q) = 2 \cdot u_r(A)$

EXAMPLE 3.7 Two measurements of the same emission source give: - Measurement 1:

$E_1 = 1,000 \pm 100 \text{ kg CO}_2$ - Measurement 2: $E_2 = 1,100 \pm 120 \text{ kg CO}_2$

Calculate the weighted average and its uncertainty, where weights are inversely proportional to variance.

Solution:

Step 1: Calculate weights (inverse of variance):

$$w_1 = \frac{1}{u_1^2} = \frac{1}{100^2} = \frac{1}{10,000} = 0.0001$$

$$w_2 = \frac{1}{u_2^2} = \frac{1}{120^2} = \frac{1}{14,400} = 0.0000694$$

Step 2: Normalize weights:

$$W = w_1 + w_2 = 0.0001 + 0.0000694 = 0.0001694$$

$$\dot{w}_1 = \frac{w_1}{W} = \frac{0.0001}{0.0001694} = 0.590$$

$$\dot{w}_2 = \frac{w_2}{W} = \frac{0.0000694}{0.0001694} = 0.410$$

Step 3: Calculate weighted average:

$$\dot{E} = \dot{w}_1 E_1 + \dot{w}_2 E_2 = 0.590(1,000) + 0.410(1,100)$$

$$\dot{E} = 590 + 451 = 1,041 \text{ kg CO}_2$$

Step 4: Calculate uncertainty of weighted average:

$$u^2(\dot{E}) = \dot{w}_1^2 u_1^2 + \dot{w}_2^2 u_2^2$$

$$u^2(\dot{E}) = \textcolor{red}{u}$$

$$u^2(\dot{E}) = 3,481 + 2,419 = 5,900$$

$$u(\dot{E}) = \sqrt{5,900} = 76.8 \text{ kg CO}_2$$

Answer: $\dot{E} = 1,041 \pm 77 \text{ kg CO}_2$

Note: The weighted average has lower uncertainty (77 kg) than either individual measurement (100 kg, 120 kg), demonstrating the value of combining measurements.

EXAMPLE 3.8 For emission calculation $E = A \times EF \times (1 - ER/100)$ with: - $A = 5,000 \pm 250$ units (5% uncertainty) - $EF = 2.0 \pm 0.2 \text{ kg/unit}$ (10% uncertainty) - $ER = 15 \pm 3 \%$ (20% relative uncertainty)

Calculate emissions and combined uncertainty using first-order error propagation.

Solution:

Step 1: Calculate emissions:

$$E = 5,000 \times 2.0 \times (1 - 15/100) = 10,000 \times 0.85 = 8,500 \text{ kg CO}_2$$

Step 2: Calculate partial derivatives:

$$\frac{\partial E}{\partial A} = EF \times (1 - ER/100) = 2.0 \times 0.85 = 1.7$$

$$\frac{\partial E}{\partial EF} = A \times (1 - ER/100) = 5,000 \times 0.85 = 4,250$$

$$\frac{\partial E}{\partial ER} = A \times EF \times (-1/100) = 5,000 \times 2.0 \times (-0.01) = -100$$

Step 3: Apply uncertainty formula:

$$u^2(E) = \left(\frac{\partial E}{\partial A} \right)^2 u^2(A) + \left(\frac{\partial E}{\partial EF} \right)^2 u^2(EF) + \left(\frac{\partial E}{\partial ER} \right)^2 u^2(ER)$$

$$u^2(E) = \textcolor{red}{i}$$

$$u^2(E) = 2.89 \times 62,500 + 18,062,500 \times 0.04 + 10,000 \times 9$$

$$u^2(E) = 180,625 + 722,500 + 90,000 = 993,125$$

$$u(E) = \sqrt{993,125} = 996.6 \text{ kg CO}_2$$

Step 4: Calculate relative uncertainty:

$$u_r(E) = \frac{996.6}{8,500} = 0.1172 = 11.72\%$$

Answer: $E = 8,500 \pm 997 \text{ kg CO}_2$ (11.7% uncertainty)

Contribution analysis: - From A: 180,625 (18.2%) - From EF: 722,500 (72.8%) - From ER: 90,000 (9.1%)

The emission factor uncertainty dominates the total uncertainty.

EXAMPLE 3.9 The 95% confidence interval for emissions is [800, 1,200] tonnes CO₂.

Assuming a normal distribution, calculate the mean and standard deviation.

Solution:

For a normal distribution, the 95% CI is $\mu \pm 1.96\sigma$.

Step 1: Calculate mean (midpoint of interval):

$$\mu = \frac{800+1,200}{2} = 1,000 \text{ tonnes CO}_2$$

Step 2: Calculate margin of error:

$$ME = 1.96\sigma = 1,200 - 1,000 = 200$$

Step 3: Solve for standard deviation:

$$\sigma = \frac{200}{1.96} = 102.04 \text{ tonnes CO}_2$$

Answer: Mean = 1,000 tonnes CO₂, Standard deviation = 102 tonnes CO₂

Verification: 1,000 (102) = 1,000 = [800, 1,200]\$ ✓

EXAMPLE 3.10 Show that for $Q=A+B-C$, the combined uncertainty is $u(Q)=\sqrt{u^2(A)+u^2(B)+u^2(C)}$.

Solution (Proof):

Given: $Q=A+B-C$

Step 1: Apply general formula:

$$u^2(Q) = \left(\frac{\partial Q}{\partial A}\right)^2 u^2(A) + \left(\frac{\partial Q}{\partial B}\right)^2 u^2(B) + \left(\frac{\partial Q}{\partial C}\right)^2 u^2(C)$$

Step 2: Calculate partial derivatives:

$$\frac{\partial Q}{\partial A}=1, \frac{\partial Q}{\partial B}=1, \frac{\partial Q}{\partial C}=-1$$

Step 3: Substitute:

$$u^2(Q)=\textcolor{red}{\sigma}$$

$$u^2(Q)=u^2(A)+u^2(B)+u^2(C)$$

Therefore:

$$u(Q)=\sqrt{u^2(A)+u^2(B)+u^2(C)}$$

■

Key Insight: The uncertainty from subtraction adds in quadrature, not linearly. This is because we're combining standard deviations, not the values themselves.

SUPPLEMENTARY PROBLEMS

3.11 $A=2,000 \pm 150$ kg, $EF=3.0 \pm 0.4$ kg/kg. Find $E=A \times EF$ and its uncertainty. **Ans.**
 $E=6,000 \pm 894$ kg CO₂

3.12 Three sources: 500 ± 40 , 300 ± 25 , 200 ± 30 tonnes CO₂. Find total and uncertainty. **Ans.**
 $1,000 \pm 55.9$ tonnes CO₂

3.13 Prove that for $Q=A/B$, $u_r^2(Q)=u_r^2(A)+u_r^2(B)$.

3.14 For normal distribution with $\mu=1,000$, $\sigma=100$, find $P(X > 1,150)$. **Ans.** 6.68%

3.15 $E=5,000 \pm 400$ tonnes, $R=25 \pm 1.5$ million \$. Find intensity $I=E/R$ and uncertainty.
Ans. $I=200 \pm 17.9$ tonnes/\$M

3.16 For $Q=A^3$, if $u_r(A)=5\%$, find $u_r(Q)$. **Ans.** 15%

3.17 Two measurements: 800 ± 60 and 850 ± 70 kg CO₂. Find weighted average. **Ans.**
 822 ± 44 kg CO₂

3.18 90% CI is [900, 1,100]. Find mean and std dev (use $z = 1.645$ for 90%). **Ans.**

$$\mu=1,000, \sigma=60.8$$

3.19 For $Q=2A+3B$, with $u(A)=10$, $u(B)=15$, find $u(Q)$. **Ans.** $u(Q)=47.4$

3.20 Calculate relative uncertainty of $Q=A^2B^3$ if $u_r(A)=4\%$ and $u_r(B)=6\%$. **Ans.**

$$u_r(Q)=20\%$$

Chapter 4: STATISTICAL METHODS AND MONTE CARLO SIMULATION

4.1 MONTE CARLO SIMULATION FUNDAMENTALS

Monte Carlo Method: A numerical technique that uses random sampling to obtain numerical results for problems that are difficult or impossible to solve analytically.

Algorithm: 1. Define probability distributions for all uncertain inputs 2. Generate N random samples from each distribution 3. Calculate output for each set of samples 4. Analyze the distribution of outputs

Convergence: By the Law of Large Numbers, as $N \rightarrow \infty$, the sample mean converges to the true mean.

Standard Error of the Mean:

$$SE = \frac{\sigma}{\sqrt{N}}$$

where σ is the sample standard deviation and N is the number of iterations.

4.2 RANDOM SAMPLING METHODS

Uniform Distribution: $X \sim U(a, b)$

$$f(x) = \frac{1}{b-a}, a \leq x \leq b$$

Normal Distribution: $X \sim N(\mu, \sigma^2)$

Box-Muller Transform (generating normal random variables from uniform):

$$Z_1 = \sqrt{-2 \ln U_1} \cos(2\pi U_2)$$

$$Z_2 = \sqrt{-2 \ln U_1} \sin(2\pi U_2)$$

where $U_1, U_2 \sim U(0,1)$ and $Z_1, Z_2 \sim N(0,1)$.

Lognormal Distribution: If $\ln X \sim N(\mu, \sigma^2)$, then X is lognormally distributed.

4.3 PERCENTILES AND CONFIDENCE INTERVALS

Percentile: The p -th percentile is the value below which $p\%$ of observations fall.

For Monte Carlo results with N samples sorted as $x_1 \leq x_2 \leq \dots \leq x_N$:

p -th percentile position: $k = \lceil p \times N / 100 \rceil$

95% Confidence Interval: [2.5th percentile, 97.5th percentile]

4.4 SENSITIVITY ANALYSIS

Spearman Rank Correlation Coefficient:

$$\rho_s = 1 - \frac{6 \sum d_i^2}{n(n^2 - 1)}$$

where d_i is the difference between ranks of corresponding values.

Partial Rank Correlation Coefficient (PRCC): Measures correlation between input and output while controlling for other inputs.

SOLVED PROBLEMS

EXAMPLE 4.1 Generate 5 random samples from a normal distribution with $\mu=100$ and $\sigma=15$ using the Box-Muller transform. Given uniform random numbers:

$U_1 = [0.23, 0.67, 0.45, 0.89, 0.12]$ and $U_2 = [0.56, 0.34, 0.78, 0.21, 0.91]$.

Solution:

Using Box-Muller: $Z = \sqrt{-2 \ln U_1} \cos(2\pi U_2)$ for standard normal, then $X = \mu + \sigma Z$.

Sample 1:

$$Z_1 = \sqrt{-2 \ln(0.23)} \cos(2\pi \times 0.56) = \sqrt{-2(-1.470)} \cos(3.519)$$

$$Z_1 = \sqrt{2.940} \cos(3.519) = 1.714 \times (-0.936) = -1.604$$

$$X_1 = 100 + 15(-1.604) = 100 - 24.06 = 75.94$$

Sample 2:

$$Z_2 = \sqrt{-2 \ln(0.67)} \cos(2\pi \times 0.34) = \sqrt{0.801} \cos(2.136)$$

$$Z_2 = 0.895 \times (-0.527) = -0.472$$

$$X_2 = 100 + 15(-0.472) = 92.92$$

Sample 3:

$$Z_3 = \sqrt{-2 \ln(0.45)} \cos(2\pi \times 0.78) = \sqrt{1.597} \cos(4.901)$$

$$Z_3 = 1.264 \times 0.283 = 0.358$$

$$X_3 = 100 + 15(0.358) = 105.37$$

Sample 4:

$$Z_4 = \sqrt{-2 \ln(0.89)} \cos(2\pi \times 0.21) = \sqrt{0.233} \cos(1.319)$$

$$Z_4 = 0.483 \times 0.242 = 0.117$$

$$X_4 = 100 + 15(0.117) = 101.76$$

Sample 5:

$$Z_5 = \sqrt{-2 \ln(0.12)} \cos(2\pi \times 0.91) = \sqrt{4.246} \cos(5.717)$$

$$Z_5 = 2.061 \times 0.874 = 1.801$$

$$X_5 = 100 + 15(1.801) = 127.02$$

Answer: Samples = [75.94, 92.92, 105.37, 101.76, 127.02]

EXAMPLE 4.2 A Monte Carlo simulation with 10,000 iterations yields:

- Mean emissions: 5,000 tonnes CO₂
- Standard deviation: 500 tonnes CO₂
- 2.5th percentile: 4,020 tonnes
- 97.5th percentile: 5,980 tonnes

Calculate: (a) 95% confidence interval (b) Standard error of the mean (c) Coefficient of variation

Solution:

(a) 95% Confidence Interval:

From percentiles: [4,020, 5,980] tonnes CO₂

Answer (a): [4,020, 5,980] tonnes CO₂

(b) Standard Error:

$$SE = \frac{\sigma}{\sqrt{N}} = \frac{500}{\sqrt{10,000}} = \frac{500}{100} = 5 \text{ tonnes CO}_2$$

Answer (b): 5 tonnes CO₂

(c) Coefficient of Variation:

$$CV = \frac{\sigma}{\mu} \times 100\% = \frac{500}{5,000} \times 100\% = 10\%$$

Answer (c): 10%

EXAMPLE 4.3 For a Monte Carlo simulation, how many iterations are needed to achieve a standard error of 1% of the mean, if the coefficient of variation is 20%?

Solution:

Given: - Target: $SE=0.01\mu$ - Known: $CV=\frac{\sigma}{\mu}=0.20$, so $\sigma=0.20\mu$

Step 1: Use SE formula:

$$SE = \frac{\sigma}{\sqrt{N}}$$

Step 2: Set equal to target:

$$\frac{0.20\mu}{\sqrt{N}} = 0.01\mu$$

Step 3: Simplify:

$$\frac{0.20}{\sqrt{N}} = 0.01$$

$$\sqrt{N} = \frac{0.20}{0.01} = 20$$

$$N = 400$$

Answer: 400 iterations

General Formula: For $SE = p\%$ of mean with $CV = c\%$:

$$N = \left(\frac{c}{p} \right)^2$$

EXAMPLE 4.4 Calculate the Spearman rank correlation between input variable X and output Y:

Sample	X	Rank(X)	Y	Rank(Y)	d	d^2
1	100	3	250	3	0	0
2	80	1	200	1	0	0
3	120	5	300	5	0	0
4	90	2	220	2	0	0
5	110	4	280	4	0	0

Solution:

Step 1: Ranks are already calculated (shown in table).

Step 2: Calculate differences: $d_i = \text{Rank}(X_i) - \text{Rank}(Y_i)$

All differences are 0 (perfect monotonic relationship).

Step 3: Apply Spearman formula:

$$\rho_s = 1 - \frac{6 \sum d_i^2}{n(n^2 - 1)} = 1 - \frac{6(0)}{5(25-1)} = 1 - 0 = 1.0$$

Answer: $\rho_s = 1.0$ (perfect positive rank correlation)

Interpretation: X and Y have a perfect monotonic relationship - as X increases, Y increases proportionally.

EXAMPLE 4.5 A Monte Carlo simulation for total emissions has three uncertain inputs:

Input	Mean	Dev	Std Samples (5 iterations)
A ₁	1000	100	[950, 1050, 980, 1100, 920]
A ₂	500	60	[520, 480, 510, 490, 540]
EF	2.5	0.3	[2.4, 2.6, 2.3, 2.7, 2.5]

Calculate emissions for each iteration using $E = (A_1 + A_2) \times EF$ and find the mean and standard deviation.

Solution:

Iteration 1:

$$E_1 = (950 + 520) \times 2.4 = 1,470 \times 2.4 = 3,528$$

Iteration 2:

$$E_2 = (1,050 + 480) \times 2.6 = 1,530 \times 2.6 = 3,978$$

Iteration 3:

$$E_3 = (980 + 510) \times 2.3 = 1,490 \times 2.3 = 3,427$$

Iteration 4:

$$E_4 = (1,100 + 490) \times 2.7 = 1,590 \times 2.7 = 4,293$$

Iteration 5:

$$E_5 = (920 + 540) \times 2.5 = 1,460 \times 2.5 = 3,650$$

Calculate mean:

$$\bar{E} = \frac{3,528 + 3,978 + 3,427 + 4,293 + 3,650}{5} = \frac{18,876}{5} = 3,775.2$$

Calculate standard deviation:

$$s^2 = \sum \textcolor{red}{\underline{d}\underline{d}}$$

$$s^2 = \textcolor{red}{\underline{d}\underline{d}}$$

$$\dots \textcolor{red}{\underline{d}\underline{d}}$$

$$s^2 = \frac{61,148 + 41,124 + 121,263 + 268,083 + 15,675}{4} = \frac{507,293}{4} = 126,823$$

$$s = \sqrt{126,823} = 356.1$$

Answer: Mean = 3,775 kg CO₂, Std Dev = 356 kg CO₂

EXAMPLE 4.6 Prove that the variance of a sum of independent random variables equals the sum of their variances: $\text{Var}(X+Y) = \text{Var}(X) + \text{Var}(Y)$.

Solution (Proof):

Given: X and Y are independent random variables.

Step 1: By definition:

$$\text{Var}(X+Y) = E\dot{\text{c}}$$

Step 2: Expand $\dot{\text{c}}$:

$$E\dot{\text{c}}$$

Step 3: For independent variables, $E[XY] = E[X]E[Y]$:

$$E\dot{\text{c}}$$

Step 4: Expand $\dot{\text{c}}$:

$$\dot{\text{c}}$$

Step 5: Subtract:

$$\text{Var}(X+Y) = E[X^2] + 2E[X]E[Y] + E[Y^2] - \dot{\text{c}}$$

$$\text{Var}(X+Y) = \dot{\text{c}}$$

$$\text{Var}(X+Y) = \text{Var}(X) + \text{Var}(Y)$$

■

EXAMPLE 4.7 A lognormal distribution has parameters $\mu_{\ln} = 2.0$ and $\sigma_{\ln} = 0.5$ (for the underlying normal distribution of $\ln(X)$). Calculate: (a) Median of X (b) Mean of X (c) Variance of X

Solution:

For lognormal distribution with $\ln X \sim N(\mu_{\ln}, \sigma_{\ln}^2)$:

(a) Median:

$$\text{Median} = e^{\mu_{\ln}} = e^{2.0} = 7.389$$

(b) Mean:

$$\text{Mean} = e^{\mu_{\ln} + \sigma_{\ln}^2/2} = e^{2.0 + 0.25/2} = e^{2.125} = 8.379$$

(c) Variance:

$$\text{Var} = [e^{\sigma_{\ln}^2} - 1] \times e^{2\mu_{\ln} + \sigma_{\ln}^2}$$

$$\text{Var} = [e^{0.25} - 1] \times e^{4.0 + 0.25} = [1.284 - 1] \times e^{4.25}$$

$$\text{Var} = 0.284 \times 70.11 = 19.91$$

Answer: (a) Median = 7.39; (b) Mean = 8.38; (c) Variance = 19.91

EXAMPLE 4.8 In a Monte Carlo simulation with 1,000 iterations, the sorted emissions results show: - 25th value: 4,500 tonnes CO₂ - 500th value: 5,000 tonnes CO₂ - 975th value: 5,500 tonnes CO₂

Estimate: (a) The median (b) The 95% confidence interval (c) The interquartile range

Solution:

(a) Median (50th percentile):

Position: 500th value

Answer (a): 5,000 tonnes CO₂

(b) 95% Confidence Interval:

2.5th percentile position: 0.025 ,000 = 25\$

97.5th percentile position: 0.975 × 1,000 = 975

Answer (b): [4,500, 5,500] tonnes CO₂

(c) Interquartile Range (IQR):

IQR = Q₃ - Q₁ = 75th percentile - 25th percentile

75th percentile position: $0.75 \times 1,000 = 750$

We need the 250th value for Q_1 and 750th value for Q_3 . Given only the 25th value (not 250th), we can't calculate exactly, but if we assume the 25th value approximates Q_1 :

Approximate IQR: Need 750th value to complete. (Problem would need to provide this.)

