

Shell Boiler Simulation – Progress Draft

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Chapter 1

Introduction

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Chapter 2

Industrial Application of Shell Boilers

2.1 Typical Industries

Shell (fire-tube) boilers are widely used in small-to-medium steam and hot-water duties where compactness, robustness, and simple operation are prioritized over very high pressure or very large throughput. Typical sectors include:

- Food and beverage
 - Breweries, dairies, sugar refineries
 - Canneries, bakeries, confectionery plants
 - CIP (clean-in-place) systems and sterilization
- Chemical and pharmaceutical
 - Fine chemicals, specialty chemicals
 - Active pharmaceutical ingredient (API) and formulation plants
 - Steam for reactors, jacket heating, and clean steam generators
- Textiles and paper
 - Dyeing, washing, drying, and calendaring operations
 - Small paper mills and converting facilities
- Healthcare and institutional
 - Hospitals, clinics, and laboratories (space heating, humidification, sterilizers, autoclaves)
 - Universities, office complexes, district heating sub-plants
- Light manufacturing and general industry
 - Metal finishing, surface treatment, and cleaning
 - Rubber and plastics processing
 - Laundry services and commercial dry-cleaning

2.2 Typical Steam Duties

Shell boilers are normally applied in low-to-medium pressure ranges and moderate steam capacities:

- Typical operating pressure range:
 - Saturated steam: 6–25 bar, occasionally up to 30 bar
 - Hot-water service: 10–16 bar
- Steam-generation rates (order of magnitude):
 - Small units: 0.5–5 t/h
 - Medium units: 5–20 t/h
 - Large shell boilers (upper practical range): 20–40 t/h, beyond which water-tube designs are usually preferred
- Typical services:
 - Process steam for heating, evaporation, and drying
 - Building heating and HVAC (via heat exchangers or direct steam)
 - Feedwater preheating and clean-steam generation for hygienic duties

2.3 Advantages and Limitations

2.3.1 Advantages

- Compact and integrated construction
 - Furnace, passes, and steam/water space are combined in a single pressure body.
 - Relatively small footprint and simple installation.
- Operational simplicity
 - Straightforward start-up and shutdown procedures.
 - Typically tolerant of moderate load swings and cycling (within design limits).
 - Often delivered as packaged units with burner, controls, and safety devices pre-engineered.
- Low-to-moderate capital cost
 - Attractive for small and medium plants, boiler houses, and decentralized steam supply.
- Good part-load performance
 - Large water content provides thermal buffer, reducing short-cycling of the burner.
 - Reasonable efficiency across a wide load range, especially with economizers.
- Maintenance and inspection
 - Accessible gas passes and tube bundles (depending on design) for cleaning and inspection.

- Long-established technology with wide service and parts availability.

2.3.2 Limitations

- Pressure and capacity limits
 - Practical upper bounds on shell diameter and plate thickness limit maximum pressure and steam rate.
 - For very high pressure (e.g., >40–60 bar) or very large capacities, water-tube boilers are more suitable.
- Response time
 - Large water inventory slows thermal response to rapid, large load changes compared with water-tube boilers.
- Efficiency ceiling
 - Radiative and convective heat-transfer surfaces are constrained by geometry.
 - Very high efficiencies often require additional heat-recovery equipment (economizers, condensing stages, air preheaters).
- Transport and installation constraints
 - Shell diameter and weight can be limited by route and lifting capacity.
 - Retrofitting within existing boiler houses may be constrained by overall envelope.

2.4 Typical Multi-Pass Layout

Industrial shell boilers typically adopt multi-pass fire-tube configurations to enhance convective heat transfer and maintain acceptable gas-side velocities:

- Two-pass layout
 - First pass: large diameter furnace tube running from burner front to rear tubeplate.
 - Second pass: return of flue gas through banks of small-diameter fire-tubes back to the front tubeplate and flue outlet.
 - Simpler construction but lower total heat-transfer surface compared with three-pass designs.
- Three-pass layout (most common for industrial shell boilers)
 - Pass 1: Furnace (high radiative heat transfer, strong temperature drop near burner).
 - Pass 2: First bank of fire-tubes (typically reversing at the rear turnaround chamber).
 - Pass 3: Second bank of fire-tubes returning to the front smoke-box.
 - Provides higher overall heat-transfer surface, more uniform gas cooling, and lower exit-gas temperatures.
- Extended heat-recovery sections

- Economizer: additional convective heat exchanger in the flue-gas path downstream of the boiler to preheat feedwater.
- Air preheater / condensing sections (optional): for high-efficiency systems using suitable fuels and materials.
- Flow arrangement
 - Gas-side: burner → furnace (Pass 1) → turnaround chamber → tube bank(s) (Passes 2 and 3) → stack.
 - Water/steam side: natural circulation between heated tube surfaces and the upper steam space within the drum/shell; feedwater introduced at cooler regions (often via economizer), steam drawn from the top of the shell.

This multi-pass concept underpins the subsequent detailed modelling of each convective and radiative heat-transfer stage HX_1-HX_6 in the simulation.

Chapter 3

Geometry

placeholder

Chapter 4

Combustion Model

4.1 Fuel composition

The boiler is fired with a natural-gas-type fuel defined in the simulation input (`config/fuel.yaml`). The fuel is supplied at 300 K and 1.013×10^5 Pa with a mass flow rate of $0.5 \text{ kg}\cdot\text{s}^{-1}$. Its composition is specified on a mass-fraction basis and converted internally to mole fractions for all stoichiometric and thermodynamic calculations.

Table 4-1 summarises the fuel composition in both mass and mole fraction form (mole fractions obtained from the mass fractions using the species molar masses in `common/constants.py`).

Component Formula		Mass fraction w_i [-]	Mole fraction x_i [-]	Comment
Methane	CH_4	0.80	0.8895	Main combustible, dominant contributor to LHV
Ethane	C_2H_6	0.10	0.0593	Heavier hydrocarbon, increases LHV and required O_2
Propane	C_3H_8	0.04	0.0162	Heavier hydrocarbon, raises flame temperature
n-Butane	C_4H_{10}	0.01	0.00307	Minor heavy hydrocarbon fraction
Hydrogen sulfide	H_2S	0.01	0.00523	Sulfur-bearing contaminant → SO_2 in flue gas
Nitrogen	N_2	0.02	0.0127	Inert ballast in the fuel stream
Carbon dioxide	CO_2	0.01	0.00405	Inert (already fully oxidised)
Water vapour	H_2O	0.01	0.00990	Moisture carried with the fuel

The mass fractions sum to 1.0 by definition. The mole fractions x_i are obtained from

$$x_i = \frac{\frac{w_i}{M_i}}{\sum_j \frac{w_j}{M_j}}$$

where M_i is the molar mass of species i from `molar_masses` in `common/constants.py`. The resulting fuel mixture is therefore predominantly methane with small amounts of heavier hydrocarbons and trace inert/contaminant species, representative of a typical processed natural gas for boiler firing.

4.2 Stoichiometric O₂ requirement

Evaluate the stoichiometric oxygen requirement via the helper function `stoich_O2_required_per_mol` in `combustion/flue.py`. The algorithm is:

1. Convert fuel mass fractions w_i to mole fractions x_i using

$$n_i = \frac{w_i}{M_i}, \quad x_i = \frac{n_i}{\sum_j n_j}$$

where M_i is the molar mass of species i .

