Water‑Vapour Concentration in Lean Combustion Products

# 1 Introduction

This note summarises the equations implemented in the accompanying Python script for estimating the water‑vapour content in the products of complete, lean combustion (φ < 1) of hydrocarbon and oxygenated fuels.

# 2 Stoichiometric oxygen requirement

For a generic fuel CxHyOz, the moles of O2 required for complete combustion per mole of fuel are

a\_st = x + y/4 – z/2

**Source**:

* *Turns, S. R. (2012).* *An Introduction to Combustion*, 3rd ed., McGraw-Hill.
* **Chapter 4**, around Section 4.1–4.2.
* This comes from the derivation of stoichiometric combustion for a generic hydrocarbon or oxygenated fuel.

# 3 Equivalence ratio and excess‑air factor

The equivalence ratio is defined as

φ = (F/A)/(F/A)\_st

and its reciprocal is the excess‑air factor λ = 1/φ. Lean combustion corresponds to λ > 1.

**Source**:

* *Turns, S. R. (2012).* *An Introduction to Combustion*, 3rd ed., McGraw-Hill.
* **Chapter 5**, typically around Sections 5.1–5.2.

# 4 Ideal combustion reaction (lean, complete)

CxHyOz + λ·a\_st (O2 + 3.76 N2) → x CO2 + y/2 H2O + (λ–1)·a\_st O2 + 3.76 λ·a\_st N2

**Source**:

* *Turns, S. R. (2012)*, again **Chapter 5**, or summary tables at the end of combustion analysis chapters.

# 5 Water‑vapour mole fraction

n\_H2O = y/2

Total moles N\_tot = n\_H2O + n\_CO2 + n\_O2(excess) + n\_N2

Mole fraction : X\_H2O = n\_H2O / N\_tot

**Source**:

* *Turns, S. R. (2012)* and consistent with general mole fraction definitions from thermodynamics.
* Also appears in *Thermal-Fluid Sciences* by Turns (2000), **Chapter on Thermodynamics of Mixtures**.

# 6 Water‑vapour mass fraction

Mass\_H2O = n\_H2O · M\_H2O

Total mass = Σ n\_i M\_i (H2O, CO2, O2, N2)

Mass fraction : w\_H2O = Mass\_H2O / Total\_mass

**Source**:

* *Heywood, J. B. (1988).* *Internal Combustion Engine Fundamentals*, McGraw-Hill.
* **Chapter 3**, covering combustion thermodynamics and gas analysis.

# 7 Example (Jet‑A, φ = 0.24)

Fuel model : C12H23

**Sources for fuel compositions**:

* *ASTM D1655-21*: Jet-A fuel specification.
* *U.S. Department of Energy AFDC*: https://afdc.energy.gov/fuels/jet\_fuel.html
* *Lefebvre & Ballal (2010)* for alternative jet fuels like HEFA-SPK, FT-SPK, etc.

a\_st = 12 + 23/4 = 17.75 mol O2/mol

λ = 1/0.24 ≈ 4.17

n\_H2O = 11.5, n\_CO2 = 12, n\_O2(excess) = 56.2, n\_N2 = 278.1

N\_tot = 357.8 → X\_H2O ≈ 0.032 (3.2 %)

w\_H2O ≈ 0.020 (2.0 %)

# 8 Assumptions & limitations

* Perfectly complete combustion; no CO, unburned fuel, NOx, SOx.
* Dissociation is neglected (reasonable for φ ≲ 0.5).
* Air composition fixed at 79 % N2 / 21 % O2 by volume.
* Lumped‑formula fuels approximate real blends (Jet‑A, HEFA‑SPK, etc.).

# 9 References

* 1. Turns, S. R. (2012). An Introduction to Combustion: Concepts and Applications (3rd ed.). McGraw-Hill.
* 2. Lefebvre, A. H., & Ballal, D. R. (2010). Gas Turbine Combustion: Alternative Fuels and Emissions (3rd ed.). CRC Press.
* 3. Heywood, J. B. (1988). Internal Combustion Engine Fundamentals. McGraw-Hill.
* 4. ASTM D1655-21. Standard Specification for Aviation Turbine Fuels. ASTM International.
* 5. U.S. Department of Energy. Alternative Fuels Data Center – Jet Fuel Properties.
* 6. Turns, S. R. (2000). Thermal-Fluid Sciences. McGraw-Hill.