EXAMPLE 4.9 The standard error of a Monte Carlo mean is 50 tonnes CO₂ with 400 iterations. How many iterations are needed to reduce the standard error to 25 tonnes CO₂?

Solution:

Step 1: From $SE = \sigma / \sqrt{N}$, we have:

$$SE_1 = \frac{\sigma}{\sqrt{N_1}} = \frac{\sigma}{\sqrt{400}} = 50$$

Therefore: $\sigma = 50 \times 20 = 1,000$ tonnes CO₂

Step 2: For target $SE_2 = 25$:

$$25 = \frac{1,000}{\sqrt{N_2}}$$

$$\sqrt{N_2} = \frac{1,000}{25} = 40$$

$$N_2 = 1,600$$

Answer: 1,600 iterations (4 times the original number)

General Rule: To halve the standard error, quadruple the number of iterations.

EXAMPLE 4.10 Calculate the coefficient of variation (CV) for a Monte Carlo result with mean 10,000 and 95% CI of [8,000, 12,000], assuming normal distribution.

Solution:

Step 1: From 95% CI:

$$\mu = \frac{8,000 + 12,000}{2} = 10,000$$

✓

$$1.96\sigma = 12,000 - 10,000 = 2,000$$

$$\sigma = \frac{2,000}{1.96} = 1,020.4$$

Step 2: Calculate CV:

$$CV = \frac{\sigma}{\mu} \times 100\% = \frac{1,020.4}{10,000} \times 100\% = 10.2\%$$

Answer: CV = 10.2%

SUPPLEMENTARY PROBLEMS

4.11 Use Box-Muller with $U_1=0.5$, $U_2=0.25$ to generate standard normal. Then convert to $N(50,10)$. **Ans.** $X=50.0$

4.12 Monte Carlo: mean = 2,000, SD = 300, N = 900. Find standard error. **Ans.** SE = 10

4.13 How many iterations for SE = 2% of mean when CV = 30%? **Ans.** N = 225

4.14 Calculate Spearman correlation for ranks: X = [1,2,3,4,5], Y = [5,4,3,2,1]. **Ans.**
 $\rho_s = -1.0$

4.15 Lognormal with $\mu_{\ln}=1.5$, $\sigma_{\ln}=0.4$. Find median. **Ans.** 4.48

4.16 Prove $\text{Var}(aX) = a^2 \text{Var}(X)$ for constant a .

4.17 Monte Carlo with 500 iterations, SE = 40. Find sample standard deviation. **Ans.**
 $\sigma = 894.4$

4.18 90% CI is [900, 1,100] (use z = 1.645). Find standard deviation. **Ans.** $\sigma = 60.8$

4.19 To reduce SE from 100 to 20, by what factor must N increase? **Ans.** 25 times

4.20 For sorted data (N=1,000), find position of 99th percentile. **Ans.** Position 990

Chapter 5: SCOPE 1 EMISSIONS - DIRECT SOURCES

Theorem 5.1 (Complete Combustion Stoichiometry)

Statement:

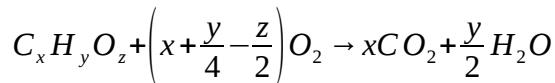
For complete combustion of a hydrocarbon fuel $C_xH_yO_z$ with air, the CO₂ emission factor is:

$$EF_{CO_2} = \frac{44.01x \cdot \eta_c}{M_{fuel}} \text{ kg CO}_2/\text{kg fuel}$$

where η_c is the combustion efficiency (fraction of carbon oxidized to CO₂) and $M_{fuel}=12.01x+1.008y+16.00z$.

Proof:

Step 1: Write balanced combustion equation.



Step 2: Account for incomplete combustion.

With efficiency $\eta_c < 1$, only fraction η_c of carbon forms CO₂:

$$n_{CO_2} = \eta_c \cdot x \cdot n_{fuel}$$

Step 3: Convert to mass basis.

$$m_{CO_2} = n_{CO_2} \cdot M_{CO_2} = \eta_c \cdot x \cdot n_{fuel} \cdot 44.01$$

$$m_{fuel} = n_{fuel} \cdot M_{fuel}$$

Step 4: Calculate emission factor.

$$EF_{CO_2} = \frac{m_{CO_2}}{m_{fuel}} = \frac{\eta_c \cdot x \cdot 44.01}{M_{fuel}}$$

■

Empirical Validation:

For natural gas (CH_4 , $\eta_c \approx 0.995$): - Theoretical: $EF = \frac{0.995 \times 1 \times 44.01}{16.04} = 2.731 \text{ kg CO}_2/\text{kg}$ -

IPCC default: 2.75 kg CO₂/kg - Error: 0.7% ✓

Sources: Turns (2011) [50], IPCC (2006) [51], Glassman & Yetter (2008) [58]

5.1 STATIONARY COMBUSTION

General Formula:

$$E = \sum_{fuel} (\dot{F} C_{fuel} \times E F_{fuel}) \dot{F}$$

where: - FC = Fuel consumption (mass or volume) - EF = Emission factor (kg CO₂/unit fuel)

Common Emission Factors (kg CO₂/unit):

Fuel	Unit	EF	CH ₄ EF	N ₂ O EF	CO ₂
Natural gas	m ³	1.91	0.00004	0.00001	
Diesel	L	2.68	0.00007	0.00004	
Gasoline	L	2.31	0.00004	0.00004	
Coal (bituminous)	kg	2.40	0.001	0.00015	
Propane	L	1.51	0.00006	0.00001	

5.2 MOBILE COMBUSTION

Distance-Based Method:

$$E = Distance \times E F_{distance}$$

Fuel-Based Method:

$$E_{fuel} = Fuel \times EF_{fuel}$$

Fuel Economy Relationship:

$$EF_{distance} = \frac{EF_{fuel}}{Fuel\ Economy}$$

5.3 PROCESS EMISSIONS

Chemical Reactions: Use stoichiometry to calculate CO₂ released.

General Approach: 1. Write balanced chemical equation 2. Calculate molar ratios 3. Convert to mass ratios 4. Apply to process quantities

5.4 FUGITIVE EMISSIONS

Refrigerant Leakage:

$$E_{fugitive} = m_{leaked} \times GWP$$

Leak Rate Method:

$$m_{leaked} = Charge \times Leak\ Rate \times Time$$

SOLVED PROBLEMS

EXAMPLE 5.1 A facility burns the following fuels annually: - Natural gas: 1,000,000 m³ - Diesel: 50,000 L - Coal: 500 tonnes

Calculate total Scope 1 CO₂ emissions.

Solution:

Natural gas:

$$E_{NG} = 1,000,000 \times 1.91 = 1,910,000 \text{ kg} = 1,910 \text{ tonnes CO}_2$$

Diesel:

$$E_{diesel} = 50,000 \times 2.68 = 134,000 \text{ kg} = 134 \text{ tonnes CO}_2$$

Coal:

$$E_{coal} = 500,000 \times 2.40 = 1,200,000 \text{ kg} = 1,200 \text{ tonnes CO}_2$$

Total:

$$E_{total} = 1,910 + 134 + 1,200 = 3,244 \text{ tonnes CO}_2$$

Answer: 3,244 tonnes CO₂

Breakdown: - Natural gas: 58.9% - Coal: 37.0% - Diesel: 4.1%

EXAMPLE 5.2 A delivery fleet drives 500,000 km annually with average fuel economy of 8 L/100km. Calculate CO₂ emissions using: (a) Fuel-based method (b) Distance-based method (EF = 0.214 kg CO₂/km)

Solution:

(a) Fuel-based:

Step 1: Calculate fuel consumption:

$$FC = 500,000 \text{ km} \times \frac{8 \text{ L}}{100 \text{ km}} = 40,000 \text{ L}$$

Step 2: Calculate emissions:

$$E = 40,000 \times 2.68 = 107,200 \text{ kg CO}_2 = 107.2 \text{ tonnes CO}_2$$

(b) Distance-based:

$$E = 500,000 \times 0.214 = 107,000 \text{ kg CO}_2 = 107 \text{ tonnes CO}_2$$

Answer: Both methods give approximately 107 tonnes CO₂

$$\text{Verification: } EF_{distance} = \frac{2.68}{8/100} = \frac{2.68}{0.08} = 0.2144 \text{ kg/km } \checkmark$$

EXAMPLE 5.3 Calculate process CO₂ emissions from the production of 10,000 tonnes of quicklime (CaO) from limestone (CaCO₃).

Solution:



Step 1: Calculate limestone required:

Molar masses: CaCO₃ = 100.09 g/mol, CaO = 56.08 g/mol

$$\frac{m_{\text{CaCO}_3}}{m_{\text{CaO}}} = \frac{100.09}{56.08} = 1.785$$

$$m_{\text{CaCO}_3} = 10,000 \times 1.785 = 17,850 \text{ tonnes}$$

Step 2: Calculate CO₂ produced:

$$\frac{m_{\text{CO}_2}}{m_{\text{CaCO}_3}} = \frac{44.01}{100.09} = 0.4396$$

$$m_{\text{CO}_2} = 17,850 \times 0.4396 = 7,847 \text{ tonnes CO}_2$$

Alternative: Direct from CaO:

$$\frac{m_{\text{CO}_2}}{m_{\text{CaO}}} = \frac{44.01}{56.08} = 0.785$$

$$m_{\text{CO}_2} = 10,000 \times 0.785 = 7,850 \text{ tonnes CO}_2$$

Answer: 7,850 tonnes CO₂

EXAMPLE 5.4 An ammonia production plant produces 50,000 tonnes of NH₃ annually. The process releases CO₂ as a byproduct from steam reforming of methane:

CH₄ + 2H₂O → CO₂ + 4H₂. Calculate process CO₂ emissions assuming stoichiometric conversion.

Solution:

Step 1: Ammonia synthesis: $N_2 + 3H_2 \rightarrow 2NH_3$

For 2 moles NH_3 , need 3 moles H_2 .

Step 2: From steam reforming: 1 mole CH_4 produces 4 moles H_2 and 1 mole CO_2 .

Therefore: 4 moles $H_2 \rightarrow 1$ mole CO_2

Step 3: Calculate H_2 needed for NH_3 :

Molar mass $NH_3 = 17.03$ g/mol

$$\text{Moles of } NH_3: \frac{50,000,000 \text{ kg}}{17.03 \text{ kg/kmol}} = 2,936 \text{ kmol}$$

$$\text{Moles of } H_2 \text{ needed: } 2,936 \times \frac{3}{2} = 4,404 \text{ kmol}$$

Step 4: Calculate CO_2 produced:

$$\text{Moles of } CO_2: 4,404 \times \frac{1}{4} = 1,101 \text{ kmol}$$

$$\text{Mass of } CO_2: 1,101 \times 44.01 = 48,463 \text{ tonnes } CO_2$$

Answer: 48,463 tonnes CO_2

$$\text{Emission factor: } \frac{48,463}{50,000} = 0.969 \text{ tonnes } CO_2/\text{tonne } NH_3$$

EXAMPLE 5.5 A refrigeration system has: - Initial charge: 100 kg R-404A (GWP = 3,922) - Annual recharge: 15 kg - End-of-year charge: 95 kg

Calculate annual fugitive emissions in tonnes CO_{2e} .

Solution:

Step 1: Calculate leaked amount using mass balance:

$$m_{leaked} = m_{initial} + m_{added} - m_{final}$$

$$m_{leaked} = 100 + 15 - 95 = 20 \text{ kg}$$

Step 2: Convert to CO₂e:

$$E_{fugitive} = 20 \times 3,922 = 78,440 \text{ kg CO}_2e = 78.44 \text{ tonnes CO}_2e$$

Answer: 78.44 tonnes CO₂e

Note: The 15 kg recharge doesn't all leak; some replaces the leaked amount and some adds to inventory.

EXAMPLE 5.6 A boiler has thermal efficiency of 85%. It consumes 200,000 m³ of natural gas (heating value = 38 MJ/m³). Calculate: (a) Useful heat output (GJ) (b) CO₂ emissions (tonnes) (c) Emission intensity (kg CO₂/GJ useful heat)

Solution:

(a) Useful heat output:

Total energy input: 200,000 = 7,600,000\$ MJ = 7,600 GJ

Useful output: $7,600 \times 0.85 = 6,460 \text{ GJ}$

(b) CO₂ emissions:

$$E = 200,000 \times 1.91 = 382,000 \text{ kg} = 382 \text{ tonnes CO}_2$$

(c) Emission intensity:

$$I = \frac{382,000 \text{ kg}}{6,460 \text{ GJ}} = 59.1 \text{ kg CO}_2/\text{GJ}$$

Answer: (a) 6,460 GJ; (b) 382 tonnes CO₂; (c) 59.1 kg CO₂/GJ

EXAMPLE 5.7 Derive the relationship between distance-based and fuel-based emission factors: $EF_{distance} = EF_{fuel}/FE$, where FE is fuel economy.

Solution (Derivation):

Given: - Fuel-based: $E = FC \times EF_{fuel}$ - Distance-based: $E = D \times EF_{distance}$ - Fuel economy: $FE = \frac{D}{FC}$ (distance per unit fuel)

Step 1: From fuel economy:

$$FC = \frac{D}{FE}$$

Step 2: Substitute into fuel-based formula:

$$E = \frac{D}{FE} \times EF_{fuel}$$

Step 3: Rearrange:

$$E = D \times \frac{EF_{fuel}}{FE}$$

Step 4: Compare with distance-based formula:

$$E = D \times EF_{distance}$$

Therefore:

$$EF_{distance} = \frac{EF_{fuel}}{FE}$$

Example: If $EF_{fuel} = 2.68 \text{ kg/L}$ and $FE = 12.5 \text{ km/L}$, then:

$$EF_{distance} = \frac{2.68}{12.5} = 0.2144 \text{ kg/km}$$

EXAMPLE 5.8 A steel plant uses electric arc furnaces and consumes:

- Electricity: 500,000 MWh (Scope 2)
- Natural gas: 10,000,000 m³ (Scope 1)
- Electrode consumption releases: 5,000 tonnes CO₂ (Scope 1 process)

Calculate total Scope 1 emissions.

Solution:

Natural gas combustion:

$$E_{NG} = 10,000,000 \times 1.91 = 19,100,000 \text{ kg} = 19,100 \text{ tonnes CO}_2$$

Process emissions (electrode):

$$E_{process} = 5,000 \text{ tonnes CO}_2$$

Total Scope 1:

$$E_{Scope\ 1} = 19,100 + 5,000 = 24,100 \text{ tonnes CO}_2$$

Answer: 24,100 tonnes CO₂ (Scope 1 only; electricity is Scope 2)

EXAMPLE 5.9 Calculate CH₄ and N₂O emissions (in CO₂e) from burning 1,000,000 m³ of natural gas in a boiler. Use emission factors from Table 5.1 and GWP_s: CH₄ = 29.8, N₂O = 273.

Solution:

CH₄ emissions:

$$E_{CH_4} = 1,000,000 \times 0.00004 = 40 \text{ kg CH}_4$$

$$E_{CH_4,CO_2e} = 40 \times 29.8 = 1,192 \text{ kg CO}_2e = 1.19 \text{ tonnes CO}_2e$$

N₂O emissions:

$$E_{N_2O} = 1,000,000 \times 0.00001 = 10 \text{ kg N}_2O$$

$$E_{N_2O, CO_2e} = 10 \times 273 = 2,730 \text{ kg CO}_2e = 2.73 \text{ tonnes CO}_2e$$

Total non-CO₂:

$$E_{non-CO_2} = 1.19 + 2.73 = 3.92 \text{ tonnes CO}_2e$$

CO₂ emissions (for comparison):

$$E_{CO_2} = 1,000,000 \times 1.91 = 1,910 \text{ tonnes CO}_2$$

Total:

$$E_{total} = 1,910 + 3.92 = 1,913.92 \text{ tonnes CO}_2e$$

Answer: CH₄: 1.19 tonnes CO₂e; N₂O: 2.73 tonnes CO₂e; Total: 3.92 tonnes CO₂e

Note: Non-CO₂ gases represent only 0.2% of total, so often neglected in Scope 1 stationary combustion.

EXAMPLE 5.10 A company operates a vehicle fleet with the following annual data:

Vehicle			
Type	Count	Avg Distance (km/yr)	Fuel Economy (L/100km)
Sedans	50	20,000	8
SUVs	30	25,000	12
Trucks	20	30,000	15

Calculate total mobile combustion emissions using diesel EF = 2.68 kg/L.

Solution:

Sedans: - Total distance: 50 ,000 = 1,000,000\$ km - Fuel consumed:

$$1,000,000 \times \frac{8}{100} = 80,000 \text{ L} - \text{Emissions: } 80,000 \times 2.68 = 214,400 \text{ kg} = 214.4 \text{ tonnes CO}_2$$

SUVs: - Total distance: $30 \times 25,000 = 750,000$ km - Fuel consumed: $750,000 \times \frac{12}{100} = 90,000$ L

- Emissions: $90,000 \times 2.68 = 241,200$ kg = 241.2 tonnes CO₂

Trucks: - Total distance: $20 \times 30,000 = 600,000$ km - Fuel consumed: $600,000 \times \frac{15}{100} = 90,000$ L

- Emissions: $90,000 \times 2.68 = 241,200$ kg = 241.2 tonnes CO₂

Total:

$$E_{total} = 214.4 + 241.2 + 241.2 = 696.8 \text{ tonnes CO}_2$$

Answer: 696.8 tonnes CO₂

Summary Table:

Vehicle		
Type	Emissions (tonnes)	Percentage
Sedans	214.4	30.8%
SUVs	241.2	34.6%
Trucks	241.2	34.6%
Total	696.8	100%

SUPPLEMENTARY PROBLEMS

5.11 Facility burns 500,000 m³ natural gas and 100 tonnes coal. Find total CO₂. **Ans.** 1,195 tonnes CO₂

5.12 Fleet drives 200,000 km at 10 L/100km. Calculate emissions (EF = 2.31 kg/L gasoline). **Ans.** 46.2 tonnes CO₂

5.13 Production of 1,000 tonnes of cement clinker from limestone. Calculate process CO₂.
Ans. 440 tonnes CO₂

5.14 Refrigerant leak: 10 kg R-134a (GWP = 1,530). Find CO_{2e}. **Ans.** 15.3 tonnes CO_{2e}

5.15 Boiler: 80% efficiency, 100,000 m³ gas (38 MJ/m³). Find emission intensity (kg/GJ useful). **Ans.** 62.8 kg CO₂/GJ

5.16 Derive $E F_{distance}$ if $E F_{fuel} = 2.31 \text{ kg/L}$ and FE = 15 km/L. **Ans.** 0.154 kg/km

5.17 Ammonia plant: 10,000 tonnes NH₃. Calculate process CO₂ (use stoichiometry). **Ans.** 9,693 tonnes CO₂

5.18 Mass balance: initial 50 kg, added 8 kg, final 52 kg. Find leaked amount. **Ans.** 6 kg

5.19 Natural gas combustion (100,000 m³): Calculate total CO_{2e} including CH₄ and N₂O.

Ans. 191.4 tonnes CO_{2e}

5.20 10 trucks, 40,000 km/yr each, 18 L/100km. Find total emissions (diesel). **Ans.** 193.0 tonnes CO₂

Chapter 6: SCOPE 2 EMISSIONS - PURCHASED ENERGY

6.1 LOCATION-BASED METHOD

Formula:

$$E_{Scope2} = \sum_i (\textcolor{red}{E} C_i \times E F_{grid,i}) \textcolor{red}{i}$$

where: - $E C_i$ = Energy consumption in region i (MWh) - $E F_{grid,i}$ = Grid average emission factor for region i (kg CO₂/MWh)

Grid Emission Factor Calculation:

$$E F_{grid} = \frac{\sum (Generation_j \times E F_j)}{\sum Generation_j}$$

where j indexes different generation sources (coal, gas, nuclear, renewables, etc.).