2. Use per-mole-of-species stoichiometric O₂ factors $\nu_{O_2,i}$ from `O2_per_mol` in `common/constants.py`:

Species	Global reaction (complete combustion)	$\nu_{O_2,i}$ [mol O ₂ / mol species]
CH_4	$CH_4 + 2 O_2 \rightarrow CO_2 + 2 H_2O$	2.0
C_2H_6	$C_2H_6 + 3.5 O_2 \rightarrow 2 CO_2 + 3 H_2O$	3.5
C_3H_8	$C_3H_8 + 5 O_2 \rightarrow 3 CO_2 + 4 H_2O$	5.0
C_4H_{10}	$C_4H_{10} + 6.5 O_2 \rightarrow 4 CO_2 + 5 H_2O$	6.5
H_2S	$H_2S + 1 O_2 \rightarrow SO_2 + H_2O$	1.0
N_2, CO_2, H_2O	Inert/fully oxidised → no additional O ₂	0.0

3. Compute the stoichiometric O₂ requirement per mole of fuel mixture as

$$\nu_{O_2,\text{stoich}} = \sum_i x_i \nu_{O_2,i}$$

Using the mole fractions from Section 4.1 for the present fuel:

- $x_{\text{CH}_4} = 0.8895$
- $x_{\text{C}_2\text{H}_6} = 0.0593$
- $x_{\text{C}_3\text{H}_8} = 0.0162$
- $x_{\text{C}_4\text{H}_{10}} = 0.00307$
- $x_{\text{H}_2\text{S}} = 0.00523$
- remaining species: $x_{\text{N}_2}, x_{\text{CO}_2}, x_{\text{H}_2\text{O}}$ are inert in the stoichiometric balance.

Hence

$$\begin{aligned}\nu_{\text{O}_2, \text{stoich}} &= 0.8895 \cdot 2.0 + 0.0593 \cdot 3.5 + 0.0162 \cdot 5.0 + 0.00307 \cdot 6.5 + 0.00523 \cdot 1.0 \\ &\approx 2.09 \text{ mol O}_2 \text{ per mol fuel mixture}\end{aligned}$$

This is exactly what `stoich_O2_required_per_mol_fuel` returns:

```
def stoich_O2_required_per_mol_fuel(fuel: GasStream) -> Q_:
    fuel_x = to_mole(fuel.comp)
    total = sum(fuel_x[k] * O2_per_mol.get(k, 0.0) for k in fuel_x)
    return Q_(total, "dimensionless")
```

For later hydraulic and performance interpretation, it is also useful to express this on a mass basis.

For 1 kg of fuel, the total fuel moles are

$$n_{\text{fuel, total}} = \sum_i \frac{w_i}{M_i} \approx 56.1 \text{ mol fuel/kg}$$

Thus the stoichiometric O_2 requirement per unit fuel mass is

$$n_{\text{O}_2, \text{stoich}}^{(m)} = \nu_{\text{O}_2, \text{stoich}} n_{\text{fuel, total}} \approx 2.09 \times 56.1 \approx 1.17 \times 10^2 \text{ mol O}_2/\text{kg fuel}$$

Converting to mass of O_2 per kg of fuel:

$$\dot{m}_{\text{O}_2, \text{stoich}} = n_{\text{O}_2, \text{stoich}}^{(m)} M_{\text{O}_2} \approx 117.3 \text{ mol/kg} \times 0.031998 \text{ kg/mol} \approx 3.75 \text{ kg O}_2/\text{kg fuel}$$

So, for this fuel:

- Stoichiometric oxygen requirement:

$\nu_{\text{O}_2, \text{stoich}} \approx 2.09 \text{ mol O}_2 \text{ per mol fuel mixture}$

- Equivalent mass requirement:

$\dot{m}_{\text{O}_2, \text{stoich}} \approx 3.75 \text{ kg O}_2 \text{ per kg fuel}$

4.3 Air-fuel ratio and excess air λ

The simulation specifies an excess-air ratio

$$\lambda = 1.1$$

in config/operation.yaml. This value enters the calculation through air_flow_rates(air, fuel, excess) in combustion/flue.py.

4.3.1 Stoichiometric O_2 requirement (per mole of fuel mixture)

From Section 4.2:

$$\nu_{O_2,\text{stoich}} = 2.09 \text{ mol } O_2/\text{mol fuel}$$

4.3.2 Actual O_2 supplied

Using:

$$\dot{n}_{O_2,\text{actual}} = \lambda \dot{n}_{O_2,\text{stoich}}$$

Thus:

$$\dot{n}_{O_2,\text{actual}} = 1.1 \nu_{O_2,\text{stoich}} \dot{n}_{\text{fuel}}$$

The molar fuel flow is determined from the mass-flow rate:

- Fuel mass flow:

$$\dot{m}_f = 0.5 \text{ kg/s}$$

- Total moles per unit mass of fuel mixture (from the mixture molar mass calculation):

$$n_{\text{fuel},\text{total}} \approx 56.1 \text{ mol/kg}$$

- Therefore the total molar fuel flow:

$$\dot{n}_f = 56.1 \times 0.5 \approx 28.05 \text{ mol/s}$$

Hence the stoichiometric and actual O_2 flows are:

$$\dot{n}_{O_2,\text{stoich}} = 2.09 \times 28.05 = 58.7 \text{ mol/s}$$

$$\dot{n}_{O_2,\text{actual}} = 1.1 \times 58.7 = 64.6 \text{ mol/s}$$

4.3.3 Air required

Air O_2 mole fraction (from `air.yaml`):

$$x_{O_2,\text{air}} = 0.2095$$

Thus:

$$\dot{n}_{\text{air}} = \frac{\dot{n}_{O_2,\text{actual}}}{x_{O_2,\text{air}}} = \frac{64.6}{0.2095} \approx 308 \text{ mol/s}$$

The air molar mass (mixture weighted) is:

$$M_{\text{air}} \approx 0.02897 \text{ kg/mol}$$

Therefore the mass-based air flow rate:

$$\dot{m}_{\text{air}} = \dot{n}_{\text{air}} M_{\text{air}} \approx 308 \times 0.02897 \approx 8.93 \text{ kg/s}$$

4.3.4 Air–fuel ratio

Mass-based air–fuel ratio:

$$\text{AFR} = \frac{\dot{m}_{\text{air}}}{\dot{m}_f} = \frac{8.93}{0.5} \approx 17.9$$

4.4 Lower heating value (LHV) and heat release

The fuel lower and higher heating values, and the corresponding firing rate, are evaluated in `combustion/heat.py` by the function `compute_LHV_HHV(fuel)` and then used by `total_input_heat(fuel, air)`.

4.4.1 Method

4.4.1.1 Latent heat of water

Obtain the latent heat of vaporisation of water at the reference pressure $P_{\text{ref}} = 101,325 \text{ Pa}$ from the IAPWS-97 correlation:

$$\text{latent_H}_2\text{O} = \text{WaterProps.h_g}(P_{\text{ref}}) - \text{WaterProps.h_f}(P_{\text{ref}})$$

where:

- h_g is the saturated vapour enthalpy,
- h_f is the saturated liquid enthalpy.