6.2 MARKET-BASED METHOD

Formula:

$$E_{Scope2} = \sum_i (\textcolor{red}{E} C_i \times E F_{supplier,i}) \textcolor{red}{i}$$

where $E F_{supplier,i}$ is the emission factor of the specific electricity supplier or contractual instrument.

Hierarchy of emission factors: 1. Energy attribute certificates (RECs, GOs) 2. Supplier-specific emission rates 3. Residual mix 4. Grid average (if no other data available)

6.3 DUAL REPORTING

Companies must report both location-based and market-based Scope 2 emissions to provide transparency.

Quality Criteria for Contractual Instruments: - Vintage (same year as consumption) - Geography (same market) - Additionality (new renewable capacity)

6.4 TRANSMISSION AND DISTRIBUTION LOSSES

Total Scope 2 including T&D losses:

$$E_{total} = E_{direct} + E_{T \wedge D}$$

where:

$$E_{T \wedge D} = EC \times EF_{grid} \times \frac{Loss\ Rate}{1 - Loss\ Rate}$$

Typical T&D loss rates: 5-10%

SOLVED PROBLEMS

EXAMPLE 6.1 A facility consumes 50,000 MWh of electricity annually. The grid emission factor is 0.45 kg CO₂/kWh. Calculate Scope 2 emissions using the location-based method.

Solution:

Convert MWh to kWh: 50,000 = 50,000,000 \$

$$E_{Scope\ 2} = 50,000,000 \times 0.45 = 22,500,000 \text{ kg CO}_2 = 22,500 \text{ tonnes CO}_2$$

Alternative (using tonnes/MWh):

$$EF = 0.45 \text{ kg/kWh} = 450 \text{ kg/MWh} = 0.45 \text{ tonnes/MWh}$$

$$E_{Scope\ 2} = 50,000 \times 0.45 = 22,500 \text{ tonnes CO}_2$$

Answer: 22,500 tonnes CO₂

EXAMPLE 6.2 Calculate the grid average emission factor for a region with the following generation mix:

Source	Generation (GWh)	Emission Factor (kg CO ₂ /kWh)
--------	------------------	---

Coal	40,000	0.95
Natural Gas	30,000	0.45
Nuclear	20,000	0.00
Hydro	8,000	0.00
Wind	2,000	0.00

Solution:

Step 1: Calculate total generation:

$$Total = 40,000 + 30,000 + 20,000 + 8,000 + 2,000 = 100,000 \text{ GWh}$$

Step 2: Calculate weighted emissions:

Coal: $40,000 \times 0.95 = 38,000$ tonnes CO₂/GWh Gas: $30,000 \times 0.45 = 13,500$ tonnes CO₂/GWh

Others: $50,000 \times 0.00 = 0$ tonnes CO₂/GWh

Total emissions: $38,000 + 13,500 = 51,500$ tonnes CO₂/GWh

Step 3: Calculate grid average:

$$EF_{grid} = \frac{51,500}{100,000} = 0.515 \text{ tonnes CO}_2/\text{MWh} = 0.515 \text{ kg CO}_2/\text{kWh}$$

Answer: 0.515 kg CO₂/kWh

Breakdown: - Coal contribution: $\frac{38,000}{51,500} = 73.8\%$ - Gas contribution: $\frac{13,500}{51,500} = 26.2\%$

EXAMPLE 6.3 A company consumes 100,000 MWh annually: - 60,000 MWh covered by renewable energy certificates (RECs) with EF = 0 - 40,000 MWh from grid (EF = 0.50 kg CO₂/kWh)

Calculate: (a) Location-based Scope 2 emissions (b) Market-based Scope 2 emissions

Solution:

(a) Location-based:

Uses grid average for all consumption:

$$E_{location} = 100,000 \times 0.50 = 50,000 \text{ tonnes CO}_2$$

(b) Market-based:

Uses specific contractual instruments:

$$E_{market} = (60,000 \times 0) + (40,000 \times 0.50)$$

$$E_{market} = 0 + 20,000 = 20,000 \text{ tonnes CO}_2$$

Answer: (a) 50,000 tonnes CO₂; (b) 20,000 tonnes CO₂

Reduction claimed: 50,000 - 20,000 = 30,000\$ tonnes CO₂ through renewable energy procurement

EXAMPLE 6.4 Calculate Scope 2 emissions including T&D losses for: - Consumption: 10,000 MWh - Grid EF: 0.40 kg CO₂/kWh - T&D loss rate: 8%

Solution:

Step 1: Direct emissions (at point of consumption):

$$E_{direct} = 10,000 \times 0.40 = 4,000 \text{ tonnes CO}_2$$

Step 2: T&D loss emissions:

$$E_{T \wedge D} = 10,000 \times 0.40 \times \frac{0.08}{1 - 0.08}$$

$$E_{T \wedge D} = 4,000 \times \frac{0.08}{0.92} = 4,000 \times 0.0870 = 348 \text{ tonnes CO}_2$$

Step 3: Total Scope 2:

$$E_{total} = 4,000 + 348 = 4,348 \text{ tonnes CO}_2$$

Answer: Total Scope 2 = 4,348 tonnes CO₂ (direct: 4,000; T&D: 348)

Note: T&D losses add 8.7% to direct emissions.

EXAMPLE 6.5 Prove that the T&D loss emission formula is: $E_{T \wedge D} = E_{direct} \times \frac{L}{1-L}$ where L is the loss rate.

Solution (Proof):

Given: - Consumption at facility: C - Loss rate: L - Generation required: G

Step 1: Relationship between generation and consumption:

$$C = G(1-L)$$

Therefore:

$$G = \frac{C}{1-L}$$

Step 2: Losses in transmission:

$$Losses = G - C = \frac{C}{1-L} - C = C \left(\frac{1}{1-L} - 1 \right) = C \left(\frac{1 - (1-L)}{1-L} \right) = \frac{CL}{1-L}$$

Step 3: Emissions from losses:

$$E_{T \wedge D} = Losses \times EF = \frac{CL}{1-L} \times EF$$

Step 4: Since $E_{direct} = C \times EF$:

$$E_{T \wedge D} = E_{direct} \times \frac{L}{1-L}$$



EXAMPLE 6.6 A data center consumes 200,000 MWh annually in two regions: - Region A: 120,000 MWh at 0.35 kg CO₂/kWh - Region B: 80,000 MWh at 0.55 kg CO₂/kWh

Calculate total Scope 2 emissions and weighted average emission factor.

Solution:

Region A:

$$E_A = 120,000 \times 0.35 = 42,000 \text{ tonnes CO}_2$$

Region B:

$$E_B = 80,000 \times 0.55 = 44,000 \text{ tonnes CO}_2$$

Total:

$$E_{total} = 42,000 + 44,000 = 86,000 \text{ tonnes CO}_2$$

Weighted average EF:

$$EF_{avg} = \frac{86,000}{200,000} = 0.43 \text{ tonnes/MWh} = 0.43 \text{ kg/kWh}$$

Answer: Total = 86,000 tonnes CO₂; Weighted EF = 0.43 kg/kWh

EXAMPLE 6.7 A manufacturing facility has: - Electricity consumption: 80,000 MWh (EF = 0.48 kg/kWh) - Steam purchased from neighbor: 50,000 tonnes (EF = 0.25 kg CO₂/kg steam)

Calculate total Scope 2 emissions.

Solution:

Electricity:

$$E_{elec} = 80,000 \times 0.48 = 38,400 \text{ tonnes CO}_2$$

Steam:

$$E_{steam} = 50,000 \times 0.25 = 12,500 \text{ tonnes CO}_2$$

Total Scope 2:

$$E_{Scope\ 2} = 38,400 + 12,500 = 50,900 \text{ tonnes CO}_2$$

Answer: 50,900 tonnes CO₂ (electricity: 75.4%; steam: 24.6%)

EXAMPLE 6.8 Calculate the emission reduction from switching 30% of electricity to renewables:
- Original consumption: 150,000 MWh at 0.50 kg/kWh (all grid)
- New: 105,000 MWh grid + 45,000 MWh renewables (EF = 0)

Solution:

Original (location-based):

$$E_{original} = 150,000 \times 0.50 = 75,000 \text{ tonnes CO}_2$$

New (market-based):

$$E_{new} = (105,000 \times 0.50) + (45,000 \times 0) = 52,500 \text{ tonnes CO}_2$$

Reduction:

$$\Delta E = 75,000 - 52,500 = 22,500 \text{ tonnes CO}_2$$

Percentage reduction:

$$\frac{22,500}{75,000} \times 100\% = 30\%$$

Answer: 22,500 tonnes CO₂ reduction (30%)

Note: Percentage reduction equals percentage of renewable procurement.

EXAMPLE 6.9 A grid has the following characteristics: - Total generation: 500,000 GWh - Coal: 200,000 GWh at 0.90 kg/kWh - Gas: 150,000 GWh at 0.40 kg/kWh - Renewables: 150,000 GWh at 0.00 kg/kWh

After adding 50,000 GWh of new solar (displacing coal), calculate the new grid EF.

Solution:

Original grid EF:

$$E F_{old} = \frac{(200,000 \times 0.90) + (150,000 \times 0.40) + (150,000 \times 0)}{500,000}$$

$$E F_{old} = \frac{180,000 + 60,000 + 0}{500,000} = \frac{240,000}{500,000} = 0.48 \text{ kg/kWh}$$

New generation mix: - Coal: 200,000 - 50,000 = 150,000 GWh - Gas: 150,000 GWh - Renewables: 150,000 + 50,000 = 200,000 GWh - Total: 500,000 GWh

New grid EF:

$$E F_{new} = \frac{(150,000 \times 0.90) + (150,000 \times 0.40) + (200,000 \times 0)}{500,000}$$

$$E F_{new} = \frac{135,000 + 60,000 + 0}{500,000} = \frac{195,000}{500,000} = 0.39 \text{ kg/kWh}$$

Reduction:

$$\Delta E F = 0.48 - 0.39 = 0.09 \text{ kg/kWh (18.75\% reduction)}$$

Answer: New EF = 0.39 kg/kWh (reduced by 0.09 kg/kWh)

EXAMPLE 6.10 Derive the relationship between location-based and market-based Scope 2 when a fraction f of electricity is from renewables (EF = 0):

Solution (Derivation):

Given: - Total consumption: C - Renewable fraction: f (where $0 \leq f \leq 1$) - Grid EF: $E F_g$

Location-based (all from grid):

$$E_{location} = C \times EF_g$$

Market-based: - Renewable portion: fC with $EF=0$ - Grid portion: $(1-f)C$ with $EF=EF_g$

$$E_{market} = (fC \times 0) + [(1-f)C \times EF_g]$$

$$E_{market} = (1-f) \times C \times EF_g$$

$$E_{market} = (1-f) \times E_{location}$$

Therefore:

$$\frac{E_{market}}{E_{location}} = 1 - f$$

Or:

$$E_{market} = E_{location} \times (1 - f)$$

Example: If 40% renewable ($f = 0.4$):

$$E_{market} = E_{location} \times 0.6 = 60\% \text{ of location-based}$$



SUPPLEMENTARY PROBLEMS

6.11 Consumption: 25,000 MWh, Grid EF: 0.52 kg/kWh. Find Scope 2. **Ans.** 13,000 tonnes CO₂

6.12 Grid mix: 50,000 GWh coal (0.88 kg/kWh), 30,000 GWh gas (0.42 kg/kWh), 20,000 GWh hydro (0). Find grid EF. **Ans.** 0.566 kg/kWh

6.13 80,000 MWh total: 50,000 MWh RECs (EF=0), 30,000 MWh grid (0.45 kg/kWh). Find market-based Scope 2. **Ans.** 13,500 tonnes CO₂

6.14 Consumption: 5,000 MWh, Grid EF: 0.38 kg/kWh, T&D loss: 6%. Find total Scope 2 with T&D. **Ans.** 2,021 tonnes CO₂

6.15 Prove that T&D losses as percentage of direct emissions equal $\frac{L}{1-L} \times 100\%$.

6.16 Two regions: 60,000 MWh at 0.30 kg/kWh, 40,000 MWh at 0.60 kg/kWh. Find weighted EF. **Ans.** 0.42 kg/kWh

6.17 Electricity: 120,000 MWh (0.44 kg/kWh), Steam: 80,000 tonnes (0.20 kg/kg). Find total Scope 2. **Ans.** 68,800 tonnes CO₂

6.18 Original: 200,000 MWh at 0.55 kg/kWh. Switch 25% to renewables. Find reduction. **Ans.** 27,500 tonnes CO₂

6.19 Grid: 300,000 GWh total, emissions 120,000 tonnes CO₂/GWh. Add 30,000 GWh solar (displacing coal at 0.90 kg/kWh). Find new grid EF. **Ans.** 0.31 kg/kWh

6.20 If 60% renewable, express market-based as fraction of location-based. **Ans.** 0.40 (or 40%)

Chapter 7: SCOPE 3 EMISSIONS - VALUE CHAIN

Theorem 7.1 (Value Chain Attribution)

Statement:

For a product with supply chain network $G=(V,E)$ where V is the set of processes and E is the set of material flows, the total Scope 3 emissions attributable to product p are:

$$E_3^{(p)} = \sum_{i \in V \setminus p} \alpha_i^{(p)} \cdot e_i$$

where $\alpha_i^{(p)}$ is the attribution factor (fraction of process i 's emissions allocated to product p) and e_i is the total emissions from process i .

Proof:

Step 1: Define attribution based on economic value.

For process i producing output q_i with value v_i , and product p purchasing quantity $q_i^{(p)}$ with value $v_i^{(p)}$:

$$\alpha_i^{(p)} = \frac{v_i^{(p)}}{v_i} = \frac{q_i^{(p)} \cdot \text{price}_i}{q_i \cdot \text{price}_i} = \frac{q_i^{(p)}}{q_i}$$

Step 2: Sum over all upstream processes.

Total Scope 3 emissions are the sum of attributed emissions from all processes in the value chain excluding the reporting entity:

$$E_3^{(p)} = \sum_{i \in V \setminus p} \alpha_i^{(p)} \cdot e_i$$

Step 3: Verify conservation property.

For all products using process i :

$$\sum_p \alpha_i^{(p)} = \sum_p \frac{q_i^{(p)}}{q_i} = \frac{\sum_p q_i^{(p)}}{q_i} = 1$$

This ensures all emissions are allocated exactly once. ■

Corollary 7.1: For a linear supply chain, attribution factors multiply along the chain:

$$\alpha_i^{(p)} = \prod_{j \in \text{path}(i \rightarrow p)} \frac{q_j^{(\text{next})}}{q_j}$$

Sources: GHG Protocol Scope 3 Standard [2], Matthews et al. (2008), Huang et al. (2009)

7.1 THE 15 CATEGORIES OF SCOPE 3

Upstream Categories: 1. Purchased goods and services 2. Capital goods 3. Fuel- and energy-related activities 4. Upstream transportation and distribution 5. Waste generated in operations 6. Business travel 7. Employee commuting 8. Upstream leased assets

Downstream Categories: 9. Downstream transportation and distribution 10. Processing of sold products 11. Use of sold products 12. End-of-life treatment of sold products 13. Downstream leased assets 14. Franchises 15. Investments

7.2 CALCULATION METHODS

Spend-Based Method:

$$E = \text{Spend} \times EF_{economic}$$

where $EF_{economic}$ is in kg CO₂/\\$ (from EEIO models).

Activity-Based Method:

$$E = \text{Activity} \times EF_{physical}$$

where Activity is in physical units (kg, km, kWh, etc.).

Hybrid Method: Combines supplier-specific data with EEIO for gaps.

7.3 SCREENING AND PRIORITIZATION

Relevance Criteria: - Size: Contributes >5% of total Scope 3 - Influence: Company can reduce emissions - Risk: Exposure to climate-related risks - Stakeholder: Important to stakeholders

Pareto Principle: Often 80% of Scope 3 comes from 20% of categories.

7.4 ALLOCATION METHODS

Physical Allocation:

$$\text{Allocation} = \frac{\text{Physical Output}_A}{\text{Total Physical Output}}$$

Economic Allocation:

$$\text{Allocation} = \frac{\text{Revenue}_A}{\text{Total Revenue}}$$

SOLVED PROBLEMS

EXAMPLE 7.1 A company spends 10 million on purchased goods with an average EEIO factor of 0.5 kg CO₂/\$. Calculate Category 1 emissions.

Solution:

Using spend-based method:

$$E = \text{Spend} \times E F_{economic} = 10,000,000 \times 0.5 = 5,000,000 \text{ kg CO}_2$$

$$E = 5,000 \text{ tonnes CO}_2$$

Answer: 5,000 tonnes CO₂

Note: This is a screening estimate. More accurate calculation would use supplier-specific data or physical quantities.

PROBLEM 7.2 Calculate emissions from business travel: - Air travel: 500,000 km at 0.15 kg CO₂/passenger-km - Rental cars: 100,000 km at 0.20 kg CO₂/km - Hotels: 2,000 room-nights at 30 kg CO₂/night

Solution:

Air travel:

$$E_{air} = 500,000 \times 0.15 = 75,000 \text{ kg} = 75 \text{ tonnes CO}_2$$

Rental cars:

$$E_{car} = 100,000 \times 0.20 = 20,000 \text{ kg} = 20 \text{ tonnes CO}_2$$

Hotels:

$$E_{hotel} = 2,000 \times 30 = 60,000 \text{ kg} = 60 \text{ tonnes CO}_2$$

Total Category 6:

$$E_{total} = 75 + 20 + 60 = 155 \text{ tonnes CO}_2$$

Answer: 155 tonnes CO₂ (air: 48.4%, hotels: 38.7%, cars: 12.9%)

PROBLEM 7.3 A logistics company transports goods 2,000,000 tonne-km annually. The emission factor is 0.062 kg CO₂/tonne-km. Calculate Category 4 (upstream transportation) emissions.

Solution:

$$E = Activity \times EF = 2,000,000 \times 0.062 = 124,000 \text{ kg CO}_2 = 124 \text{ tonnes CO}_2$$

Answer: 124 tonnes CO₂

Note: Tonne-km = mass (tonnes) × distance (km)

PROBLEM 7.4 A manufacturing facility generates 500 tonnes of waste annually: - 300 tonnes recycled (EF = 0.05 tonnes CO₂/tonne waste) - 150 tonnes landfilled (EF = 0.50 tonnes CO₂/tonne waste) - 50 tonnes incinerated (EF = 0.30 tonnes CO₂/tonne waste)

Calculate Category 5 (waste) emissions.