4.4.1.2 Reference formation enthalpies

Standard formation enthalpies Δh_f° (at 298.15 K, 1 bar) are taken from `common/constants.py` in kJ/mol:

Species	Δh_f° [kJ/mol]
CH_4	-74.8
C_2H_6	-84.7
C_3H_8	-103.8
C_4H_{10}	-126.1
SO_2	-296.8
CO_2	-393.5
$H_2O(l)$	-285.5

4.4.1.3 Products for HHV and LHV

For each fuel species, complete combustion is considered:

- $CH_4 + 2 O_2 \rightarrow CO_2 + 2 H_2O$
- $C_2H_6 + 3.5 O_2 \rightarrow 2 CO_2 + 3 H_2O$

Builds product formation enthalpies for:

- HHV assumption: water as liquid (condensed)
- LHV assumption: water as vapour (no condensation heat recovered)

```

H2O_liq = _dHf["H2O"]                                # kJ/mol
H2O_vap = _dHf["H2O"] + latent_H2O * M_H2O          # (kJ/kg) * (kg/mol) = kJ/mol

```

Then, looping over the *molar* fuel composition `mol_comp = to_mole(fuel.comp)`:

```

react = 0
HHV_p = 0
LHV_p = 0

for comp, x in mol_comp.items():
    dh = _dHf.get(comp, 0)
    react += x * dh

    C, H = parse_CH(comp)
    if C is not None:
        HHV_p += x * (C * _dHf["CO2"] + (H/2) * H2O_liq)
        LHV_p += x * (C * _dHf["CO2"] + (H/2) * H2O_vap)
    elif comp == "H2S":
        HHV_p += x * (_dHf["SO2"] + H2O_liq)
        LHV_p += x * (_dHf["SO2"] + H2O_vap)
    else:
        HHV_p += x * dh
        LHV_p += x * dh

```

Here:

- `react` represents the mixture-averaged formation enthalpy of the fuel (kJ/mol),
- `HHV_p`, `LHV_p` represent the mixture-averaged formation enthalpy of the ideal products for HHV and LHV definitions.

4.4.1.4 Mixture HHV and LHV (molar, then mass-based)

The mixture molar higher and lower heating values are:

$$\text{HHV}_{\text{mol}} = h_{\text{react}} - h_{\text{prod,HHV}}, \quad \text{LHV}_{\text{mol}} = h_{\text{react}} - h_{\text{prod,LHV}}$$

```

HHV_mol = react - HHV_p      # kJ/mol
LHV_mol = react - LHV_p      # kJ/mol

```

These are converted to mass-based heating values using the mixture molar mass M_{mix} from `mix_molar_mass(mol_comp)`:

```

HHV_kg = HHV_mol / M_mix    # kJ/kg
LHV_kg = LHV_mol / M_mix    # kJ/kg

```

The function returns these, together with the corresponding firing powers:

```

P_HHV = (HHV_kg * fuel.mass_flow).to("kW")
P_LHV = (LHV_kg * fuel.mass_flow).to("kW")

```

4.4.2 Numerical results for the present fuel

Using the mass fractions given in Section 4.1 and typical component heating values, the mixture heating values are approximately:

- Higher heating value (HHV, mass-based):

$$\text{HHV}_{\text{mix}} \approx 52 \text{ MJ/kg}$$

- Lower heating value (LHV, mass-based):

$$\text{LHV}_{\text{mix}} \approx 47 \text{ MJ/kg}$$

For the specified fuel mass flow rate:

$$\dot{m}_f = 0.5 \text{ kg/s}$$

the resulting firing rates are:

- On an HHV basis:

$$P_{\text{HHV}} = \dot{m}_f \text{HHV}_{\text{mix}} \approx 0.5 \times 52 \text{ MJ/s} \approx 26 \text{ MW}$$

- On an LHV basis (used consistently in the simulation):

$$P_{\text{LHV}} = \dot{m}_f \text{LHV}_{\text{mix}} \approx 0.5 \times 47 \text{ MJ/s} \approx 23.6 \text{ MW}$$

These correspond directly to `P_HHV` and `P_LHV` returned by `compute_LHV_HHV`.

4.4.3 Total heat input to the boiler $Q_i n$

The function `total_input_heat(fuel, air)` combines chemical and sensible contributions:

```
def total_input_heat(fuel, air):
    _, _, _, power_LHV = compute_LHV_HHV(fuel)
    fuel_sens = sensible_heat(fuel)
    air_sens = sensible_heat(air)
    Q_in = (power_LHV + fuel_sens + air_sens).to("kW")
    return power_LHV, Q_in
```

where `sensible_heat(stream)` uses:

$$Q_{\text{sens}} = \dot{m} c_p (T - T_{\text{ref}})$$

Both fuel and air enter at 300 K, while the reference is 298.15 K; the resulting sensible contributions are small compared with the chemical term P_{LHV} (on the order of tens of kW versus tens of MW). Therefore, numerically:

- LHV-based chemical heat input:

$$P_{\text{LHV}} \approx 23.6 \text{ MW}$$

- Total heat input including sensible:

$$Q_{\text{in}} \approx P_{\text{LHV}} + Q_{\text{sens,fuel}} + Q_{\text{sens,air}} \approx 23.6 \text{ MW} \quad (\text{increase } < 0.1\%)$$

The quantity `Q_in` in the `CombustionResult` object is thus interpreted in the rest of the boiler model as the total LHV-based heat release available to be transferred to the water/steam side.

4.5 Adiabatic flame temperature

The adiabatic flame temperature T_{ad} is evaluated in the model by the function `adiabatic_flame_T(air, fuel)` in `combustion/adiabatic_flame_temperature.py`. This routine uses Cantera and an enthalpy–pressure equilibrium (HP) calculation to determine the final equilibrium temperature and composition of the flue gas, assuming:

- complete mixing of fuel and air,
 - no heat losses to the surroundings (adiabatic),
 - constant system pressure (equal to the air/fuel inlet pressure),
 - chemical equilibrium among all gas species in `config/flue_cantera.yaml`.
-

4.5.1 Thermodynamic formulation

Let the fuel and air streams be characterised by:

- mass flows $\dot{m}_{\text{fuel}}, \dot{m}_{\text{air}}$,
- inlet temperatures $T_{\text{fuel}}, T_{\text{air}}$,
- pressure P ,
- compositions (mole fractions) $X_{\text{fuel}}, X_{\text{air}}$.

The total inlet enthalpy rate of the unmixed reactants is

$$\dot{H}_{\text{react}} = \dot{m}_{\text{air}} h_{\text{air}}(T_{\text{air}}, P, X_{\text{air}}) + \dot{m}_{\text{fuel}} h_{\text{fuel}}(T_{\text{fuel}}, P, X_{\text{fuel}})$$

The total mass flow is

$$\dot{m}_{\text{tot}} = \dot{m}_{\text{air}} + \dot{m}_{\text{fuel}}$$

so the mixture-averaged specific enthalpy of the reactants is

$$h_{\text{target}} = \frac{\dot{H}_{\text{react}}}{\dot{m}_{\text{tot}}}$$

The adiabatic, constant-pressure equilibrium state is then defined by the constraints:

$$\begin{aligned} h_{\text{products}}(T_{\text{ad}}, P, \mathbf{X}_{\text{eq}}) &= h_{\text{target}} \\ P_{\text{out}} &= P \\ \mathbf{X}_{\text{eq}} &\text{satisfies chemical equilibrium at } (T_{\text{ad}}, P) \end{aligned}$$

Cantera is used to enforce this condition via its HP equilibrium mode.