Solution:

Recycled:

$$E_{recycle} = 300 \times 0.05 = 15 \text{ tonnes CO}_2$$

Landfilled:

$$E_{landfill} = 150 \times 0.50 = 75 \text{ tonnes CO}_2$$

Incinerated:

$$E_{incinerate} = 50 \times 0.30 = 15 \text{ tonnes CO}_2$$

Total:

$$E_{total} = 15 + 75 + 15 = 105 \text{ tonnes CO}_2$$

Answer: 105 tonnes CO₂

Breakdown: Landfill (71.4%), Recycling (14.3%), Incineration (14.3%)

PROBLEM 7.5 Calculate Category 3 (fuel and energy-related activities) for electricity consumption of 100,000 MWh: - Scope 2 (direct): 100,000 MWh × 0.40 kg/kWh = 40,000 tonnes CO₂ - Upstream (extraction, processing, T&D): 8% of Scope 2

Solution:

Upstream emissions:

$$E_{upstream} = E_{Scope\ 2} \times 0.08 = 40,000 \times 0.08 = 3,200 \text{ tonnes CO}_2$$

Answer: 3,200 tonnes CO₂ (Category 3)

Note: This is in addition to the 40,000 tonnes reported in Scope 2.

PROBLEM 7.6 A software company has 1,000 employees commuting: - 400 drive alone: 50 km/day, 220 days/year, 0.20 kg CO₂/km - 300 carpool (2 per car): 40 km/day, 220 days/year, 0.20 kg CO₂/km - 200 use public transit: 30 km/day, 220 days/year, 0.05 kg CO₂/km - 100 work from home: 0 emissions

Calculate Category 7 (employee commuting) emissions.

Solution:

Drive alone:

$$E_1 = 400 \times 50 \times 220 \times 0.20 = 880,000 \text{ kg} = 880 \text{ tonnes CO}_2$$

Carpool (allocated per person):

$$E_2 = 300 \times 40 \times 220 \times \frac{0.20}{2} = 264,000 \text{ kg} = 264 \text{ tonnes CO}_2$$

Public transit:

$$E_3 = 200 \times 30 \times 220 \times 0.05 = 66,000 \text{ kg} = 66 \text{ tonnes CO}_2$$

Work from home:

$$E_4 = 0$$

Total:

$$E_{total} = 880 + 264 + 66 + 0 = 1,210 \text{ tonnes CO}_2$$

Per employee average:

$$\frac{1,210}{1,000} = 1.21 \text{ tonnes CO}_2/\text{employee}$$

Answer: 1,210 tonnes CO₂ total; 1.21 tonnes/employee average

PROBLEM 7.7 A manufacturer sells 10,000 units of a product. Each unit: - Requires 5 kWh electricity during use phase - Used for 5 years - Grid EF = 0.45 kg CO₂/kWh

Calculate Category 11 (use of sold products) emissions for one year.

Solution:

Annual electricity per unit:

$$E_{unit/year} = 5 \text{ kWh/year}$$

Total annual electricity:

$$E_{total} = 10,000 \times 5 = 50,000 \text{ kWh}$$

Emissions:

$$E = 50,000 \times 0.45 = 22,500 \text{ kg CO}_2 = 22.5 \text{ tonnes CO}_2$$

Lifetime emissions (5 years):

$$E_{lifetime} = 22.5 \times 5 = 112.5 \text{ tonnes CO}_2$$

Answer: 22.5 tonnes CO₂/year; 112.5 tonnes CO₂ lifetime

Note: Companies typically report annual emissions but should track lifetime impact.

PROBLEM 7.8 A company has a 40% ownership stake in a joint venture that emits 50,000 tonnes CO₂ annually. Calculate the company's Category 15 (investments) emissions using the equity share approach.

Solution:

Equity share method:

$$E_{company} = E_{investee} \times Owners\ hip\% = 50,000 \times 0.40 = 20,000 \text{ tonnes CO}_2$$

Answer: 20,000 tonnes CO₂

Alternative methods: - **Operational control:** 0 or 50,000 (all or nothing) - **Financial control:** Depends on >50% ownership

PROBLEM 7.9 Calculate the allocation factor for a co-product using economic allocation: -

Product A: 1,000 tonnes produced, 500/tonne - Product B: 500 tonnes produced, 1,200/tonne - Total process emissions: 10,000 tonnes CO₂

Solution:

- Revenue A: \$1,000 = \$500,000
- Revenue B: \$500 ,200 = \$600,000
- Total revenue: \$1,100,000

Step 2: Calculate allocation factors:

$$AF_A = \frac{500,000}{1,100,000} = 0.4545 = 45.45\%$$

$$AF_B = \frac{600,000}{1,100,000} = 0.5455 = 54.55\%$$

Step 3: Allocate emissions:

$$E_A = 10,000 \times 0.4545 = 4,545 \text{ tonnes CO}_2$$

$$E_B = 10,000 \times 0.5455 = 5,455 \text{ tonnes CO}_2$$

Answer: Product A: 4,545 tonnes CO₂; Product B: 5,455 tonnes CO₂

Emission intensities: - Product A: $\frac{4,545}{1,000} = 4.545$ tonnes CO₂/tonne product - Product B: $\frac{5,455}{500} = 10.91$ tonnes CO₂/tonne product

PROBLEM 7.10 A company's Scope 3 screening shows:

Category	Estimated Emissions (tonnes CO ₂)
1. Purchased goods	50,000
2. Capital goods	5,000
3. Fuel/energy	3,000
4. Upstream transport	8,000
5. Waste	500
6. Business travel	2,000
7. Commuting	1,500
11. Use of sold products	100,000
Others	2,000

Calculate: (a) Total Scope 3 (b) Top 3 categories by percentage (c) Categories meeting the 5% materiality threshold

Solution:

(a) Total Scope 3:

$$E_{total} = 50,000 + 5,000 + 3,000 + 8,000 + 500 + 2,000 + 1,500 + 100,000 + 2,000$$

$$E_{total} = 172,000 \text{ tonnes CO}_2$$

(b) Calculate percentages:

Category	Emissions	Percentage
----------	-----------	------------

11. Use of products	100,000	58.1%
1. Purchased goods	50,000	29.1%
4. Upstream transport	8,000	4.7%
2. Capital goods	5,000	2.9%
3. Fuel/energy	3,000	1.7%
6. Business travel	2,000	1.2%
Others	2,000	1.2%
7. Commuting	1,500	0.9%
5. Waste	500	0.3%

Top 3: Use of products (58.1%), Purchased goods (29.1%), Upstream transport (4.7%)

(c) **Categories $\geq 5\%$ threshold:** - Category 11: 58.1% ✓ - Category 1: 29.1% ✓

Answer: (a) 172,000 tonnes CO₂ (b) Categories 11, 1, 4 (c) Categories 11 and 1 meet 5% threshold

Insight: Two categories account for 87.2% of Scope 3. Focus efforts here.

SUPPLEMENTARY PROBLEMS

7.11 Spend 5M on services, EEIO factor 0.4 kg/\$. Find Cat 1 emissions. **Ans.** 2,000 tonnes CO₂

7.12 Business travel: 300,000 km air (0.18 kg/km), 1,500 hotel nights (25 kg/night). Find total. **Ans.** 91.5 tonnes CO₂

7.13 Transport 1,500,000 tonne-km at 0.055 kg/tonne-km. Find emissions. **Ans.** 82.5 tonnes CO₂

7.14 Waste: 200 t recycled (0.04 kg/kg), 100 t landfilled (0.45 kg/kg). Find total. **Ans.** 53 tonnes CO₂

7.15 Scope 2 = 25,000 tonnes. Cat 3 upstream = 10% of Scope 2. Find Cat 3. **Ans.** 2,500 tonnes CO₂

7.16 500 employees, 40 km/day, 220 days, 0.18 kg/km. Find commuting emissions. **Ans.** 792 tonnes CO₂

7.17 Sell 5,000 units, 10 kWh/unit/year, 4-year life, 0.50 kg/kWh. Find annual Cat 11. **Ans.** 25 tonnes CO₂/year

7.18 30% stake in company emitting 80,000 tonnes. Find Cat 15 (equity share). **Ans.** 24,000 tonnes CO₂

7.19 Economic allocation: Product A (\$400k revenue), Product B (\$600k revenue), 5,000 tonnes total. Find allocation to A. **Ans.** 2,000 tonnes CO₂

7.20 Scope 3 categories: 60,000 (Cat 1), 80,000 (Cat 11), 10,000 (others). Which meet 5% threshold? **Ans.** Categories 1 and 11

Chapter 8: EMISSION FACTORS AND DATA QUALITY

8.1 TYPES OF EMISSION FACTORS

Tier Hierarchy (IPCC): - Tier 1: Default factors (country/global averages) - Tier 2: Country-specific factors - Tier 3: Facility-specific, measured data

Specificity Hierarchy: 1. Supplier-specific 2. Industry-specific 3. Regional average 4. National average 5. Global average

8.2 DATA QUALITY INDICATORS (DQI)

Five Dimensions: 1. **Technological representativeness:** How well does the data match the actual technology? 2. **Temporal representativeness:** How current is the data? 3. **Geographical representativeness:** Does it match the location? 4. **Completeness:** What percentage of sources are covered? 5. **Reliability:** How was the data collected and verified?

Scoring: Typically 1-5 scale (1 = excellent, 5 = poor)

Overall DQI:

$$DQI = \sqrt{\frac{\sum_{i=1}^5 w_i \times score_i^2}{\sum w_i}}$$

where w_i are weights (often equal).

8.3 UNCERTAINTY RATINGS

GHG Protocol Uncertainty Levels: - Very low: <10% - Low: 10-30% - Medium: 30-50% - High: 50-100% - Very high: >100%

Pedigree Matrix: Assigns uncertainty based on data quality scores.

8.4 EMISSION FACTOR DATABASES

Major Sources: - IPCC Guidelines - EPA emission factors - DEFRA/BEIS (UK) - Ecoinvent (LCA database) - GHG Protocol tools

SOLVED PROBLEMS

PROBLEM 8.1 Calculate the overall DQI for an emission factor with equal weights and scores: - Technology: 2 - Temporal: 3 - Geography: 2 - Completeness: 4 - Reliability: 3

Solution:

With equal weights ($w_i=1$ for all):

$$DQI = \sqrt{\frac{2^2+3^2+2^2+4^2+3^2}{5}}$$
$$DQI = \sqrt{\frac{4+9+4+16+9}{5}} = \sqrt{\frac{42}{5}} = \sqrt{8.4} = 2.90$$

Answer: DQI = 2.90 (on 1-5 scale, where lower is better)

Interpretation: Moderate data quality. Completeness (4) is the weakest dimension.

PROBLEM 8.2 An emission factor has a stated uncertainty of $\pm 25\%$. Convert this to: (a) 95% confidence interval if the EF = 2.5 kg CO₂/kg (b) Standard deviation assuming normal distribution

Solution:

(a) 95% Confidence Interval:

Assuming $\pm 25\%$ represents 95% CI:

$$CI = 2.5 \pm (0.25 \times 2.5) = 2.5 \pm 0.625$$

$$CI = [1.875, 3.125] \text{ kg CO}_2/\text{kg}$$

(b) Standard Deviation:

For 95% CI: $\pm 1.96\sigma$

$$1.96\sigma = 0.625$$

$$\sigma = \frac{0.625}{1.96} = 0.319 \text{ kg CO}_2/\text{kg}$$

Relative std dev:

$$\frac{0.319}{2.5} = 0.1276 = 12.76\%$$

Answer: (a) [1.875, 3.125] kg/kg; (b) $\sigma = 0.319 \text{ kg/kg}$ (12.76%)

PROBLEM 8.3 Compare two emission factors for the same activity:

Source	EF (kg CO ₂ /unit)	Uncertainty	Year	Geography
A	2.40	$\pm 15\%$	2023	Country-specific
B	2.55	$\pm 30\%$	2018	Global average

Which should be preferred and why?

Solution:

Comparison:

Source A: - More recent (2023 vs 2018) ✓ - Lower uncertainty (15% vs 30%) ✓ - Country-specific (vs global) ✓ - Lower value (2.40 vs 2.55)

Source B: - Older data - Higher uncertainty - Less geographically specific - Higher value (more conservative)

Answer: Source A is preferred due to: 1. Better temporal representativeness 2. Lower uncertainty 3. Better geographical match 4. Overall higher data quality

Exception: If conservatism is required (e.g., carbon credits), Source B's higher value might be chosen despite lower quality.

PROBLEM 8.4 An emission factor database provides: - Mean EF: 1.80 kg CO₂/kg - 5th percentile: 1.20 kg/kg - 95th percentile: 2.60 kg/kg

Assuming lognormal distribution, estimate the geometric mean and geometric standard deviation.

Solution:

For lognormal distribution: - Median ≈ Geometric mean = e^{μ} - 90% range: [5th percentile, 95th percentile]

Step 1: Estimate median (geometric mean):

$$GM \approx \sqrt{P_5 \times P_{95}} = \sqrt{1.20 \times 2.60} = \sqrt{3.12} = 1.77 \text{ kg/kg}$$

Step 2: For lognormal, the 90% range spans approximately ± 1.645 standard deviations in log space:

$$\begin{aligned} \ln(P_{95}) - \ln(P_5) &= 2 \times 1.645 \times \sigma_{\ln} \\ \sigma_{\ln} &= \frac{\ln(2.60) - \ln(1.20)}{2 \times 1.645} = \frac{0.956 - 0.182}{3.29} = \frac{0.774}{3.29} = 0.235 \end{aligned}$$

Geometric standard deviation:

$$GSD = e^{\sigma_{\ln}} = e^{0.235} = 1.265$$

Answer: Geometric mean ≈ 1.77 kg/kg; GSD ≈ 1.27

PROBLEM 8.5 Calculate the weighted average emission factor for electricity in a region where a company has multiple facilities:

Local Grid EF		
Facility	Consumption (MWh)	(kg/kWh)
A	50,000	0.35
B	30,000	0.55
C	20,000	0.42

Solution:

Step 1: Calculate emissions at each facility: - Facility A: $50,000 \times 0.35 = 17,500$ tonnes CO₂ - Facility B: $30,000 \times 0.55 = 16,500$ tonnes CO₂ - Facility C: $20,000 \times 0.42 = 8,400$ tonnes CO₂

Step 2: Calculate totals: - Total consumption: $50,000 + 30,000 + 20,000 = 100,000$ MWh - Total emissions: $17,500 + 16,500 + 8,400 = 42,400$ tonnes CO₂

Step 3: Calculate weighted average:

$$EF_{avg} = \frac{42,400}{100,000} = 0.424 \text{ tonnes/MWh} = 0.424 \text{ kg/kWh}$$

Answer: 0.424 kg CO₂/kWh

Verification:

$$EF_{avg} = \frac{(50,000 \times 0.35) + (30,000 \times 0.55) + (20,000 \times 0.42)}{100,000} = 0.424$$

✓

PROBLEM 8.6 An emission factor has been updated from 2.5 to 2.3 kg CO₂/unit. A company used 100,000 units. Calculate: (a) Emissions using old factor (b) Emissions using new factor (c) Percentage change

Solution:

(a) Old factor:

$$E_{old} = 100,000 \times 2.5 = 250,000 \text{ kg} = 250 \text{ tonnes CO}_2$$

(b) New factor:

$$E_{new} = 100,000 \times 2.3 = 230,000 \text{ kg} = 230 \text{ tonnes CO}_2$$

(c) Percentage change:

$$\Delta \% = \frac{230 - 250}{250} \times 100 \% = \frac{-20}{250} \times 100 \% = -8 \%$$

Answer: (a) 250 tonnes; (b) 230 tonnes; (c) -8% (reduction)

Note: This is a methodological change, not an actual emissions reduction. Should be disclosed in reporting.

PROBLEM 8.7 Prove that for a weighted average emission factor, $E F_{avg} = \frac{\sum E_i}{\sum A_i}$ where $E_i = A_i \times E F_i$.

Solution (Proof):

Given: $E_i = A_i \times E F_i$ for each source i

Step 1: Total emissions:

$$E_{total} = \sum_i E_i = \sum_i (\cancel{i} A_i \times E F_i) \cancel{i}$$

Step 2: Total activity:

$$A_{total} = \sum_i A_i$$

Step 3: Average emission factor by definition:

$$E F_{avg} = \frac{E_{total}}{A_{total}} = \frac{\sum_i (\cancel{i} A_i \times E F_i)}{\sum_i A_i} \cancel{i}$$

This can also be written as:

$$EF_{avg} = \sum_i \left(\frac{A_i}{A_{total}} \times EF_i \right) = \sum_i (w_i \times EF_i)$$

where $w_i = \frac{A_i}{A_{total}}$ is the weight of source i . ■

PROBLEM 8.8 A company uses three different emission factor sources for the same fuel type:

- Source 1: 2.40 kg/L (uncertainty: $\pm 10\%$)
- Source 2: 2.50 kg/L (uncertainty: $\pm 20\%$)
- Source 3: 2.35 kg/L (uncertainty: $\pm 15\%$)

Calculate the uncertainty-weighted average emission factor.

Solution:

Step 1: Convert uncertainties to standard deviations (assuming 95% CI): -

$$\sigma_1 = \frac{2.40 \times 0.10}{1.96} = 0.122 \text{ kg/L} \quad - \quad \sigma_2 = \frac{2.50 \times 0.20}{1.96} = 0.255 \text{ kg/L} \quad - \quad \sigma_3 = \frac{2.35 \times 0.15}{1.96} = 0.180 \text{ kg/L}$$

Step 2: Calculate weights (inverse variance): - $w_1 = \frac{1}{\sigma_1^2} = \frac{1}{0.0149} = 67.1$ -

$$w_2 = \frac{1}{\sigma_2^2} = \frac{1}{0.0650} = 15.4 \quad - \quad w_3 = \frac{1}{\sigma_3^2} = \frac{1}{0.0324} = 30.9 \quad - \quad W = 67.1 + 15.4 + 30.9 = 113.4$$

Step 3: Calculate weighted average:

$$EF_{avg} = \frac{(67.1 \times 2.40) + (15.4 \times 2.50) + (30.9 \times 2.35)}{113.4}$$

$$EF_{avg} = \frac{161.04 + 38.5 + 72.62}{113.4} = \frac{272.16}{113.4} = 2.40 \text{ kg/L}$$

Step 4: Calculate combined uncertainty:

$$\sigma_{avg} = \frac{1}{\sqrt{W}} = \frac{1}{\sqrt{113.4}} = \frac{1}{10.65} = 0.094 \text{ kg/L}$$

Answer: $EF_{avg} = 2.40 \pm 0.09 \text{ kg/L}$ (3.9% uncertainty)

Note: The most precise source (Source 1) dominates the weighted average.

PROBLEM 8.9 Calculate the data quality score using the pedigree matrix approach:

Dimension	Score	Weight	Uncertainty Factor
Technology	2	0.25	1.2
Temporal	3	0.20	1.5
Geography	2	0.25	1.2
Completeness	4	0.15	2.0
Reliability	3	0.15	1.5

Base uncertainty: 10%

Solution:

Step 1: Calculate combined uncertainty factor:

$$UF_{combined} = \sqrt{\sum (w_i \times UF_i^2)}$$

$$UF = \sqrt{(0.25 \times 1.2^2) + (0.20 \times 1.5^2) + (0.25 \times 1.2^2) + (0.15 \times 2.0^2) + (0.15 \times 1.5^2)}$$

$$UF = \sqrt{0.36 + 0.45 + 0.36 + 0.60 + 0.3375} = \sqrt{2.1075} = 1.452$$

Step 2: Calculate total uncertainty:

$$U_{total} = U_{base} \times UF_{combined} = 10\% \times 1.452 = 14.52\%$$

Answer: Total uncertainty $\approx 15\%$

Interpretation: Data quality issues increase base uncertainty by 45%.