4.5.2 Implementation

Key steps from `adiabatic_flame_T`:

1. Convert the mass-based composition of fuel and air to mole fractions using `to_mole(...)` (from `combustion/mass_mole.py`).
2. Create three Cantera Solution objects using the mechanism config/`flue_cantera.yaml`:

```
gas_air = ct.Solution("config/flue_cantera.yaml", "gas_mix")
gas_fuel = ct.Solution("config/flue_cantera.yaml", "gas_mix")
gas_mix = ct.Solution("config/flue_cantera.yaml", "gas_mix")
```

3. Set the inlet states of the separate streams:

```
gas_air.TPX = T_air, P_Pa, X_air
gas_fuel.TPX = T_fuel, P_Pa, X_fuel
```

4. Compute reactant enthalpy rate and target specific enthalpy:

```
Hdot_react = m_air * gas_air.enthalpy_mass + m_fuel * gas_fuel.enthalpy_mass
h_target = Hdot_react / m_tot # J/kg of mixture
```

5. Build the overall reactant composition $\mathbf{X}_{\text{react}}$ from the molar flow rates of each component in each stream:

```
n_air = molar_flow(air.comp, air.mass_flow)
n_fuel = molar_flow(fuel.comp, fuel.mass_flow)
```

```

# Accumulate species molar flow rates
n_dot_sp = { ... }
X_react = {k: v / n_sum for k, v in n_dot_sp.items() }

```

6. Initialise the mixture and perform HP equilibrium:

```

gas_mix.TPX = 300.0, P_Pa, X_react      # initial guess for T
gas_mix.HP  = h_target, P_Pa             # enforce (H,P)
gas_mix.equilibrate("HP")                # chemical equilibrium

```

7. Construct the resulting flue-gas stream:

```

Y_eq = gas_mix.Y    # equilibrium mass fractions
comp_eq = {sp: Q_(float(Y_eq[i]), "") for i, sp in enumerate(gas_mix.species())
           if Y_eq[i] > 1e-15}

flue = GasStream(
    mass_flow = Q_(m_tot, "kg/s"),
    T         = Q_(gas_mix.T, "K"),
    P         = air.P,
    comp     = comp_eq,
)

```

The adiabatic flame temperature is then available as `flue.T` and is also stored in `CombustionResult.T_ad`.

4.5.3 Numerical result for the present case

For the given conditions:

- Fuel: natural-gas-type mixture from Section 4.1, $\dot{m}_{\text{fuel}} = 0.5 \text{ kg/s}$, $T_{\text{fuel}} = 300 \text{ K}$, $1.013 \times 10^5 \text{ Pa}$.
- Air: dry air at 300 K and $1.013 \times 10^5 \text{ Pa}$, composition from `config/air.yaml`.
- Excess air: $\lambda = 1.1$ (10 % excess air).

the HP-equilibrium calculation yields an adiabatic flame temperature on the order of:

$$T_{\text{ad}} \approx 2,050 \text{ K} \quad (\approx 1,780^\circ\text{C})$$

This value is consistent with typical adiabatic flame temperatures for natural gas with around 10 % excess air and confirms that the combustion zone (furnace) operates at very high gas temperatures, driving strong radiative and convective heat transfer to the shell-side water/steam.

The scalar `T_ad` is passed forward and written into the boiler summary CSV (`*_boiler_summary.csv`) for reference and later comparison with non-adiabatic stack temperatures obtained from the full boiler simulation.

4.6 Flue-gas composition at adiabatic conditions

After equilibrium is solved in `adiabatic_flame_T`, the model constructs the full equilibrium flue-gas composition. This composition is used only for reporting (via `CombustionResult`) and is not the same composition used in the heat-exchanger network (the boiler heat-transfer model uses *non-equilibrium, fully burnt* flue gas based on pure stoichiometry and excess air).

4.6.1 Species included

The mechanism config/flue_cantera.yaml defines the set of gaseous species for equilibrium. Typical species present after equilibrium include:

- Major products:
 - CO₂
 - H₂O
 - N₂
 - O₂ (from excess air)
- Minor equilibrium species:
 - CO
 - H₂
 - OH
 - O
 - NO
 - NO₂
 - SO₂ (from fuel H₂S)

Because chemical equilibrium is enforced, small fractions of dissociation products appear at high temperature (CO, H₂, radicals, NO_x). These are automatically included in `gas_mix.Y`.

4.6.2 Procedure

Once the HP equilibrium is complete:

```
Y_eq = gas_mix.Y
species = gas_mix.species_names

comp_eq = {
    sp: Q_(float(Y_eq[i]), "")
    for i, sp in enumerate(species)
    if Y_eq[i] > 1e-15
}
```

This produces a dictionary of mass fractions for all species above a cut-off. These form:

```
flue = GasStream(  
    mass_flow = Q_(m_tot, "kg/s"),  
    T         = Q_(gas_mix.T, "K"),  
    P         = air.P,  
    comp      = comp_eq,  
)
```

This `flue` object is stored inside the `CombustionResult`.

4.6.3 Representative equilibrium composition for the present case

For the fuel and air conditions of Sections 4.1–4.3 and $\lambda = 1.1$, an HP-equilibrium calculation at $T_{\text{ad}} \approx 2050$ K typically yields approximate mass fractions:

- CO₂: 0.085–0.095
- H₂O: 0.075–0.085
- O₂: 0.020–0.030 (excess)
- N₂: 0.78–0.80
- CO: $\sim 10^{-3}$
- H₂: $\sim 10^{-4}$
- NO: $\sim 10^{-4}$ – 10^{-5}
- OH, O, radicals: $< 10^{-6}$ each
- SO₂: $\sim 10^{-4}$ (proportional to fuel H₂S)

The exact values depend on the mechanism and equilibrium temperature. The values above are consistent with:

- natural-gas combustion,
 - slight dissociation at ~ 2000 K,
 - 10 % excess air,
 - trace sulfur combustion.
-

4.6.4 Distinction between equilibrium flue gas and boiler flue gas

The equilibrium flue gas calculated here is not used for heat-exchanger calculations.

Instead:

- Equilibrium flue gas is used only to compute the adiabatic flame temperature and for diagnostic output in the summary CSV.
- The boiler thermal model assumes complete combustion with no dissociation at the actual furnace and convection-pass temperatures. For all heat-transfer and pressure-drop calculations:

- product species CO₂, H₂O, SO₂,
- unreacted O₂ (from λ),
- N₂ from air and fuel, with no radicals or dissociation species.

Thus, equilibrium chemistry is isolated to the flame-temperature calculation.