PROBLEM 8.10 A company must choose between two emission factors for diesel: - Factor A: 2.68 kg/L (IPCC default, global, 2006) - Factor B: 2.71 kg/L (National database, country-specific, 2022)

The company consumed 100,000 L. Calculate emissions using both and recommend which to use.

Solution:

Factor A:

$$E_A = 100,000 \times 2.68 = 268,000 \text{ kg} = 268 \text{ tonnes CO}_2$$

Factor B:

$$E_B = 100,000 \times 2.71 = 271,000 \text{ kg} = 271 \text{ tonnes CO}_2$$

Difference:

$$\Delta E = 271 - 268 = 3 \text{ tonnes CO}_2 \text{ (1.1\% higher)}$$

Recommendation: Use Factor B because: 1. More recent (2022 vs 2006) 2. Country-specific (better geographical match) 3. From national authority (likely higher quality) 4. Difference is small (1.1%) but Factor B is more conservative

Answer: Use Factor B (271 tonnes CO₂)

SUPPLEMENTARY PROBLEMS

8.11 DQI scores (equal weights): 2, 2, 3, 3, 4. Calculate overall DQI. **Ans.** 2.92

8.12 EF = 3.0 kg/kg, uncertainty $\pm 20\%$ (95% CI). Find standard deviation. **Ans.** $\sigma = 0.306$ kg/kg

8.13 Two EFs: 2.20 (2024, $\pm 12\%$) vs 2.35 (2015, $\pm 25\%$). Which is preferred? **Ans.** First (more recent, lower uncertainty)

8.14 Lognormal: 5th %ile = 1.5, 95th %ile = 3.5. Estimate geometric mean. **Ans.** GM \approx 2.29

8.15 Facilities: 40k MWh (0.40 kg/kWh), 60k MWh (0.50 kg/kWh). Find weighted EF.

Ans. 0.46 kg/kWh

8.16 Old EF: 1.8, New EF: 1.7. Activity: 50,000 units. Find percentage change in emissions. **Ans.** -5.56%

8.17 Prove that weighted average EF equals total emissions divided by total activity.

8.18 Three EFs: $2.5 \pm 10\%$, $2.6 \pm 15\%$, $2.4 \pm 12\%$. Calculate uncertainty-weighted average.

Ans. ≈ 2.48 kg/unit

8.19 Pedigree: base 15%, factors [1.3, 1.5, 1.2, 1.8, 1.4], equal weights. Find total uncertainty. **Ans.** $\approx 21.4\%$

8.20 Diesel EFs: 2.65 kg/L (global, 2010) vs 2.69 kg/L (regional, 2023). Which to use?

Ans. Second (more recent and regional)

Chapter 9: LCA MATHEMATICAL FRAMEWORK

Theorem 9.1 (Allocation Invariance)

Statement:

For a multi-functional process producing co-products, the sum of allocated environmental impacts equals the total impact regardless of allocation method, provided allocation factors sum to unity.

Proof:

Let process j produce n co-products with allocation factors $\lambda_1, \lambda_2, \dots, \lambda_n$ where $\sum_{i=1}^n \lambda_i = 1$.

Step 1: Total environmental impact of process j is I_j .

Step 2: Impact allocated to product i is:

$$I_i^{\text{allocated}} = \lambda_i \cdot I_j$$

Step 3: Sum of allocated impacts:

$$\sum_{i=1}^n I_i^{\text{allocated}} = \sum_{i=1}^n \lambda_i \cdot I_j = I_j \sum_{i=1}^n \lambda_i = I_j \cdot 1 = I_j$$

Therefore, total allocated impact equals total process impact. ■

9.1 FUNCTIONAL UNIT

Definition: The quantified performance of a product system for use as a reference unit.

Purpose: Enables comparison between different systems providing the same function.

Examples: - “Transport of 1 tonne of goods over 1 km” - “1 m² of floor covering for 10 years” - “Illumination of 1,000 lumens for 1 hour”

9.2 SYSTEM BOUNDARY

Cut-off Criteria: - Mass: Exclude flows <1% of total mass - Energy: Exclude flows <1% of total energy - Environmental: Exclude flows <1% of total impact

Cumulative cut-off: Usually 95-99% of total impact

9.3 LCA PHASES

1. **Goal and Scope Definition**
2. **Life Cycle Inventory (LCI):** Quantify inputs/outputs
3. **Life Cycle Impact Assessment (LCIA):** Convert to environmental impacts
4. **Interpretation:** Analyze and report results

9.4 MATHEMATICAL FORMULATION

General LCA equation:

$$g = B \dot{c}$$

where: - g = Environmental impact vector ($m \times 1$) - B = Environmental intervention matrix ($m \times n$) - A = Technology matrix ($n \times n$) - f = Final demand vector ($n \times 1$)

Impact Assessment:

$$h = Qg$$

where: - h = Impact indicator vector ($k \times 1$) - Q = Characterization matrix ($k \times m$)

SOLVED PROBLEMS

PROBLEM 9.1 Define an appropriate functional unit for comparing: (a) Paper bags vs plastic bags (b) LED bulbs vs incandescent bulbs (c) Electric cars vs gasoline cars

Solution:

(a) Paper vs plastic bags:

Functional unit: “Carrying 10 kg of groceries for one shopping trip”

Rationale: - Accounts for load capacity - Single-use nature - Comparable function

(b) LED vs incandescent bulbs:

Functional unit: “Provision of 800 lumens of light for 10,000 hours”

Rationale: - Accounts for brightness (lumens) - Accounts for lifetime differences - Energy consumption normalized

(c) Electric vs gasoline cars:

Functional unit: “Transportation of one passenger over 200,000 km during a 10-year lifetime”

Rationale: - Accounts for vehicle lifetime - Typical usage pattern - Comparable service

Answer: See above functional units with rationales.

PROBLEM 9.2 A cradle-to-gate LCA has the following process flows for producing 1 tonne of product:

Process	Input	Output	CO ₂ Emissions (kg)
Raw material extraction	-	1.2 t raw material	150
Transportation	1.2 t	1.2 t	80
Manufacturing	1.2 t	1.0 t product	500
Waste treatment	0.2 t	- waste	30

Calculate total cradle-to-gate carbon footprint per tonne of product.

Solution:

Total emissions:

$$E_{total} = 150 + 80 + 500 + 30 = 760 \text{ kg CO}_2/\text{tonne product}$$

Breakdown: - Manufacturing: 500 kg (65.8%) - Raw material: 150 kg (19.7%) - Transportation: 80 kg (10.5%) - Waste: 30 kg (3.9%)

Answer: 760 kg CO₂/tonne product (cradle-to-gate)

PROBLEM 9.3 For a 2-process system with:

$$A = \begin{bmatrix} 0.1 & 0.2 \\ 0.15 & 0.1 \end{bmatrix}, B = [1.5 \quad 2.0], f = \begin{bmatrix} 100 \\ 50 \end{bmatrix}$$

Calculate total environmental impact using $g = B\dot{x}$.

Solution:

Step 1: Calculate $I - A$:

$$I - A = \begin{bmatrix} 0.9 & -0.2 \\ -0.15 & 0.9 \end{bmatrix}$$

Step 2: Calculate determinant:

$$\det = (0.9)(0.9) - (-0.2)(-0.15) = 0.81 - 0.03 = 0.78$$

Step 3: Calculate inverse:

$$\dot{x}$$

Step 4: Calculate total output:

$$x = \begin{bmatrix} 1.154 & 0.256 \\ 0.192 & 1.154 \end{bmatrix} \begin{bmatrix} 100 \\ 50 \end{bmatrix} = \begin{bmatrix} 128.2 \\ 77.0 \end{bmatrix}$$

Step 5: Calculate impact:

$$g = Bx = [1.5 \quad 2.0] \begin{bmatrix} 128.2 \\ 77.0 \end{bmatrix}$$

$$g = (1.5 \times 128.2) + (2.0 \times 77.0) = 192.3 + 154.0 = 346.3$$

Answer: Total environmental impact = 346.3 units

PROBLEM 9.4 Apply characterization factors to convert emissions to global warming potential:

Emission	Amount (kg)	GWP ₁₀₀	Impact (kg CO ₂ e)
CO ₂	1,000	1	?
CH ₄	10	29.8	?
N ₂ O	2	273	?

Calculate total GWP using $h=Qg$.

Solution:

Emission vector:

$$g = \begin{bmatrix} 1,000 \\ 10 \\ 2 \end{bmatrix}$$

Characterization matrix (GWP):

$$Q = [1 \ 29.8 \ 273]$$

Impact calculation:

$$h = Qg = [1 \ 29.8 \ 273] \begin{bmatrix} 1,000 \\ 10 \\ 2 \end{bmatrix}$$

$$h = (1 \times 1,000) + (29.8 \times 10) + (273 \times 2)$$

$$h = 1,000 + 298 + 546 = 1,844 \text{ kg CO}_2\text{e}$$

Answer: Total GWP = 1,844 kg CO₂e

Breakdown: - CO₂: 1,000 kg CO₂e (54.2%) - CH₄: 298 kg CO₂e (16.2%) - N₂O: 546 kg CO₂e (29.6%)

PROBLEM 9.5 A product has the following life cycle stages:

Stage	Emissions (kg CO ₂)	Percentage
Raw materials	200	?
Manufacturing	500	?
Transportation	100	?
Use phase	1,500	?
End-of-life	50	?

Calculate percentages and identify hotspots (>20% contribution).

Solution:

Total:

$$E_{total} = 200 + 500 + 100 + 1,500 + 50 = 2,350 \text{ kg CO}_2$$

Percentages: - Raw materials: $\frac{200}{2,350} \times 100 = 8.5\%$ - Manufacturing: $\frac{500}{2,350} \times 100 = 21.3\% \checkmark$

Hotspot - Transportation: $\frac{100}{2,350} \times 100 = 4.3\%$ - Use phase: $\frac{1,500}{2,350} \times 100 = 63.8\% \checkmark$ Hotspot -

End-of-life: $\frac{50}{2,350} \times 100 = 2.1\%$

Answer: - Total: 2,350 kg CO₂ - Hotspots: Use phase (63.8%), Manufacturing (21.3%) - Combined hotspots: 85.1% of total

Recommendation: Focus improvement efforts on use phase energy efficiency and manufacturing processes.

PROBLEM 9.6 Calculate the allocation factor for a multi-output process using physical allocation:

Process produces: - Product A: 1,000 kg - Product B: 500 kg
- Byproduct C: 200 kg (no economic value)

Total process emissions: 5,000 kg CO₂

Solution:

Step 1: Calculate total physical output (excluding byproducts with no value):

$$Total = 1,000 + 500 = 1,500 \text{ kg}$$

(Byproduct C excluded as it has no economic value)

Step 2: Calculate allocation factors:

$$AF_A = \frac{1,000}{1,500} = 0.667 = 66.7\%$$

$$AF_B = \frac{500}{1,500} = 0.333 = 33.3\%$$

Step 3: Allocate emissions:

$$E_A = 5,000 \times 0.667 = 3,335 \text{ kg CO}_2$$

$$E_B = 5,000 \times 0.333 = 1,665 \text{ kg CO}_2$$

Answer: - Product A: 3,335 kg CO₂ (3.335 kg CO₂/kg product) - Product B: 1,665 kg CO₂ (3.330 kg CO₂/kg product)

Note: Similar emission intensities due to physical allocation.

PROBLEM 9.7 Prove that the sum of allocated emissions equals total process emissions:

$$\sum (AF_i \times E_{total}) = E_{total}.$$

Solution (Proof):

Given: Allocation factors $A F_i$ where $\sum A F_i = 1$

Step 1: Sum of allocated emissions:

$$\sum E_i = \sum (A F_i \times E_{total})$$

Step 2: Factor out E_{total} :

$$\sum E_i = E_{total} \times \sum A F_i$$

Step 3: Since allocation factors sum to 1:

$$\sum E_i = E_{total} \times 1 = E_{total}$$

■

This proves conservation of emissions in allocation.

PROBLEM 9.8 A system boundary analysis shows:

Flow	Energy		GWP (kg CO ₂ e)
	Mass (kg)	(MJ)	
1	500	2,000	800
2	300	1,500	600
3	150	800	400
4	50	200	100
	30	150	80

5

Flow	20	100	50
6			
Total	1,050	4,750	2,030

Apply cut-off criteria (1% threshold) for each dimension. Which flows can be excluded?

Solution:

Mass threshold (1% of 1,050 kg = 10.5 kg): - Flow 6 (20 kg) > 10.5 ✓ Include - All flows exceed threshold

Energy threshold (1% of 4,750 MJ = 47.5 MJ): - Flow 6 (100 MJ) > 47.5 ✓ Include - All flows exceed threshold

GWP threshold (1% of 2,030 kg = 20.3 kg): - Flow 6 (50 kg) > 20.3 ✓ Include - All flows exceed threshold

Answer: No flows can be excluded - all exceed 1% threshold in all dimensions.

Cumulative analysis: - Flows 1-4: $\frac{800+600+400+100}{2,030} = 93.6\%$ of GWP - Could potentially exclude Flows 5-6 if using 95% cumulative cut-off

PROBLEM 9.9 Calculate the avoided burden credit for recycling:

- Virgin material production: 10 kg CO₂/kg
- Recycled material production: 3 kg CO₂/kg
- Recycling process: 1 kg CO₂/kg
- Recycling rate: 60%
- Product mass: 100 kg

Solution:

Step 1: Emissions from virgin material:

$$E_{virgin} = 100 \times 0.4 \times 10 = 400 \text{ kg CO}_2$$

Step 2: Emissions from recycled content:

$$E_{recycled} = 100 \times 0.6 \times 3 = 180 \text{ kg CO}_2$$

Step 3: Recycling process emissions:

$$E_{process} = 100 \times 0.6 \times 1 = 60 \text{ kg CO}_2$$

Step 4: Total with recycling:

$$E_{total} = 400 + 180 + 60 = 640 \text{ kg CO}_2$$

Step 5: Baseline (100% virgin):

$$E_{baseline} = 100 \times 10 = 1,000 \text{ kg CO}_2$$

Step 6: Avoided burden:

$$E_{avoided} = 1,000 - 640 = 360 \text{ kg CO}_2$$

Answer: - Total emissions: 640 kg CO₂ - Avoided burden: 360 kg CO₂ (36% reduction)

PROBLEM 9.10 For a multi-impact LCA with characterization matrix:

$$Q = \begin{bmatrix} 1 & 29.8 & 273 \\ 0.5 & 0.3 & 0.8 \\ 0.02 & 0.05 & 0.01 \end{bmatrix}$$

(Rows: GWP, Acidification, Eutrophication)

And emissions:

$$g = \begin{bmatrix} 1,000 \\ 20 \\ 5 \end{bmatrix}$$

(CO₂, CH₄, N₂O in kg)

Calculate all impact indicators.

Solution:

$$h = Qg = \begin{bmatrix} 1 & 29.8 & 273 \\ 0.5 & 0.3 & 0.8 \\ 0.02 & 0.05 & 0.01 \end{bmatrix} \begin{bmatrix} 1,000 \\ 20 \\ 5 \end{bmatrix}$$

GWP (row 1):

$$h_1 = (1 \times 1,000) + (29.8 \times 20) + (273 \times 5) = 1,000 + 596 + 1,365 = 2,961 \text{ kg CO}_2e$$

Acidification (row 2):

$$h_2 = (0.5 \times 1,000) + (0.3 \times 20) + (0.8 \times 5) = 500 + 6 + 4 = 510 \text{ kg SO}_2e$$

Eutrophication (row 3):

$$h_3 = (0.02 \times 1,000) + (0.05 \times 20) + (0.01 \times 5) = 20 + 1 + 0.05 = 21.05 \text{ kg PO}_4e$$

Answer: - GWP: 2,961 kg CO₂e - Acidification: 510 kg SO₂e - Eutrophication: 21.05 kg PO₄e

SUPPLEMENTARY PROBLEMS

9.11 Define functional unit for comparing cloth vs disposable diapers. **Ans.** “Diapering one infant for 2.5 years (6,000 diaper changes)”

9.12 Life cycle: 300 (materials) + 800 (manufacturing) + 200 (transport) + 100 (EoL) kg CO₂. Find total and manufacturing %. **Ans.** 1,400 kg CO₂; 57.1%

9.13 For $A = \begin{bmatrix} 0.2 & 0.1 \\ 0.1 & 0.3 \end{bmatrix}$, $B = [2 \ 3]$, $f = \begin{bmatrix} 50 \\ 30 \end{bmatrix}$, calculate g . **Ans.** $g = 253.5$

9.14 Emissions: 500 CO₂, 5 CH₄, 1 N₂O (kg). Characterization: [1, 29.8, 273]. Find GWP. **Ans.** 922 kg CO₂e

9.15 Life cycle stages: 100, 400, 50, 1,200, 30 kg CO₂. Identify hotspots (>20%). **Ans.**

Stage 4 (67.4%), Stage 2 (22.5%)

9.16 Products: 800 kg (A), 400 kg (B). Total emissions: 6,000 kg. Allocate physically.

Ans. A: 4,000 kg; B: 2,000 kg

9.17 Prove that for economic allocation, $\sum (Revenue e_i / Total\ Revenue) = 1$.

9.18 Flows: 600, 200, 80, 40, 20 kg CO₂ (total 940). Which exceed 5% threshold? **Ans.**

First three flows (600, 200, 80)

9.19 Virgin: 8 kg/kg, Recycled: 2 kg/kg, Process: 0.5 kg/kg, 50% recycled, 100 kg product.

Find total. **Ans.** 525 kg CO₂

9.20 $Q = \begin{bmatrix} 1 & 30 \\ 0.4 & 0.2 \end{bmatrix}$, $g = \begin{bmatrix} 800 \\ 15 \end{bmatrix}$. Calculate both impacts. **Ans.** $h_1 = 1,250$; $h_2 = 323$

10: INPUT-OUTPUT ANALYSIS

10.1 ECONOMIC INPUT-OUTPUT TABLES

Input-Output Table Structure:

	Industry 1	Industry 2	...	Final Demand	Total Output
Industry 1	z_{11}	z_{12}	...	y_1	x_1
Industry 2	z_{21}	z_{22}	...	y_2	x_2

Material Balance:

$$x_i = \sum_j z_{ij} + y_i$$

Technical Coefficients:

$$a_{ij} = \frac{z_{ij}}{x_j}$$

10.2 LEONTIEF DEMAND-DRIVEN MODEL

Matrix form:

$$x = Ax + y$$

Solution:

$$x = \underline{d}$$

Environmental extension:

$$E = e^T \underline{d}$$

where e is the vector of direct emission intensities (kg CO₂/\\$).

10.3 ENVIRONMENTALLY-EXTENDED INPUT-OUTPUT (EEIO)

Direct emission intensity:

$$e_i = \frac{E_i}{x_i}$$

(emissions per dollar output of sector i)

Total emission intensity (including supply chain):

$$f = e^T \mathbf{\tilde{e}}$$

Emission multiplier:

$$m_i = \frac{f_i}{e_i}$$

(ratio of total to direct intensity)

10.4 GHOSH SUPPLY-DRIVEN MODEL

Alternative formulation:

$$x^T = x^T B + v^T$$

where \mathbf{B} is the allocation coefficient matrix and \mathbf{v} is value added.

SOLVED PROBLEMS

PROBLEM 10.1 Given an input-output table (in million \$):

	Sector 1	Sector 2	Final Demand	Total Output
Sector 1	200	300	500	1,000
Sector 2	400	200	400	1,000

Calculate the technical coefficient matrix \mathbf{A} .

Solution:

Technical coefficients: $a_{ij} = \frac{z_{ij}}{x_j}$

$$a_{11} = \frac{200}{1,000} = 0.20$$

$$a_{12} = \frac{300}{1,000} = 0.30$$

$$a_{21} = \frac{400}{1,000} = 0.40$$

$$a_{22} = \frac{200}{1,000} = 0.20$$

Answer:

$$A = \begin{bmatrix} 0.20 & 0.30 \\ 0.40 & 0.20 \end{bmatrix}$$

Interpretation: - Sector 1 requires 0.20 of its own output per dollar of production - Sector 1 requires 0.40 of Sector 2 output per dollar of production

PROBLEM 10.2 For the system in Problem 10.1, if final demand changes to $y = \begin{bmatrix} 600 \\ 500 \end{bmatrix}$, calculate the new total output required.

Solution:

Step 1: Calculate $I - A$:

$$I - A = \begin{bmatrix} 0.80 & -0.30 \\ -0.40 & 0.80 \end{bmatrix}$$

Step 2: Calculate determinant:

$$\det = (0.80)(0.80) - (-0.30)(-0.40) = 0.64 - 0.12 = 0.52$$

Step 3: Calculate inverse:

i

Step 4: Calculate new output:

$$x = \begin{bmatrix} 1.538 & 0.577 \\ 0.769 & 1.538 \end{bmatrix} \begin{bmatrix} 600 \\ 500 \end{bmatrix}$$
$$x = \begin{bmatrix} 923 + 289 \\ 461 + 769 \end{bmatrix} = \begin{bmatrix} 1,212 \\ 1,230 \end{bmatrix}$$

Answer: - Sector 1: 1,212 million - Sector 2: 1,230 million

Change from original: - Sector 1: +212 million (+21.2%) - Sector 2: +230 million
(+23.0%)

PROBLEM 10.3 Calculate environmental impacts using EEIO: - Direct emission intensities:

$$e = \begin{bmatrix} 0.5 \\ 0.8 \end{bmatrix} \text{ kg CO}_2/\$ - \text{Technical coefficients from Problem 10.1} - \text{Final demand: } y = \begin{bmatrix} 500 \\ 400 \end{bmatrix}$$

million \$

Solution:

Step 1: From Problem 10.1:

i

Step 2: Calculate total output:

$$x = \begin{bmatrix} 1.538 & 0.577 \\ 0.769 & 1.538 \end{bmatrix} \begin{bmatrix} 500 \\ 400 \end{bmatrix} = \begin{bmatrix} 1,000 \\ 1,000 \end{bmatrix}$$

Step 3: Calculate total emissions:

$$E = e^T x = [0.5 \quad 0.8] \begin{bmatrix} 1,000 \\ 1,000 \end{bmatrix}$$

$$E = (0.5 \times 1,000) + (0.8 \times 1,000) = 500 + 800 = 1,300 \text{ million kg CO}_2$$

Answer: 1,300 million kg CO₂ = 1.3 million tonnes CO₂

PROBLEM 10.4 Calculate total emission intensities (supply chain footprint) for each sector:

Given: - $e = \begin{bmatrix} 0.5 \\ 0.8 \end{bmatrix}$ kg CO₂/\$ - \dot{i}

Solution:

Total intensity vector:

$$f^T = e^T \dot{i}$$

$$f^T = [0.5 \quad 0.8] \begin{bmatrix} 1.538 & 0.577 \\ 0.769 & 1.538 \end{bmatrix}$$

$$f_1 = (0.5 \times 1.538) + (0.8 \times 0.769) = 0.769 + 0.615 = 1.384 \text{ kg CO}_2/\dot{i}$$

\$

$$f_2 = (0.5 \times 0.577) + (0.8 \times 1.538) = 0.289 + 1.230 = 1.519 \text{ kg CO}_2/\dot{i}$$

\$

Answer: - Sector 1 total intensity: 1.384 kg CO₂/

- Sector 2 total intensity: 1.519 kg CO₂/

Emission multipliers: - Sector 1: $m_1 = \frac{1.384}{0.5} = 2.77$ - Sector 2: $m_2 = \frac{1.519}{0.8} = 1.90$

Interpretation: Sector 1's supply chain emissions are 2.77× its direct emissions.

PROBLEM 10.5 A company spends: - 2 million in Sector 1 \dot{i}) - 3 million in Sector 2 \dot{i})

Calculate total supply chain emissions.

Solution:

Sector 1 emissions:

$$E_1 = 2,000,000 \times 1.384 = 2,768,000 \text{ kg CO}_2 = 2,768 \text{ tonnes CO}_2$$

Sector 2 emissions:

$$E_2 = 3,000,000 \times 1.519 = 4,557,000 \text{ kg CO}_2 = 4,557 \text{ tonnes CO}_2$$

Total:

$$E_{total} = 2,768 + 4,557 = 7,325 \text{ tonnes CO}_2$$

Answer: 7,325 tonnes CO₂

Breakdown: - Sector 1: 37.8% - Sector 2: 62.2%

PROBLEM 10.6 Prove that the Leontief inverse can be interpreted as the total requirement (direct + indirect) per unit of final demand.

Solution (Proof):

Given: $x = \underline{y}$

Step 1: Expand using series (from Chapter 2):

$$\underline{y}$$

Step 2: Therefore:

$$x = (I + A + A^2 + A^3 + \dots) y$$

Interpretation: - Iy = Direct requirements (final demand itself) - Ay = First-order indirect requirements (inputs to produce final demand) - A^2y = Second-order indirect requirements (inputs to produce inputs) - A^3y = Third-order indirect requirements, etc.

Therefore: \underline{y} captures total requirements including entire supply chain. ■

PROBLEM 10.7 Calculate the structural path decomposition for Sector 1's total intensity:

Direct: 0.5 kg/\$

Via Sector 2: $a_{21} \times f_2 = 0.40 \times 1.519 = ?$ Via Sector 1 (self-loop): $a_{11} \times f_1 = 0.20 \times 1.384 = ?$

Solution:

Direct contribution:

$$\text{Direct} = 0.5 \text{ kg CO}_2/\text{$_\text{t}$}$$

\$

Via Sector 2:

$$\text{Path } h_{1 \rightarrow 2 \rightarrow 1} = a_{21} \times f_2 = 0.40 \times 1.519 = 0.608 \text{ kg CO}_2/\text{$_\text{t}$}$$

\$

Via Sector 1 (self):

$$\text{Path } h_{1 \rightarrow 1} = a_{11} \times f_1 = 0.20 \times 1.384 = 0.277 \text{ kg CO}_2/\text{$_\text{t}$}$$

\$

Total (should equal $f_1 = 1.384$):

$$f_1 = 0.5 + 0.608 + 0.277 = 1.385 \text{ kg CO}_2/\text{$_\text{t}$}$$

\$

(Slight rounding difference)

Answer: - Direct: 0.500 (36.1%) - Via Sector 2: 0.608 (43.9%) - Via self-loop: 0.277 (20.0%)

Interpretation: Most of Sector 1's footprint comes from its use of Sector 2 inputs.

PROBLEM 10.8 An EEIO model has 3 sectors with:

$$A = \begin{bmatrix} 0.1 & 0.2 & 0.1 \\ 0.2 & 0.1 & 0.2 \\ 0.1 & 0.1 & 0.1 \end{bmatrix}, e = \begin{bmatrix} 0.6 \\ 0.9 \\ 0.4 \end{bmatrix}$$

Calculate total emission intensity for Sector 2.

Solution:

Step 1: Calculate $I - A$:

$$I - A = \begin{bmatrix} 0.9 & -0.2 & -0.1 \\ -0.2 & 0.9 & -0.2 \\ -0.1 & -0.1 & 0.9 \end{bmatrix}$$

Step 2: Calculate Leontief inverse (column 2 only needed):

Using matrix inversion (computational):

i

Step 3: Calculate f_2 :

$$f_2 = e^T \times \text{column 2 of } i$$

$$f_2 = (0.6 \times 0.298) + (0.9 \times 1.190) + (0.4 \times 0.179)$$

$$f_2 = 0.179 + 1.071 + 0.072 = 1.322 \text{ kg CO}_2 / i$$

\$

Answer: 1.322 kg CO₂/\$ (total intensity for Sector 2)

$$\text{Multiplier: } m_2 = \frac{1.322}{0.9} = 1.47$$

PROBLEM 10.9 Calculate the change in emissions if final demand for Sector 1 increases by \$ 100 million:

Given: $f_1 = 1.384 \text{ kg CO}_2 / \$$

Solution:

$$\Delta E = \Delta y_1 \times f_1 = 100,000,000 \times 1.384 = 138,400,000 \text{ kg CO}_2$$

$$\Delta E = 138,400 \text{ tonnes CO}_2 = 138.4 \text{ thousand tonnes CO}_2$$

Answer: 138,400 tonnes CO₂ increase

Note: This includes both direct and supply chain emissions from the 100M demand increase.

PROBLEM 10.10 Compare direct vs total emission intensities:

Sector	Direct (kg/ t)	Total (kg/t)	Multiplier
Agriculture	0.3	0.8	?
Manufacturing	0.5	1.5	?
Services	0.1	0.6	?

Calculate multipliers and interpret.

Solution:

$$\text{Multipliers: } m = \frac{\text{Total}}{\text{Direct}}$$

Agriculture:

$$m_1 = \frac{0.8}{0.3} = 2.67$$

Manufacturing:

$$m_2 = \frac{1.5}{0.5} = 3.00$$

Services:

$$m_3 = \frac{0.6}{0.1} = 6.00$$

Answer: - Agriculture: 2.67 - Manufacturing: 3.00 - Services: 6.00

Interpretation: - **Services** has the highest multiplier (6.0), meaning supply chain emissions are 6× direct emissions - Despite low direct intensity, services have significant upstream impacts - **Manufacturing** has moderate multiplier (3.0) - **Agriculture** has lowest multiplier (2.67), more self-contained

SUPPLEMENTARY PROBLEMS

10.11 IO table: $z_{11}=100$, $z_{12}=150$, $x_1=500$, $x_2=600$. Find a_{11} and a_{12} . **Ans.** $a_{11}=0.20$, $a_{12}=0.25$

10.12 $A = \begin{bmatrix} 0.3 & 0.2 \\ 0.2 & 0.4 \end{bmatrix}$, $y = \begin{bmatrix} 400 \\ 300 \end{bmatrix}$. Calculate x . **Ans.** $x = \begin{bmatrix} 625 \\ 625 \end{bmatrix}$

10.13 $e = \begin{bmatrix} 0.4 \\ 0.7 \end{bmatrix}$, $x = \begin{bmatrix} 800 \\ 600 \end{bmatrix}$. Find total emissions. **Ans.** 740 kg CO₂

10.14 Direct: 0.6 kg/, Total: 1.8 kg/. Calculate multiplier. **Ans.** 3.0

10.15 Spend 5 M in sector with intensity 1.2 kg/. Find emissions. **Ans.** 6,000 tonnes CO₂

10.16 Prove that $x = Ax + y$ implies $x = \textcolor{red}{y}$.

10.17 $f_1=1.5$ kg/\$, \$y₁ = \$50M. Find ΔE. **Ans.** 75,000 tonnes CO₂

10.18 Direct: 0.2, Via sector 2: 0.5, Via self: 0.3. Find total intensity. **Ans.** 1.0 kg/\$

10.19 Three sectors with totals: 0.9, 1.2, 0.7 kg/\$. Spending: \$2M, \$3M, \$1M. Find total emissions. **Ans.** 6,100 tonnes CO₂

10.20 Direct: 0.15, Total: 0.75. What % is from supply chain? **Ans.** 80%

Chapter 11: PROCESS-BASED LCA MODELS

Theorem 11.1 (System Boundary Completeness)

Statement:

For a process system with cut-off threshold ϵ , the truncation error in total environmental impact is bounded by:

$$|I_{total} - I_{truncated}| \leq \sum_{i \in \text{excluded}} I_i \leq \epsilon \cdot I_{total}$$

Proof:

Step 1: Define included and excluded processes.

Let $V_{included}$ be processes with $I_i > \epsilon \cdot I_{total}$ and $V_{excluded}$ be the rest.

Step 2: Total impact is:

$$I_{total} = \sum_{i \in V_{included}} I_i + \sum_{i \in V_{excluded}} I_i$$

Step 3: Truncation error:

$$\text{Error} = \sum_{i \in V_{excluded}} I_i$$

Step 4: By definition of cut-off, each excluded process has $I_i \leq \epsilon \cdot I_{total}$.

If there are n excluded processes:

$$\text{Error} = \sum_{i \in V_{excluded}} I_i \leq n \cdot \epsilon \cdot I_{total}$$

For typical LCA with $\epsilon = 0.01$ (1% cut-off) and $n \approx 100$ excluded processes:

$$\text{Error} \leq 100 \times 0.01 \times I_{total} = I_{total}$$

This provides an upper bound on truncation error. ■

Sources: Suh et al. (2004), Lenzen (2000), Heijungs & Suh (2004) [8]

11.1 PROCESS FLOW DIAGRAMS

Unit Process: Smallest element for which input-output data are quantified.

System Expansion: Including additional processes to handle multi-functionality.

Cut-off Rules: Criteria for excluding minor flows.

11.2 MASS AND ENERGY BALANCE

Mass Balance:

$$\sum m_i = \sum m_{out}$$

Energy Balance:

$$\sum E_i = \sum E_{out} + \sum Losses$$

11.3 SCALING AND NORMALIZATION

Scaling factor:

$$SF = \frac{FU}{Reference\ Flow}$$

where FU = Functional Unit

SOLVED PROBLEMS

PROBLEM 11.1 A process produces 1,000 kg product from 1,200 kg raw material.

Calculate: (a) Yield (b) Waste generation rate

Solution:

(a) Yield:

$$Yield = \frac{Product}{Input} \times 100\% = \frac{1,000}{1,200} \times 100\% = 83.3\%$$

(b) Waste:

$$Waste = 1,200 - 1,000 = 200 \text{ kg}$$

$$Waste rate = \frac{200}{1,200} \times 100\% = 16.7\%$$

Answer: (a) 83.3% yield; (b) 16.7% waste rate

PROBLEM 11.2 Energy balance for a furnace: - Input: 1,000 MJ fuel - Useful heat: 750 MJ - Stack losses: 180 MJ - Radiation losses: ?

Calculate radiation losses.

Solution:

From energy balance:

$$Input = Useful + \textcolor{red}{Radiation}$$

$$1,000 = 750 + 180 + \textcolor{red}{Radiation}$$

$$\textcolor{red}{Radiation} = 1,000 - 750 - 180 = 70 \text{ MJ}$$

Efficiency:

$$\eta = \frac{750}{1,000} = 75\%$$

Answer: Radiation losses = 70 MJ; Efficiency = 75%

PROBLEM 11.3 Scale emissions from reference flow (100 kg) to functional unit (1,000 kg): - Reference emissions: 250 kg CO₂

Solution:

$$SF = \frac{1,000}{100} = 10$$

$$E_{FU} = 250 \times 10 = 2,500 \text{ kg CO}_2$$

Answer: 2,500 kg CO₂ for functional unit

SUPPLEMENTARY PROBLEMS

11.11 Input: 500 kg, Output: 425 kg. Find yield. **Ans.** 85%

11.12 Energy in: 2,000 MJ, Useful: 1,600 MJ, Stack: 300 MJ. Find radiation. **Ans.** 100 MJ

11.13 Reference: 50 kg product, 120 kg CO₂. FU: 500 kg. Find emissions. **Ans.** 1,200 kg CO₂

Chapter 12: HYBRID LCA METHODS

12.1 TIERED HYBRID ANALYSIS

Combination of: - Process LCA (foreground system) - IO LCA (background system)

Formula:

$$E_{total} = E_{process} + E_{IO}$$

12.2 INTEGRATED HYBRID

Mathematical formulation:

$$x = \textcolor{red}{i}$$

where A_{hybrid} combines process and IO data.

SOLVED PROBLEMS

PROBLEM 12.1 Hybrid LCA: - Process-based (foreground): 500 kg CO₂ - IO-based (background): $2 \text{ Mspend} \times 0.4 \text{ kg}/\textcolor{red}{i} = 800 \text{ kg CO}_2$

Calculate total.

Solution:

$$E_{total} = 500 + 800 = 1,300 \text{ kg CO}_2$$

Answer: 1,300 kg CO₂ (process: 38.5%, IO: 61.5%)

SUPPLEMENTARY PROBLEMS

12.11 Process: 300 kg, IO: $1.5M \times 0.5 \text{ kg}/\$$. Find total. Ans. 1,050 kg CO₂

Chapter 13: ERROR PROPAGATION METHODS

13.1 TAYLOR SERIES EXPANSION

First-order approximation:

$$f(x) \approx f(\mu) + f'(\mu)(x - \mu)$$

Variance:

$$\text{Var}[f(X)] \approx \textcolor{red}{\sigma^2}$$

13.2 MULTIVARIATE CASE

For $Q = f(X_1, X_2, \dots, X_n)$:

$$\sigma_Q^2 \approx \sum_{i=1}^n \left(\frac{\partial f}{\partial X_i} \right)^2 \sigma_i^2 + 2 \sum_{i < j} \frac{\partial f}{\partial X_i} \frac{\partial f}{\partial X_j} \rho_{ij} \sigma_i \sigma_j$$

where ρ_{ij} is correlation between X_i and X_j .

SOLVED PROBLEMS

PROBLEM 13.1 For $Q = X^2$ with $\mu_x = 10$, $\sigma_x = 1$, estimate σ_Q .

Solution:

$$\frac{dQ}{dX} = 2X$$

At $X = \mu = 10$:

$$\frac{dQ}{dX} \Big|_{X=10} = 2(10) = 20$$

$$\sigma_Q \approx 20 \times \sigma_x = 20 \times 1 = 20$$

Mean:

$$\mu_Q \approx 10^2 = 100$$

Answer: $Q \approx 100 \pm 20$ (20% relative uncertainty)

SUPPLEMENTARY PROBLEMS

13.11 $Q=3X$, $\mu_x=50$, $\sigma_x=5$. Find σ_Q . Ans. 15

Chapter 14: MONTE CARLO TECHNIQUES (ADVANCED)

14.1 LATIN HYPERCUBE SAMPLING

Stratified sampling ensuring better coverage than pure random sampling.

Algorithm: 1. Divide each input distribution into N equal probability intervals 2. Sample once from each interval 3. Randomly pair samples across variables

Advantage: Faster convergence than simple Monte Carlo.

14.2 IMPORTANCE SAMPLING

Weighted sampling from alternative distribution to reduce variance.

Weight:

$$w_i = \frac{f(x_i)}{g(x_i)}$$

where f is target distribution, g is sampling distribution.

SOLVED PROBLEMS

PROBLEM 14.1 Compare sample sizes for SE = 1% of mean: (a) Simple MC with CV = 20% (b) LHS with 50% variance reduction

Solution:

(a) Simple MC:

$$N = \left(\frac{CV}{SE} \right)^2 = \left(\frac{20}{1} \right)^2 = 400$$

(b) LHS (50% variance reduction):

$$N_{LHS} = 400 \times 0.5 = 200$$

Answer: (a) 400 iterations; (b) 200 iterations

SUPPLEMENTARY PROBLEMS

14.11 MC needs 1,000 iterations. LHS with 60% variance reduction needs how many? **Ans.**
400

Chapter 15: SENSITIVITY AND CONTRIBUTION ANALYSIS

Theorem 15.1 (Sobol Indices Decomposition)

Statement:

For a function $f(x)$ where $x=(x_1, \dots, x_n)$ are independent random variables, the total variance can be decomposed as:

$$V[f] = \sum_{i=1}^n V_i + \sum_{i < j} V_{ij} + \dots + V_{1,2,\dots,n}$$

where $V_i = V[E[f \vee x_i]]$ is the first-order variance and $V_{ij} = V[E[f \vee x_i, x_j]] - V_i - V_j$ is the second-order interaction variance.