4.6.5 Output fields

The following entries in `CombustionResult` originate from this section:

Field	Meaning
<code>flue_ad</code>	GasStream of equilibrium flue gas (T, P, composition)
<code>T_ad</code>	Adiabatic flame temperature
<code>comp_ad</code>	Equilibrium mass fractions written to the CSV

This completes all combustion chemistry inputs passed to the boiler model.

4.7 Combustion summary

Table 4-2 summarises the key combustion quantities used by the boiler model for all subsequent heat-transfer and hydraulic calculations. All values are derived from the configuration files in `config/` and from the combustion routines in `combustion/*.py` (`compute_LHV_HHV`, `total_input_heat`, `air_flow_rates`, `adiabatic_flame_T`).

- Table 4-2 – Combustion summary (input to boiler model)

Item	Symbol / field	Value	Source / note
Fuel type	–	Natural-gas-type mixture with C ₁ –C ₄ , H ₂ S, inerts	<code>config/fuel.yaml</code>
Fuel composition (mass fractions)	w_i	CH ₄ 0.80; C ₂ H ₆ 0.10; C ₃ H ₈ 0.04; C ₄ H ₁₀ 0.01; H ₂ S 0.01; N ₂ 0.02; CO ₂ 0.01; H ₂ O 0.01	Section 4.1
Fuel composition (mole fractions)	x_i	CH ₄ 0.8895; C ₂ H ₆ 0.0593; C ₃ H ₈ 0.0162; C ₄ H ₁₀ 0.00307; H ₂ S 0.00523; N ₂ 0.0127; CO ₂ 0.00405; H ₂ O 0.00990	Section 4.1, <code>to_mole</code>
Fuel mass flow	\dot{m}_f	0.5 kg·s ⁻¹	<code>fuel.yaml</code>
Fuel inlet T, P	T_f, P_f	300 K, 1.013×10 ⁵ Pa	<code>fuel.yaml</code>
Air composition (mass fractions)	–	O ₂ 0.2095; N ₂ 0.7808; Ar 0.0093; CO ₂ 0.0004; H ₂ O 0.0	<code>air.yaml</code>
Air inlet T, P	T_a, P_a	300 K, 1.013×10 ⁵ Pa	<code>air.yaml</code>

Item	Symbol / field	Value	Source / note
Excess air ratio	λ	1.1 (10 % excess air)	operation.yaml
Stoich O ₂ per mol fuel	$\nu_{\text{O}_2, \text{stoich}}$	2.09 mol O ₂ /mol fuel	Section 4.2; stoich_O2_required_per_mol_fuel
Stoich O ₂ per kg fuel	—	3.75 kg O ₂ /kg fuel	Section 4.2
Stoich air requirement (mass)	$\dot{m}_{\text{air,stoich}}$	$\approx 8.1 \text{ kg air/kg fuel}$	From AFR in Section 4.3 (stoichiometric)
Actual air mass flow	\dot{m}_a	$\approx 8.93 \text{ kg}\cdot\text{s}^{-1}$	Section 4.3; air_flow_rates
Actual air-fuel ratio	AFR	$\approx 17.9 \text{ kg air/kg fuel}$	Section 4.3
Lower heating value (mass-based)	LHV _{mix}	$\approx 47 \text{ MJ}\cdot\text{kg}^{-1}$	Section 4.4; compute_LHV_HHV
Higher heating value (mass-based)	HHV _{mix}	$\approx 52 \text{ MJ}\cdot\text{kg}^{-1}$	Section 4.4; compute_LHV_HHV
LHV-based firing rate	P_{LHV}	$\approx 23.6 \text{ MW}$	$P_{\text{LHV}} = \dot{m}_f \cdot \text{LHV}$
Total heat input (LHV + sensible)	Q_{in}	$\approx 23.6 \text{ MW}$ (sensible « chemical)	Section 4.4; total_input_heat
Adiabatic flame temperature	T_{ad}	$\approx 2050 \text{ K} (\approx 1780 \text{ }^{\circ}\text{C})$	Section 4.5; adiabatic_flame_T (Cantera, HP-equilibrium)
Equilibrium flue gas (major species, mass fractions)	—	$\text{CO}_2 \approx 0.09; \text{H}_2\text{O} \approx 0.08; \text{O}_2 \approx 0.02\text{--}0.03; \text{N}_2 \approx 0.78\text{--}0.80; \text{SO}_2, \text{CO}, \text{H}_2, \text{NO} \square 1\% \text{ each}$	Section 4.6; Cantera HP-equilibrium at T_{ad}
Flue-gas mass flow (equilibrium stream)	\dot{m}_{flue}	$\dot{m}_{\text{flue}} = \dot{m}_f + \dot{m}_a$	Constructed in adiabatic_flame_T as GasStream(m_tot, T_ad, P, comp)

In the implementation, these quantities are wrapped in a `CombustionResult` dataclass (`common/results.py`):

```
@dataclass(frozen=True)
class CombustionResult:
    LHV: Q_
    Q_in: Q_
        # LHV-based firing power [kW]
        # total heat input (LHV + sensible) [kW]
```

```

T_ad: Q_          # adiabatic flame temperature [K]
flue: GasStream   # flue-gas stream at adiabatic conditions
fuel_LHV_mass: Q_ | None = None    # LHV_mix [kJ/kg]
fuel_P_LHV:     Q_ | None = None    # P_LHV [kW]

```

This object is created in `Combustor.run()` and passed to the boiler solver:

- to define the total available heat Q_{in} ,
- to initialise the flue-gas stream entering the first heat-transfer stage (HX_1),
- and to provide diagnostic quantities (LHV , T_{ad}) for the boiler performance summary.

Chapter 5

Heat-Transfer Calculations

5.1 Fundamental heat-balance equations

The boiler is modelled as a one-dimensional counter-current heat exchanger composed of six stages (HX_1–HX_6). Heat transfer is resolved along the gas flow direction x , while water flows in the opposite direction. Each stage is discretized into segments of length dx ; all local quantities are defined per unit length.

- Notation (per segment)
 - x – axial coordinate along the gas flow [m]
 - dx – marching step in x [m]
 - \dot{m}_g, \dot{m}_w – gas and water mass flow rates [kg/s]
 - $T_g(x), T_w(x)$ – bulk gas and water temperatures [K]
 - $T_{gw}(x), T_{ww}(x)$ – gas-side and water-side wall temperatures [K]
 - $h_g(x), h_w(x)$ – total gas-side and water-side heat-transfer coefficients [$\text{W}/\text{m}^2 \cdot \text{K}$]
 - P_g, P_w – gas-side and water-side wetted perimeters [m]
 - $q'(x)$ – linear heat flux (heat per unit length) [W/m]
 - $UA'(x)$ – overall conductance per unit length [$\text{W}/\text{K}/\text{m}$]
-

5.2 Local energy balance

For each differential segment of length dx , the model enforces a one-dimensional steady-state energy balance between the gas, the water and the tube wall:

- Heat transferred across the wall:

$$q'(x) = UA'(x) [T_g(x) - T_w(x)]$$

- Relation to the segment duty:

$$dQ(x) = q'(x) dx$$

- Gas stream:

$$dQ(x) = -\dot{m}_g dh_g(x) \Rightarrow \frac{dh_g}{dx} = -\frac{q'(x)}{\dot{m}_g}$$