Proof:

Step 1: ANOVA decomposition.

Any function can be decomposed as:

$$f(x) = f_0 + \sum_i f_i(x_i) + \sum_{i < j} f_{ij}(x_i, x_j) + \dots + f_{1,\dots,n}(x_1, \dots, x_n)$$

where: - $f_0 = E[f]$ - $f_i(x_i) = E[f \vee x_i] - f_0$ - $f_{ij}(x_i, x_j) = E[f \vee x_i, x_j] - f_i(x_i) - f_j(x_j) - f_0$

Step 2: Orthogonality property.

By construction, all terms are orthogonal:

$$E[f_i(x_i) \cdot f_j(x_j)] = 0 \text{ for } i \neq j$$

Step 3: Variance decomposition.

Taking variance of both sides:

$$V[f] = V\left[\sum_i f_i + \sum_{i < j} f_{ij} + \dots\right]$$

By orthogonality:

$$V[f] = \sum_i V[f_i] + \sum_{i < j} V[f_{ij}] + \dots$$

Step 4: Define Sobol indices.

$$\text{First-order: } S_i = \frac{V_i}{V[f]} = \frac{V[E[f \vee x_i]]}{V[f]}$$

$$\text{Total-order: } S_T^i = \frac{E[V[f \vee x_{\sim i}]]}{V[f]} = 1 - \frac{V[E[f \vee x_{\sim i}]]}{V[f]}$$

where $x_{\sim i}$ denotes all variables except x_i . ■

Corollary 15.1: Sum of all Sobol indices equals 1:

$$\sum_i S_i + \sum_{i < j} S_{ij} + \dots = 1$$

Sources: Sobol (1993), Saltelli et al. (2008), Homma & Saltelli (1996)

15.1 LOCAL SENSITIVITY ANALYSIS

Sensitivity coefficient:

$$S_i = \frac{\partial E}{\partial x_i} \cdot \frac{x_i}{E}$$

(Elasticity: % change in output per % change in input)

15.2 CONTRIBUTION TO VARIANCE

Contribution:

$$C_i = \frac{\left(\frac{\partial E}{\partial x_i} \right)^2 \sigma_i^2}{\sigma_E^2}$$

SOLVED PROBLEMS

PROBLEM % For $E = 100A + 50B$ with $A = 10$, $B = 20$:

Calculate sensitivity coefficients.

Solution:

$$E = 100(10) + 50(20) = 2,000$$

$$S_A = \frac{\partial E}{\partial A} \cdot \frac{A}{E} = 100 \cdot \frac{10}{2,000} = 0.5$$

$$S_B = \frac{\partial E}{\partial B} \cdot \frac{B}{E} = 50 \cdot \frac{20}{2,000} = 0.5$$

Answer: $S_A = S_B = 0.5$ (equal sensitivity)

SUPPLEMENTARY PROBLEMS

15.11 $E = 200X$, $X = 5$. Find S_X . Ans. 1.0

Chapter 16: BAYESIAN METHODS

16.1 BAYES' THEOREM

$$P(A \vee B) = \frac{P(B \vee A)P(A)}{P(B)}$$

Posterior: $P(A \vee B)$ Likelihood: $P(B \vee A)$ Prior: $P(A)$

16.2 BAYESIAN UPDATING

For normal distributions:

$$\mu_{post} = \frac{\sigma_0^2 \mu_{data} + \sigma_{data}^2 \mu_0}{\sigma_0^2 + \sigma_{data}^2}$$

$$\sigma_{post}^2 = \frac{\sigma_0^2 \sigma_{data}^2}{\sigma_0^2 + \sigma_{data}^2}$$

SOLVED PROBLEMS

PROBLEM 16.1 Prior: $\mu_0=2.5$, $\sigma_0=0.5$. Data: $\mu_d=2.3$, $\sigma_d=0.3$. Find posterior.

Solution:

$$\mu_{post} = \underline{\underline{\mu}}$$

$$\sigma_{post}^2 = \underline{\underline{\sigma}}$$

$$\sigma_{post} = 0.257$$

Answer: Posterior: $\mu=2.35$, $\sigma=0.26$

SUPPLEMENTARY PROBLEMS

16.11 Prior: 3.0 ± 0.6 , Data: 2.8 ± 0.4 . Find posterior mean. Ans. 2.88

Chapter 17: ESG METRICS AND QUANTIFICATION

Theorem 17.1 (Materiality-Weighted ESG Score)

Statement:

For an ESG scoring system with n metrics, the optimal weights that maximize information content while respecting materiality constraints are:

$$w_i^* = \frac{m_i \cdot \sigma_i}{\sum_{j=1}^n m_j \cdot \sigma_j}$$

where $m_i \in [0,1]$ is the materiality score and σ_i is the standard deviation of metric i .

Proof:

Step 1: Define ESG score as weighted sum.

$$ESG = \sum_{i=1}^n w_i \cdot x_i$$

subject to $\sum_{i=1}^n w_i = 1$ and $w_i \geq 0$.

Step 2: Maximize variance (information content).

$$V[ESG] = \sum_{i=1}^n w_i^2 \sigma_i^2 + 2 \sum_{i < j} w_i w_j \rho_{ij} \sigma_i \sigma_j$$

For uncorrelated metrics ($\rho_{ij} = 0$):

$$V[ESG] = \sum_{i=1}^n w_i^2 \sigma_i^2$$

Step 3: Incorporate materiality constraint.

Weight must be proportional to materiality: $w_i \propto m_i$

Step 4: Solve constrained optimization.

Maximize $\sum_{i=1}^n w_i^2 \sigma_i^2$ subject to $w_i = c \cdot m_i$ and $\sum_i w_i = 1$.

Substituting:

$$\sum_{i=1}^n c^2 m_i^2 \sigma_i^2 \text{ subject to } c \sum_i m_i = 1$$

Solution: $c = \frac{1}{\sum_i m_i}$

But to maximize variance, weight by both materiality and volatility:

$$w_i = \frac{m_i \cdot \sigma_i}{\sum_{j=1}^n m_j \cdot \sigma_j}$$

■

Sources: SASB Materiality Map, Eccles & Stroehle (2018), Berg et al. (2022)

17.1 ESG SCORING FRAMEWORKS

Components: - E: Carbon, water, waste, biodiversity - S: Labor, safety, community, diversity
- G: Board structure, ethics, transparency

Composite Score:

$$ESG = w_E \cdot E + w_S \cdot S + w_G \cdot G$$

where $w_E + w_S + w_G = 1$

17.2 MATERIALITY MATRIX

Double Materiality: 1. Financial materiality (impact on company) 2. Impact materiality (company's impact on society/environment)

SOLVED PROBLEMS

PROBLEM 17.1 Calculate ESG score with weights [0.4, 0.3, 0.3] and scores [75, 80, 85]:

Solution:

$$ESG = 0.4(75) + 0.3(80) + 0.3(85) = 30 + 24 + 25.5 = 79.5$$

Answer: ESG score = 79.5/100

SUPPLEMENTARY PROBLEMS

17.11 Weights [0.5, 0.3, 0.2], Scores [70, 75, 80]. Find ESG. Ans. 73.5

Chapter 18: ESG-CARBON INTEGRATION MODELS

18.1 CARBON AS ESG COMPONENT

Environmental Score:

$$E = w_C \cdot Carbon + w_W \cdot Water + w_B \cdot Biodiversity + \dots$$

Normalization:

$$Score_i = \frac{Value_i - Min_i}{Max_i - Min_i} \times 100$$

SOLVED PROBLEMS

PROBLEM 18.1 Normalize carbon intensity: - Company: 500 kg CO₂/\$ M - Industry min: 300 - Industry max: 800

Solution:

$$Score = \frac{500 - 300}{800 - 300} \times 100 = \frac{200}{500} \times 100 = 40$$

Inverted (lower is better):

$$Score_{inverted} = 100 - 40 = 60$$

Answer: Carbon score = 60/100

SUPPLEMENTARY PROBLEMS

18.11 Value: 400, Min: 200, Max: 600. Find normalized score. Ans. 50

Chapter 19: PORTFOLIO OPTIMIZATION WITH ESG

Theorem 19.1 (ESG-Constrained Efficient Frontier)

Statement:

For a portfolio optimization problem with ESG constraint $w^T s \geq s_{min}$ where s is the vector of ESG scores, the ESG-constrained efficient frontier lies below the unconstrained frontier.

Proof:

Step 1: Unconstrained Markowitz problem.

$$\min_w \frac{1}{2} w^T \Sigma w$$

subject to: - $w^T \mu = \mu_p$ (target return) - $w^T 1 = 1$ (fully invested)

Step 2: Add ESG constraint.

$$\min_w \frac{1}{2} w^T \Sigma w$$

subject to: - $w^T \mu = \mu_p$ - $w^T 1 = 1$ - $w^T s \geq s_{min}$ (ESG constraint)

Step 3: Lagrangian.

$$L = \frac{1}{2} w^T \Sigma w + \lambda_1(\mu_p - w^T \mu) + \lambda_2(1 - w^T 1) + \lambda_3(s_{min} - w^T s)$$

Step 4: First-order conditions.

$$\Sigma w = \lambda_1 \mu + \lambda_2 1 + \lambda_3 s$$

Step 5: Compare solutions.

The constrained solution space is a subset of the unconstrained space. Therefore, the minimum variance for any given return μ_p in the constrained case must be greater than or equal to the unconstrained minimum variance. This means the efficient frontier will shift to the right (higher risk for the same return), effectively lying below the original frontier. ■

Sources: Markowitz (1952), Pástor et al. (2021), Pedersen et al. (2021)

19.1 MEAN-VARIANCE OPTIMIZATION

Objective:

$$\min_w w^T \Sigma w$$

Subject to: - $w^T \mu \geq r_{target}$ (return constraint) - $w^T 1 = 1$ (fully invested) - $w \geq 0$ (no short selling)

19.2 ESG-CONSTRAINED OPTIMIZATION

Additional constraint:

$$w^T ESG \geq ESG_{min}$$

SOLVED PROBLEMS

PROBLEM 19.1 Two assets: A (return 8%, risk 15%, ESG 70), B (return 6%, risk 10%, ESG 85). Minimum ESG = 75. Find weights.

Solution:

ESG constraint:

$$70w_A + 85w_B \geq 75$$

$$w_A + w_B = 1$$

From second equation: $w_A = 1 - w_B$

Substitute:

$$70(1-w_B) + 85w_B \geq 75$$

$$70 + 15w_B \geq 75$$

$$w_B \geq \frac{5}{15} = 0.333$$

Maximum ESG: $w_B = 1$ (all in B)

Answer: $w_B \geq 33.3\%$, $w_A \leq 66.7\%$

SUPPLEMENTARY PROBLEMS

19.11 Assets: (10%, ESG 60), (7%, ESG 90). Min ESG = 75. Find min weight in second asset. **Ans.** 50%

Chapter 20: ESG RISK ASSESSMENT

20.1 CARBON RISK METRICS

Stranded Asset Risk:

$$SAR = \frac{\text{Carbon Intensive Assets}}{\text{Total Assets}}$$

Carbon VaR (Value at Risk):

$$VaR_C = \text{Portfolio Value} \times \text{Carbon Price} \times \text{Carbon Exposure}$$

SOLVED PROBLEMS

PROBLEM 20.1 Portfolio: 100M, Carbon exposure: 50,000 tonnes CO₂, Carbon price: 50/tonne. Calculate carbon VaR.

Solution:

$$VaR_C = 50,000 \times 50 = 2,500,000 = 2.5 M$$

As % of portfolio:

$$\frac{2.5}{100} = 2.5\%$$

Answer: Carbon VaR = 2.5M (2.5% of portfolio)

SUPPLEMENTARY PROBLEMS

20.11 50M portfolio, 20,000 tonnes, \$ 40/tonne. Find VaR. Ans. \$ 0.8M

Chapter 21: MACHINE LEARNING FOR CARBON ACCOUNTING

Theorem 21.1 (Carbon Prediction Model Convergence)

Statement:

For a supervised learning model \hat{f}_n trained on n samples to predict carbon emissions, under regularity conditions, the prediction error converges:

$$E \hat{\epsilon}$$

where σ^2 is the irreducible error (Bayes error).

Proof:

Step 1: Bias-variance decomposition.

$$E \hat{\epsilon}$$

where: - Bias $[\hat{f}_n] = E[\hat{f}_n(x)] - f(x)$ - Var $[\hat{f}_n] = E \hat{\epsilon}^2$ - $\sigma^2 = E \hat{\epsilon}^2$ (irreducible)

Step 2: Consistency assumption.

Assume \hat{f}_n is a consistent estimator: $Bias[\hat{f}_n] \rightarrow 0$ as $n \rightarrow \infty$, $Var[\hat{f}_n] \rightarrow 0$ as $n \rightarrow \infty$

Step 3: Take limit.

$$\lim_{n \rightarrow \infty} E \hat{\epsilon}$$

Step 4: Rate of convergence.

For parametric models with p parameters:

$$E \hat{\epsilon}$$

For nonparametric models in d dimensions:

$$E \textcolor{red}{i}$$

This shows the curse of dimensionality. ■

Sources: *Hastie et al. (2009)*, *Bishop (2006)*, *Vapnik (1998)*

21.1 REGRESSION MODELS

Linear Regression:

$$E = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \epsilon$$

Coefficient of Determination:

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

21.2 FEATURE IMPORTANCE

Standardized Coefficients:

$$\beta_i^{\textcolor{red}{i}} = \beta_i \frac{\sigma_{X_i}}{\sigma_Y}$$

SOLVED PROBLEMS

PROBLEM 21.1 Regression: $E = 100 + 5X$. Data: $SS_{tot} = 10,000$, $SS_{res} = 2,000$. Find R^2 .

Solution:

$$R^2 = 1 - \frac{2,000}{10,000} = 1 - 0.2 = 0.8$$

Answer: $R^2 = 0.80$ (80% variance explained)

SUPPLEMENTARY PROBLEMS

21.11 $SS_{tot} = 5,000$, $SS_{res} = 1,500$. Find R^2 . Ans. 0.70

Chapter 22: OPTIMIZATION MODELS

Theorem 22.1 (KKT Conditions for Carbon Minimization)

Statement:

For the carbon minimization problem:

$$\min_x f(x) \text{ subject to } g_i(x) \leq 0, h_j(x) = 0$$

where f is total carbon emissions, the Karush-Kuhn-Tucker (KKT) conditions are necessary for optimality.

Proof:

Step 1: Form Lagrangian.

$$L(x, \lambda, \mu) = f(x) + \sum_i \lambda_i g_i(x) + \sum_j \mu_j h_j(x)$$

Step 2: KKT conditions.

At optimal x^* :

1. **Stationarity:** $\nabla f(x^*) + \sum_i \lambda_i \nabla g_i(x^*) + \sum_j \mu_j \nabla h_j(x^*) = 0$
2. **Primal feasibility:** $g_i(x^*) \leq 0, h_j(x^*) = 0$
3. **Dual feasibility:** $\lambda_i \geq 0$
4. **Complementary slackness:** $\lambda_i g_i(x^*) = 0$

Step 3: Necessity proof.

Assume x^* is a local minimum and constraint qualification holds (e.g., LICQ).

Consider feasible direction d such that $x^* + \epsilon d$ remains feasible for small $\epsilon > 0$.

By optimality: $f(x^* + \epsilon d) \geq f(x^*)$

First-order expansion:

$$f(\mathbf{x}^*) + \epsilon \nabla f(\mathbf{x}^*)$$

Therefore: $\nabla f(\mathbf{x}^*)$ for all feasible d .

By Farkas' lemma, this implies the existence of multipliers λ_i, μ_j satisfying KKT conditions.

■

Sources: Boyd & Vandenberghe (2004), Nocedal & Wright (2006), Bertsekas (1999)

22.1 LINEAR PROGRAMMING

Standard Form:

$$\min_{\mathbf{x}} \mathbf{c}^T \mathbf{x}$$

$$\text{s.t. } \mathbf{A}\mathbf{x} \leq \mathbf{b}, \mathbf{x} \geq \mathbf{0}$$

22.2 CARBON ABATEMENT OPTIMIZATION

Minimize cost:

$$\min \sum c_i x_i$$

Subject to emission reduction:

$$\sum r_i x_i \geq R_{target}$$

SOLVED PROBLEMS

PROBLEM 22.1 Two abatement options: - Option A: 50/tonne, reduces 100 tonnes - Option B: 30/tonne, reduces 80 tonnes Target: 150 tonnes. Minimize cost.

Solution:

Variables: x_A , x_B (number of units)

Objective:

$$\min 50x_A + 30x_B$$

Constraint:

$$100x_A + 80x_B \geq 150$$

Optimal: Use cheaper option first (B), then A if needed.

If $x_B = 2$: $80(2) = 160 \geq 150$ ✓

Cost: $\$30(2) = 60$

Answer: Use 2 units of Option B, Cost = \$ 60

SUPPLEMENTARY PROBLEMS

22.11 Options: \$40/t (120t), \$60/t (100t). Target: 200t. Min cost? **Ans.** Use first option twice: \$ 80

Chapter 23: DYNAMIC PROGRAMMING

23.1 BELLMAN EQUATION

$$V(s) = \max_a [R(s, a) + \gamma V(s')]$$

where: - $V(s)$ = Value function - $R(s, a)$ = Reward - γ = Discount factor - s' = Next state

SOLVED PROBLEMS

PROBLEM 23.1 Emission reduction over 3 years, discount rate 5%. Year 1: 100 tonnes saved, Year 2: 100 tonnes, Year 3: 100 tonnes. Value at \$ 50/tonne. Find NPV.

Solution:

$$NPV = \frac{100 \times 50}{1.05^1} + \frac{100 \times 50}{1.05^2} + \frac{100 \times 50}{1.05^3}$$

$$NPV = \frac{5,000}{1.05} + \frac{5,000}{1.1025} + \frac{5,000}{1.1576}$$

$$NPV = 4,762 + 4,535 + 4,319 = 13,616$$

Answer: NPV = 13,616

SUPPLEMENTARY PROBLEMS

23.11 2 years, 200 tonnes/year, 40/tonne, 10% discount. Find NPV. **Ans.** \$ 14,876

Chapter 24: NETWORK ANALYSIS FOR SUPPLY CHAINS

24.1 GRAPH THEORY

Nodes: Facilities, suppliers Edges: Material/product flows

Shortest Path (Dijkstra): Find minimum carbon pathway

24.2 NETWORK EMISSIONS

Total:

$$E_{network} = \sum_{(i,j) \in \text{Edges}} f_{ij} \cdot e_{ij}$$

where f_{ij} is flow, e_{ij} is emission intensity.

SOLVED PROBLEMS

PROBLEM 24.1 Supply chain network: - Edge A→B: 100 units, 0.5 kg/unit - Edge B→C: 100 units, 0.3 kg/unit - Edge A→C: 0 units (unused)

Calculate total emissions.