- Water stream:

$$dQ(x) = +\dot{m}_w dh_w(x) \Rightarrow \frac{dh_w}{dx} = +\frac{q'(x)}{\dot{m}_w}$$

In the numerical implementation these equations are applied in finite-difference form over each marching step:

$$Q_{\text{step}} = q'(x) \Delta x$$

$$\Delta h_g = -\frac{Q_{\text{step}}}{\dot{m}_g}, \quad \Delta h_w = +\frac{Q_{\text{step}}}{\dot{m}_w}$$

5.3 Overall conductance and resistance network

The overall conductance per unit length $UA'(x)$ is obtained from a radial series of thermal resistances per unit length:

- Gas-side convection:

$$R'_g = \frac{1}{h_g(x) P_g}$$

- Gas-side fouling:

$$R'_{fg} = R'_{fi}(P_g) \quad (\text{from specified fouling thickness and conductivity})$$

- Tube wall:

$$R'_w = \frac{\ln(D_o/D_i)}{2\pi k_w}$$

- Water-side fouling:

$$R'_{fc} = R'_{fo}(P_w)$$

- Water-side convection:

$$R'_c = \frac{1}{h_w(x) P_w}$$

where D_i and D_o are the tube inner and outer diameters and k_w is the tube wall thermal conductivity. Combining these contributions:

$$\frac{1}{UA'(x)} = R'_g + R'_{fg} + R'_w + R'_{fc} + R'_c$$

or equivalently,

$$UA'(x) = \left[\frac{1}{h_g P_g} + R'_{fg} + R'_w + R'_{fc} + \frac{1}{h_w P_w} \right]^{-1}$$

The linear heat flux then follows directly:

$$q'(x) = UA'(x) [T_g(x) - T_w(x)]$$

5.4 Stage- and boiler-level duties

For a stage of length L_j , the stage heat duty and stage-level conductance are obtained by integrating the local quantities along x :

$$Q_{\text{stage},j} = \int_0^{L_j} q'(x) dx \approx \sum_i q'_i \Delta x_i$$

$$(UA)_j = \int_0^{L_j} UA'(x) dx \approx \sum_i UA'_i \Delta x_i$$

The total useful boiler duty is the sum of all stage duties:

$$Q_{\text{useful}} = \sum_{j=1}^6 Q_{\text{stage},j}$$

These integrated quantities are later used in the performance and efficiency evaluation (Section 7) and for constructing stage-wise summary tables.

5.5 Gas-side

Gas-side heat transfer is computed with geometry-aware correlations based on local gas properties from Cantera (GasProps) and stage-specific geometry from the GeometryBuilder. For each marching step, the total gas-side HTC is split into a convective and a radiative contribution:

$$h_{g,\text{tot}} = h_{g,\text{conv}} + h_{g,\text{rad}}$$

The implementation uses the helper `gas_htc_parts(g, spec, T_{gw})`, which returns $(h_{g,\text{conv}}, h_{g,\text{rad}})$ in $\text{W/m}^2\cdot\text{K}$, and then sums them in `gas_htc`.

5.5.1 Single-tube and reversal-chamber

Stages of kind "single_tube" and "reversal_chamber" are treated as internal forced convection in a circular duct. The characteristic quantities are:

- Diameter: $D = D_i$ (tube inner diameter)
- Length: L (stage inner length)
- Flow area: $A = A_{\text{hot,flow}}$ (from geometry builder)
- Velocity:

$$V = \frac{\dot{m}_g}{\rho_g A}$$

- Reynolds and Prandtl numbers:

$$\text{Re} = \frac{\rho_g V D}{\mu_g}, \quad \text{Pr} = \frac{c_{p,g} \mu_g}{k_g}$$

Local gas properties $\rho_g, \mu_g, k_g, c_{p,g}$ are obtained from the Cantera mixture at the local gas temperature and pressure.

Laminar/developing flow (Graetz-type)

For $\text{Re} < 2300$, uses a Graetz correlation for thermally developing laminar flow:

$$Gz = \text{Re} \text{Pr} \frac{D}{L}$$

$$\text{Nu} = 3.66 + \frac{0.0668 Gz}{1 + 0.04 Gz^{2/3}}$$

(Incropera et al. 2011)

Turbulent flow (Gnielinski with Petukhov friction factor)

For $\text{Re} \geq 2300$, the Gnielinski correlation is applied with a Petukhov friction factor:

$$f = (0.79 \ln \text{Re} - 1.64)^{-2}$$

(Munson et al. 2013)

$$\text{Nu} = \frac{\frac{f}{8}(\text{Re} - 1000) \text{Pr}}{1 + 12.7 \sqrt{\frac{f}{8} (\text{Pr}^{2/3} - 1)}}$$

(Incropera et al. 2011) The local convective heat-transfer coefficient is then:

$$h_{g,\text{conv}} = \frac{\text{Nu} k_g}{D}$$

(Incropera et al. 2011)

This same internal correlation is used for "single_tube", "reversal_chamber" and "tube_bank" gas-side flow (see below).

5.5.2 Tube-bank

Stages "tube_bank" correspond to tube bundles inside the shell. In this model, the gas side is still treated as internal flow inside the tubes:

- Hot side (gas): inside tubes (inner diameter D_i), using the same internal forced convection model as in Section 5.2.1.

Thus the gas-side convective HTC in tube-bank stages is:

$$h_{g,\text{conv}}^{(\text{HX3,5})} = \frac{\text{Nu}_{\text{internal}}(\text{Re}, \text{Pr}) k_g}{D_i}$$

with $\text{Nu}_{\text{internal}}$ given by the Graetz/Gnielinski formulation above, and Re , Pr computed from the local gas properties and tube hydraulic diameter.

5.5.3 Economizer (external)

The economizer "economiser" stage reverses the roles: gas flows outside the tubes in cross-flow, while water flows inside. The gas-side convection is then modelled as external crossflow over a tube bank.

Key geometry quantities (from `GeometryBuilder` for the economizer):

- Tube outer diameter: $D = D_o$

- Gas-side crossflow area: $A_{\text{bulk}} = A_{\text{hot,flow}}$
- Optional maximum/mean velocity factor:

$$V_{\text{bulk}} = \frac{\dot{m}_g}{\rho_g A_{\text{bulk}}}, \quad V = u_{\max} V_{\text{bulk}}$$

where u_{\max} is calculated depending on the tube bank arrangement and spacing between tubes.

- Reynolds and Prandtl numbers:

$$\text{Re} = \frac{\rho_g V D}{\mu_g}, \quad \text{Pr} = \frac{c_{p,g} \mu_g}{k_g}$$

For "economiser" stages the primary correlation is a banded Zukauskas form for crossflow over tube banks:

$$\text{Nu} = C \text{Re}^m \text{Pr}^n$$

(Incropera et al. 2011)

where the coefficients C, m are selected from standard bands as a function of Reynolds number and tube arrangement (inline vs staggered), and the exponent n is:

$$n = \begin{cases} 0.36, & \text{Pr} \leq 10 \\ 0.25, & \text{Pr} > 10 \end{cases}$$

If Re falls outside the tabulated bands, the model falls back to the Churchill–Bernstein correlation for crossflow over a single cylinder:

$$\text{Nu} = 0.3 + \frac{0.62 \text{Re}^{1/2} \text{Pr}^{1/3}}{\left[1 + (0.4/\text{Pr})^{2/3}\right]^{1/4}} \left[1 + \left(\frac{\text{Re}}{282000}\right)^{5/8}\right]^{4/5}$$

(Incropera et al. 2011) The gas-side convective HTC in the economizer is then:

$$h_{g,\text{conv}}^{(\text{HX6})} = \frac{\text{Nu} k_g}{D_o}$$

(Incropera et al. 2011)

5.5.4 Gas radiation model

Radiative heat transfer from the flue gas to the furnace surfaces is explicitly accounted for by a participating-medium model for the H₂O/CO₂ mixture. The implementation follows a simplified Smith–Shen–Friedman style four-gray model.

For each step, the gas emissivity is computed as:

1. Partial pressures of participating species:

$$p_{\text{H}_2\text{O}} = y_{\text{H}_2\text{O}} P, \quad p_{\text{CO}_2} = y_{\text{CO}_2} P$$

(Modest 2013) where y_i are molar (or mass-fraction-equivalent) composition entries from the flue gas stream, and P is the local gas pressure.

2. Mean beam length:

$$L_b = \begin{cases} L_{\text{rad},\text{override}}, & \text{if specified in the stage} \\ 0.9 D_{h,\text{gas}}, & \text{otherwise} \end{cases}$$

(Modest 2013) with $D_{h,\text{gas}}$ the gas-side hydraulic diameter.

3. Effective optical thickness in each gray band:

$$p_{\text{ratio}} = \frac{p_{\text{H}_2\text{O}} + p_{\text{CO}_2}}{P_{\text{atm}}}$$

(Modest 2013)

$$\tau_j = K_j \left(\frac{T}{1000 \text{ K}} \right)^{T_{\text{exp}}} p_{\text{ratio}} L_b$$

(Modest 2013)

where K_j and weighting factors A_j are fixed band coefficients, T is the gas temperature, and T_{exp} is a temperature exponent (default 0.65, configurable per stage via `rad_Texp`).

4. Total gas emissivity:

$$\varepsilon_g = 1 - \sum_{j=1}^4 A_j \exp(-\tau_j)$$

(Modest 2013) with ε_g constrained to [0, 1].

A mean-film temperature is used for the linearized radiative HTC:

$$T_{\text{film}} = \frac{T_g + T_{gw}}{2}$$

$$h_{g,\text{rad}} = 4 \sigma F \varepsilon_g T_{\text{film}}^3$$

(Modest 2013)

where:

- σ is the Stefan–Boltzmann constant,
- F is an effective view factor (default 1.0 or stage-specific `rad_F`).

The gas-side total HTC reported and used in the resistance network is then:

$$h_{g,\text{tot}} = h_{g,\text{conv}} + h_{g,\text{rad}}$$

and the corresponding convective/radiative contributions to the linear heat flux are tracked via:

$$q'_{\text{conv}} = q' \frac{h_{g,\text{conv}}}{h_{g,\text{tot}}}, \quad q'_{\text{rad}} = q' - q'_{\text{conv}}$$

These diagnostics are later integrated on a per-stage basis to quantify the share of convective vs radiative heat transfer in each section of the boiler.

5.6 Water-side

Water-side heat transfer is modelled with geometry-dependent correlations using local water properties from the `WaterProps` helper. The water side appears in two configurations:

1. Water inside tubes (single-tube, reversal chamber, economizer)
2. Water outside tubes in crossflow (tube-bank stages `HX_3` and `HX_5`)

The total water-side HTC is computed at each marching step as:

$$h_w = h_{w,\text{conv}}$$

Water-side radiation is neglected.

In the present work, the water-side model is used in two distinct regimes:

- `HX*1–HX_5` are treated as boiling surfaces in contact with a pool at saturation temperature. In these stages the bulk water temperature is forced to $T * \text{sat}(p)$ and the heat-transfer coefficient is obtained from a pure pool-boiling correlation.
- `HX_6` (economizer) is treated as a single-phase / flow-boiling tube bundle with water flowing inside the tubes and heated by the flue-gas crossflow.

The underlying implementation is more general (it contains a full Chen-type flow-boiling formulation valid for internal forced convection), but for the final boiler calculations this capability is only

used in the economizer; in HX_1–HX_5 the water side is deliberately simplified to a pool-boiling model.

5.6.1 Economizer (internal)

For the economiser stage (kind "economiser", HX_6), where water flows inside the tubes, the model uses standard internal-flow correlations augmented with a viscosity-ratio correction and, when needed, a Chen-type flow-boiling enhancement. The tube inner diameter D_i is used as characteristic length.

5.6.1.1 Velocity and nondimensional groups

$$V_w = \frac{\dot{m}_w}{\rho_w A_{\text{cold,flow}}}$$

$$\text{Re}_w = \frac{\rho_w V_w D_i}{\mu_w}, \quad \text{Pr}_w = \frac{c_{p,w} \mu_w}{k_w}$$

Local water-side properties $\rho_w, \mu_w, k_w, c_{p,w}$ are evaluated at the bulk water temperature.

5.6.1.2 Laminar regime ($\text{Re} < 2300$)

For fully developed laminar internal flow in a circular tube:

$$\text{Nu}_w = 3.66$$

(Incropera et al. 2011) For developing laminar flow, the same Graetz form used on the gas side is applied:

$$\text{Gz}_w = \text{Re}_w \text{Pr}_w \frac{D_i}{L}$$

$$\text{Nu}_w = 3.66 + \frac{0.0668 \text{Gz}_w}{1 + 0.04 \text{Gz}_w^{2/3}}$$

(Incropera et al. 2011)

5.6.1.3 Turbulent regime ($\text{Re} \geq 2300$)

The Gnielinski correlation is used:

$$f_w = (0.79 \ln \text{Re}_w - 1.64)^{-2}$$

(Munson et al. 2013)

$$\text{Nu}_w = \frac{\frac{f_w}{8}(\text{Re}_w - 1000)\text{Pr}_w}{1 + 12.7\sqrt{\frac{f_w}{8}}(\text{Pr}_w^{2/3} - 1)}$$

(Incropera et al. 2011) In the implementation, the Nusselt number is multiplied by a viscosity-ratio correction $(\mu_b/\mu_w)^{0.11}$ evaluated at bulk and wall temperatures, following the common Gnielinski extension for heated internal flow.

Finally:

$$h_{w,\text{conv}} = \frac{\text{Nu}_w k_w}{D_i}$$

(Incropera et al. 2011)

5.6.2 Tube-banks (external)

In the boiling sections (HX*1–HX_5) the water occupies the shell-side region around the heated tubes. When a crossflow description is needed (e.g. in HX_3 and HX_5), a Zukauskas-type correlation is applied for flow over a tube bundle on the water side, using the outer tube diameter D_o and the cold-side flow area $A * \text{cold,flow}$ supplied by the geometry builder.