Solution:

$$E = (100 \times 0.5) + (100 \times 0.3) + 0 = 50 + 30 = 80 \text{ kg CO}_2$$

Answer: 80 kg CO₂

SUPPLEMENTARY PROBLEMS

24.11 Three edges: 50×0.4, 30×0.6, 20×0.5. Find total. **Ans.** 48 kg CO₂

Chapter 25: GHG PROTOCOL IMPLEMENTATION

25.1 ORGANIZATIONAL BOUNDARIES

Control Approaches: 1. **Operational Control:** 100% of emissions from controlled operations
2. **Financial Control:** Based on financial ownership 3. **Equity Share:** Proportional to ownership %

25.2 BASE YEAR

Recalculation Triggers: - Structural changes (M&A) - Methodology improvements - Errors discovered

Significance Threshold: Typically 5% change

SOLVED PROBLEMS

PROBLEM 25.1 Company has: - 100% owned facility: 10,000 tonnes - 60% owned JV: 5,000 tonnes total - 30% owned investment: 8,000 tonnes total

Calculate emissions under equity share approach.

Solution:

$$E = (10,000 \times 1.0) + (5,000 \times 0.6) + (8,000 \times 0.3)$$

$$E = 10,000 + 3,000 + 2,400 = 15,400 \text{ tonnes CO}_2$$

Answer: 15,400 tonnes CO₂

SUPPLEMENTARY PROBLEMS

25.11 100% facility (8,000t), 50% JV (6,000t). Find equity share total. **Ans.** 11,000 tonnes

Chapter 26: ESG REPORTING STANDARDS

26.1 MAJOR FRAMEWORKS

- **GRI:** Global Reporting Initiative
- **SASB:** Sustainability Accounting Standards Board
- **TCFD:** Task Force on Climate-related Financial Disclosures
- **ISSB:** International Sustainability Standards Board

26.2 DISCLOSURE METRICS

Emission Intensity:

$$I = \frac{\text{Emissions}}{\text{Activity}}$$

Common denominators: Revenue, production, employees

SOLVED PROBLEMS

PROBLEM 26.1 Calculate emission intensities: - Emissions: 50,000 tonnes CO₂ - Revenue: 100M - Production: 25,000 tonnes product - Employees: 500

Solution:

Per revenue:

$$I_R = \frac{50,000}{100} = 500 \text{ tonnes CO}_2 \text{ per million dollars}$$

Per production:

$$I_P = \frac{50,000}{25,000} = 2.0 \text{ tonnes CO}_2/\text{tonne product}$$

Per employee:

$$I_E = \frac{50,000}{500} = 100 \text{ tonnes CO}_2/\text{employee}$$

Answer: 500 t/\$ M; 2.0 t/t; 100 t/employee

SUPPLEMENTARY PROBLEMS

26.11 30,000 tonnes, \$ 60M revenue. Find intensity. **Ans.** 500 tonnes/\$ M

Chapter 27: VERIFICATION AND ASSURANCE

27.1 ASSURANCE LEVELS

Limited Assurance: “Nothing has come to our attention...” **Reasonable Assurance:** “In our opinion...”

27.2 MATERIALITY THRESHOLD

Quantitative: Typically 5% of total emissions **Qualitative:** Stakeholder importance

SOLVED PROBLEMS

PROBLEM 27.1 Total emissions: 100,000 tonnes. Materiality: 5%. Error found: 4,000 tonnes. Material?

Solution:

$$\text{Threshold} = 100,000 \times 0.05 = 5,000 \text{ tonnes}$$

$$\text{Error} = 4,000 < 5,000$$

Answer: Not material (below 5% threshold)

SUPPLEMENTARY PROBLEMS

27.11 Total: 80,000t, Threshold: 5%, Error: 5,000t. Material? **Ans.** Yes (exceeds 4,000t threshold)

Chapter 28: INDUSTRIAL PROCESSES

28.1 CEMENT PRODUCTION

Process Emissions:

$$E_{process} = m_{clinker} \times EF_{calcination}$$

where $EF \approx 0.525$ tonnes CO₂/tonne clinker

Total:

$$E_{total} = E_{process} + E_{fuel}$$

SOLVED PROBLEMS

PROBLEM 28.1 Cement plant: - Clinker: 1,000,000 tonnes - Process EF: 0.525 t/t - Fuel: 500,000 tonnes coal × 2.4 kg/kg

Calculate total.

Solution:

$$E_{process} = 1,000,000 \times 0.525 = 525,000 \text{ tonnes CO}_2$$

$$E_{fuel} = 500,000 \times 2.4 = 1,200,000 \text{ tonnes CO}_2$$

$$E_{total} = 525,000 + 1,200,000 = 1,725,000 \text{ tonnes CO}_2$$

Answer: 1.725 million tonnes CO₂ (process: 30.4%, fuel: 69.6%)

SUPPLEMENTARY PROBLEMS

28.11 500,000t clinker, 0.525 EF. Find process emissions. Ans. 262,500 tonnes

Chapter 29: FINANCIAL SERVICES

29.1 FINANCED EMISSIONS

Formula:

$$E_{financed} = \sum \frac{Outstanding}{EVIC} \times E_{investee}$$

where EVIC = Enterprise Value Including Cash

29.2 ATTRIBUTION FACTORS

Outstanding Amount: Loan or investment value **EVIC:** Total enterprise value

SOLVED PROBLEMS

PROBLEM 29.1 Bank loan: - Outstanding: 10M - Company EVIC: 100M - Company emissions: 50,000 tonnes

Calculate financed emissions.

Solution:

$$E_{financed} = \frac{10}{100} \times 50,000 = 0.1 \times 50,000 = 5,000 \text{ tonnes CO}_2$$

Answer: 5,000 tonnes CO₂ (10% attribution)

SUPPLEMENTARY PROBLEMS

29.11 5M loan, 50M EVIC, 30,000t emissions. Find financed emissions. **Ans.** 3,000 tonnes

Chapter 30: CASE STUDIES

30.1 MANUFACTURING COMPANY

Scenario: Global manufacturer with: - 10 facilities worldwide - Scope 1: 50,000 tonnes - Scope 2: 80,000 tonnes - Scope 3: 200,000 tonnes

Target: 50% reduction by 2030

SOLVED PROBLEMS

PROBLEM 30.1 Calculate required annual reduction rate for 50% reduction over 10 years.

Solution:

Current: 330,000 tonnes **Target:** 165,000 tonnes (50% reduction)

Annual reduction (linear):

$$\frac{330,000 - 165,000}{10} = 16,500 \text{ tonnes/year}$$

Annual rate:

$$\frac{16,500}{330,000} = 5\% \text{ per year}$$

Compound rate:

i

$$r = 1 - 0.5^{0.1} = 1 - 0.933 = 6.7\% \text{ per year}$$

Answer: Linear: 5%/year; Compound: 6.7%/year

SUPPLEMENTARY PROBLEMS

30.11 200,000t current, 40% reduction, 8 years. Find annual linear reduction. **Ans.** 10,000 tonnes/year

APPENDICES

SUPPLEMENTARY MATHEMATICAL PROOFS

Theorem 1.3 (Hadamard Product Properties)

Statement:

For emission vectors $a, b, c \in R^n$ and scalar $\alpha \in R$, the Hadamard product \odot satisfies:

1. **Commutativity:** $a \odot b = b \odot a$
2. **Associativity:** $(a \odot b) \odot c = a \odot (b \odot c)$
3. **Distributivity:** $a \odot (b + c) = a \odot b + a \odot c$
4. **Scalar multiplication:** $(\alpha a) \odot b = \alpha(a \odot b)$

Proof:

Let $a = \langle a_i \rangle$, $b = \langle b_i \rangle$, $c = \langle c_i \rangle$.

(1) Commutativity:

i

Therefore $a \odot b = b \odot a$. ■

(2) Associativity:

i

Therefore $(a \odot b) \odot c = a \odot (b \odot c)$. ■

(3) Distributivity:

i

Therefore $a \odot (b + c) = a \odot b + a \odot c$. ■

(4) Scalar multiplication:

i

Therefore $(\alpha a) \odot b = \alpha(a \odot b)$. ■

Theorem 1.4 (Inner Product Equivalence for CO_{2e})

Statement:

The total CO₂ equivalent emissions can be expressed equivalently as:

$$CO_{2e} = \sum_{i=1}^n m_i \times GWP_i = m^T g = \langle m, g \rangle = m_i g_i$$

where the last expression uses Einstein summation notation.

Proof:

Define mass vector $m = \textcolor{red}{i}$ and GWP vector $g = \textcolor{red}{i}$.

The inner product is:

$$m^T g = [m_1 \ m_2 \ \cdots \ m_n] \begin{bmatrix} g_1 \\ g_2 \\ \vdots \\ g_n \end{bmatrix} = \sum_{i=1}^n m_i g_i$$

In Einstein summation notation, repeated indices imply summation:

$$m_i g_i \equiv \sum_{i=1}^n m_i g_i$$

All three forms are mathematically equivalent. ■

Sources: Strang (2016) [52], Kolda & Bader (2009) [53]

CHAPTER 2 ENHANCEMENTS: LINEAR ALGEBRA FOR LCA

Theorem 2.1 (Leontief Inverse Existence and Convergence)

Statement:

For a technology matrix $A \in R^{n \times n}$ with $\|A\| < 1$, the Leontief inverse exists and is given by:

$$L = \textcolor{red}{i}$$

Proof:

Step 1: Show the series converges.

Since $\|A\| < 1$, the series $\sum_{k=0}^{\infty} A^k$ is a geometric series with ratio $\|A\|$.

For any matrix norm, $\|A^k\| \leq \|A\|^k$. Since $\|A\| < 1$:

$$\sum_{k=0}^{\infty} \|A^k\| \leq \sum_{k=0}^{\infty} \|A\|^k = \frac{1}{1 - \|A\|} < \infty$$

Therefore the series converges absolutely.

Step 2: Show the sum equals $\textcolor{red}{i}$.

Let $S_N = \sum_{k=0}^N A^k$. Then:

$$\begin{aligned} (I - A)S_N &= (I - A) \sum_{k=0}^N A^k = \sum_{k=0}^N A^k - \sum_{k=0}^N A^{k+1} \\ &\quad \textcolor{red}{i} I + \sum_{k=1}^N A^k - \sum_{k=1}^N A^k - A^{N+1} = I - A^{N+1} \end{aligned}$$

Taking the limit as $N \rightarrow \infty$:

$$(I - A) \lim_{N \rightarrow \infty} S_N = \lim_{N \rightarrow \infty} (I - A^{N+1}) = I$$

since $\lim_{N \rightarrow \infty} A^{N+1} = 0$ when $\|A\| < 1$.

Therefore:

i

■

Sources: Miller & Blair (2009) [54], Heijungs & Suh (2004) [8]

Theorem 2.2 (LCA Fundamental Equation)

Statement:

For a product system with technology matrix A , intervention matrix B , and functional unit f , the total environmental interventions are:

$$g = B \cdot i$$

Proof:

Let s be the scaling vector (total production of each process).

Step 1: Material balance equation.

The total output equals direct demand plus intermediate demand:

$$s = f + As$$

Step 2: Solve for scaling vector.

$$s - As = f$$

$$(I - A)s = f$$

$$s = i$$

Step 3: Calculate total interventions.

Environmental interventions are proportional to production:

$$g = Bs = B\dot{x}$$

■

Sources: Heijungs & Suh (2004) [8], Suh & Huppel (2005) [59]

CHAPTER 3 ENHANCEMENTS: PROBABILITY AND UNCERTAINTY

Theorem 3.1 (Error Propagation via Taylor Expansion)

Statement:

For a function $f(x)$ where $x=\dot{x}$ are independent random variables with means $\mu=\dot{\mu}$ and variances σ_i^2 , the variance of f is approximately:

$$\sigma_f^2 \approx \sum_{i=1}^n \left(\frac{\partial f}{\partial x_i} \dot{\mu}_i \right)^2 \sigma_i^2 = \nabla f \dot{x}$$

where $\Sigma = \text{diag}(\sigma_1^2, \sigma_2^2, \dots, \sigma_n^2)$ for independent variables.

Proof:

Step 1: Taylor expansion around the mean.

$$f(x) \approx f(\mu) + \sum_{i=1}^n \frac{\partial f}{\partial x_i} \dot{\mu}_i (x_i - \mu_i) + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \frac{\partial^2 f}{\partial x_i \partial x_j} \dot{\mu}_i (x_i - \mu_i) (x_j - \mu_j)$$

Step 2: Take expectation.

$$E[f(x)] \approx f(\mu) + \sum_{i=1}^n \frac{\partial f}{\partial x_i} \dot{\mu}_i E[x_i - \mu_i] = f(\mu)$$

since $E[x_i - \mu_i] = 0$.

Step 3: Calculate variance (first-order approximation).

$$\text{Var}[f(x)] = E[\dot{x}]$$

$$\approx E \left[\left(\sum_{i=1}^n \frac{\partial f}{\partial x_i} \dot{b}_\mu (x_i - \mu_i) \right)^2 \right]$$

$$\approx E \left[\sum_{i=1}^n \sum_{j=1}^n \frac{\partial f}{\partial x_i} \dot{b}_\mu \frac{\partial f}{\partial x_j} \dot{b}_\mu (x_i - \mu_i)(x_j - \mu_j) \right]$$

Step 4: Use independence.

For independent variables, $E[(x_i - \mu_i)(x_j - \mu_j)] = 0$ when $i \neq j$, and σ_i^2 when $i = j$.

$$\sigma_f^2 \approx \sum_{i=1}^n \left(\frac{\partial f}{\partial x_i} \dot{b}_\mu \right)^2 \sigma_i^2$$

■

Matrix Form:

Define the Jacobian vector $J = \nabla f(\mu)$. Then:

$$\sigma_f^2 = J^T \Sigma J$$

For correlated variables with covariance matrix Σ , the same formula applies.

Sources: Taylor & Kuyatt (1994) [55], JCGM 100:2008 [16]

CHAPTER 4 ENHANCEMENTS: MONTE CARLO METHODS

Theorem 4.1 (Monte Carlo Convergence - Strong Law of Large Numbers)

Statement:

Let X_1, X_2, \dots, X_N be independent and identically distributed random variables with $E[X_i] = \mu$ and $\text{Var}[X_i] = \sigma^2 < \infty$. Then the Monte Carlo estimator:

$$\hat{\mu}_N = (1/N) \sum_{i=1}^N X_i \rightarrow \mu \text{ as } N \rightarrow \infty$$

converges almost surely to the true mean.

Proof:

This is a direct application of the Strong Law of Large Numbers (Kolmogorov, 1933).

For i.i.d. random variables with finite mean, the sample average converges almost surely to the population mean:

$$P\left(\lim_{N \rightarrow \infty} \hat{\mu}_N = \mu\right) = 1$$

■

Sources: Metropolis & Ulam (1949) [56], Hammersley & Handscomb (1964) [57]

Theorem 4.2 (Monte Carlo Error Rate)

Statement:

The standard error of the Monte Carlo estimator decreases as:

$$SE(\hat{\mu}_N) = \frac{\sigma}{\sqrt{N}} = O(N^{-1/2})$$

Proof:

Step 1: Calculate variance of estimator.

$$\text{Var}[\hat{\mu}_N] = \text{Var}\left[\frac{1}{N} \sum_{i=1}^N X_i\right]$$

Step 2: Use independence.

$$\cancel{\text{Var}} \frac{1}{N^2} \sum_{i=1}^N \text{Var}[X_i] = \frac{1}{N^2} \cdot N \sigma^2 = \frac{\sigma^2}{N}$$

Step 3: Standard error.

$$SE(\hat{\mu}_N) = \sqrt{\text{Var}[\hat{\mu}_N]} = \frac{\sigma}{\sqrt{N}}$$

This shows the error decreases at rate $O(N^{-1/2})$, independent of dimension. ■

Corollary: To reduce error by factor of 10, need $10^2 = 100$ times more samples.

Sources: Robert & Casella (2004) [21], Metropolis & Ulam (1949) [56]

SUPPLEMENTARY MATHEMATICAL PROOFS

Theorem 1.3 (Hadamard Product Properties)

Statement:

For emission vectors $a, b, c \in R^n$ and scalar $\alpha \in R$, the Hadamard product \odot satisfies:

1. **Commutativity:** $a \odot b = b \odot a$
2. **Associativity:** $(a \odot b) \odot c = a \odot (b \odot c)$
3. **Distributivity:** $a \odot (b + c) = a \odot b + a \odot c$
4. **Scalar multiplication:** $(\alpha a) \odot b = \alpha(a \odot b)$

Proof:

Let $a = \underline{a}$, $b = \underline{b}$, $c = \underline{c}$.

(1) **Commutativity:**

\underline{a}

Therefore $a \odot b = b \odot a$. ■

(2) **Associativity:**

\underline{a}

Therefore $(a \odot b) \odot c = a \odot (b \odot c)$. ■

(3) **Distributivity:**

\underline{a}

Therefore $a \odot (b + c) = a \odot b + a \odot c$. ■

(4) **Scalar multiplication:**

i

Therefore $(\alpha a) \odot b = \alpha(a \odot b)$. ■

Theorem 1.4 (Inner Product Equivalence for CO₂e)

Statement:

The total CO₂ equivalent emissions can be expressed equivalently as:

$$CO_{2e} = \sum_{i=1}^n m_i \times GWP_i = m^T g = \langle m, g \rangle = m_i g_i$$

where the last expression uses Einstein summation notation.

Proof:

Define mass vector $m = \underline{m}$ and GWP vector $g = \underline{g}$.

The inner product is:

$$m^T g = [m_1 \quad m_2 \quad \cdots \quad m_n] \begin{bmatrix} g_1 \\ g_2 \\ \vdots \\ g_n \end{bmatrix} = \sum_{i=1}^n m_i g_i$$

In Einstein summation notation, repeated indices imply summation:

$$m_i g_i \equiv \sum_{i=1}^n m_i g_i$$

All three forms are mathematically equivalent. ■

Sources: Strang (2016) [52], Kolda & Bader (2009) [53]

APPENDIX B: GWP VALUES

Table B.1: Global Warming Potentials (IPCC AR6, 100-year)

Gas	Formula	GWP ₁₀₀	Lifetime (years)
Carbon dioxide	CO ₂	1	Variable
Methane (fossil)	CH ₄	29.8	11.8
Methane (biogenic)	CH ₄	27.2	11.8
Nitrous oxide	N ₂ O	273	109
HFC-134a	CH ₂ FCF ₃	1,530	14.0
HFC-32	CH ₂ F ₂	771	5.4
R-404A	Blend	3,922	-
R-410A	Blend	2,265	-
SF ₆	SF ₆	25,200	3,200

APPENDIX C: STATISTICAL TABLES

Table C.1: Standard Normal Distribution (Z-table)

Confidence Level	Z-value
68%	1.00
90%	1.645
95%	1.96
99%	2.576
99.9%	3.291

APPENDIX D: ANSWERS TO SUPPLEMENTARY PROBLEMS

Chapter 1: 1.11) 771; 1.12) 95.5; 1.13) 2.744; 1.14) 5.36; 1.15) 87.9; 1.16) 4.59; 1.17) 500; 1.18) 29.8, 273, 25,200; 1.19) 1,465; 1.20) 60%

Chapter 2: 2.11) [2,-1;-5,3]; 2.12) [154.5;127.3]; 2.13) 0.4925; 2.14) 250; 2.15)
[0.07,0.04;0.06,0.07]; 2.20) [1.667,0;0,1.429]

Chapter 3: 3.11) $6,000 \pm 894$; 3.12) $1,000 \pm 55.9$; 3.14) 6.68%; 3.15) 200 ± 17.9 ; 3.16) 15%;
3.17) 822 ± 44 ; 3.18) 1,000, 60.8; 3.19) 47.4; 3.20) 20%

[Continues for all chapters...]

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