5.6.2.1 Geometry inputs from `GeometryBuilder`

- Tube outer diameter: D_o
- Cold-side flow area: $A_{\text{cold,flow}}$
- Water velocity:

$$V_w = \frac{\dot{m}_w}{\rho_w A_{\text{cold,flow}}}$$

- Reynolds and Prandtl numbers:

$$\text{Re}_w = \frac{\rho_w V_w D_o}{\mu_w}, \quad \text{Pr}_w = \frac{c_{p,w} \mu_w}{k_w}$$

5.6.2.2 Zukauskas banded correlation

$$\text{Nu}_w = C \text{Re}_w^m \text{Pr}_w^n$$

Coefficient selection:

- C, m chosen based on the Reynolds band and bundle arrangement (inline or staggered).
- Exponent n :

$$n = \begin{cases} 0.36, & \text{Pr}_w \leq 10 \\ 0.25, & \text{Pr}_w > 10 \end{cases}$$

If the Reynolds number lies outside the valid Zukauskas range, the model falls back to Churchill–Bernstein:

$$\text{Nu}_w = 0.3 + \frac{0.62 \text{Re}_w^{1/2} \text{Pr}_w^{1/3}}{\left[1 + (0.4/\text{Pr}_w)^{2/3}\right]^{1/4}} \left[1 + \left(\frac{\text{Re}_w}{282000}\right)^{5/8}\right]^{4/5}$$

(Incropera et al. 2011)

The external HTC is then:

$$h_{w,\text{conv}} = \frac{\text{Nu}_w k_w}{D_o}$$

5.6.3 Treatment of boiling

Boiling is treated differently in the pool-boiling stages (HX_1–HX_5) and in the economiser (HX_6).

5.6.3.1 Pool-boiling

For stages flagged as `pool_boiling = true` (HX_1–HX_5), the water side is deliberately simplified to a pure pool-boiling model:

- The bulk water temperature entering the wall-energy balance is fixed at the saturation temperature corresponding to the local pressure:

$$T_w = T_{\text{sat}}(p_w).$$

- The water-side heat-transfer coefficient is taken from a Cooper-type pool-boiling correlation:

$$h_{w,\text{nb}} = h_{\text{Cooper}}(p_w, q'')$$

(Incropera et al. 2011) where q'' is the local heat flux on the water side and the roughness of the boiling surface enters through the correlation.

- This nucleate-boiling coefficient is used directly as the water-side HTC:

$$h_w = h_{w,\text{nb}},$$

and the region is always tagged as “boiling” in the post-processing.

In other words, HX_1–HX_5 are modelled as heated surfaces immersed in a saturated pool, with boiling controlled by the local heat flux and surface roughness rather than by a detailed prediction of the liquid velocity. This reflects the natural-circulation behavior of the boiler riser and furnace sections and follows the modelling simplification requested for the thesis.

5.6.3.2 Economizer

For the economizer stage HX_6 (`pool_boiling = false`), the model uses a more general internal-flow formulation that can represent both single-phase convection and flow boiling:

1. Boiling detection.

A helper function checks whether the local state falls into the saturation enthalpy interval $[h_f(p), h_g(p)]$ or, for slightly subcooled liquid, whether the wall superheat exceeds a threshold. If neither condition is met, the flow is treated as single-phase liquid.

2. Single-phase regime.

In single-phase operation, the water-side HTC is computed from an internal forced-convection correlation (Gnielinski with viscosity-ratio correction), as described in Section 5.3.1.

3. Flow-boiling regime (Chen-type model).

When boiling is detected, the HTC is assembled from a liquid-only contribution and a nucleate-boiling contribution:

$$h_{lo} = \text{single-phase liquid HTC at } T_{sat}(p),$$

$$h_{nb} = h_{Cooper}(p, q''),$$

$$h_w = F h_{lo} + S h_{nb}.$$

(Incropera et al. 2011) The factor F accounts for the effect of two-phase flow on the convective heat transfer (via a Martinelli-type parameter), while S modulates the nucleate-boiling contribution as a function of Reynolds number and mass flux. Both are bounded to remain within reasonable engineering limits.

In the present thesis, this full Chen-type flow-boiling capability is only exercised in the economizer stage. In the main boiling sections (HX_1–HX_5), where circulation is dominated by buoyancy and the flow pattern is closer to pool boiling, the simpler pool-boiling representation described above is preferred.

5.7 Per-step resistance insertion

The water-side resistance per unit length used in the overall UA' assembly is:

$$R'_c = \frac{1}{h_w P_w}$$

where the wetted perimeter is:

- $P_w = \pi D_i$ when water is inside the tubes.
- $P_w = N_{\text{tubes}} \pi D_o$ effective per bundle pitch when water is outside tubes, handled automatically by GeometryBuilder.

Fouling is added in series:

$$R'_{fc} = \frac{\delta_{f,\text{water}}}{k_{f,\text{water}} P_w}$$

Total water-side contribution:

$$R'_{w,\text{side}} = R'_{fc} + R'_c$$

This resistance is passed into the overall conductance formulation (Section 5.1.2).

5.8 Wall-temperature update and thermal convergence

The tube wall temperatures on the gas and water sides, T_{gw} and T_{ww} , are updated using a two-node wall model in each marching step.

Given $q'(x)$, the wall-side energy balances yield:

$$T_{gw} = T_g - \frac{q'}{h_{g,\text{tot}}}$$

$$T_{ww} = T_w + \frac{q'}{h_w}$$

The wall conduction temperature drop is:

$$\Delta T_{\text{wall}} = T_{gw} - T_{ww}$$

which is also equal to:

$$\Delta T_{\text{wall}} = q' [R'_{fg} + R'_w + R'_{fc}]$$

A consistency check is applied; if the implied wall temperature difference from conduction differs from the one implied by convection, the marching solver iterates the HTC evaluation once with relaxed updates (default under-relaxation factor 0.35). Full Picard iteration is omitted for performance reasons.

In the actual implementation this consistency check is performed by iterating on T_{gw} , T_{ww} , and q' using the full resistance network (gas convection, gas fouling, wall, water fouling, water convection), with an under-relaxation factor applied to both wall temperatures and the linear heat flux.

If temperature overshoot (negative film coefficient, reversed driving force) is detected within a step, the step is automatically halved and recomputed.

Chapter 6

Hydraulic Calculations

Hydraulic behaviour is extracted directly from the solver through the per-step pressure-drop decomposition implemented in

`heat/solver.py` (`_gas_dp_components`, `pressure_drop_gas`) and accumulated at the stage level in

`heat/solver.py::solve_stage` and in the boiler summary computed by `heat/postproc.py::su`

The model divides gas-side pressure losses into:

- Frictional losses:

Computed by Colebrook–White (turbulent), laminar $64/\text{Re}$, and a linear transitional blend for
 $2300 < \text{Re}$

- < 4000).

The per-step drop is

$$\Delta P_{\text{fric}} = -f \frac{\Delta x}{D_h} \left(\frac{\rho V^2}{2} \right)$$

where f is obtained from `_friction_factor()` and hydraulic diameter, velocity, and density come from the local gas state.

- Minor losses:

Applied using per-stage catalogue K -values.

For reversal chambers, inlet/outlet nozzle K plus bend-equivalent loss are included; tube-banks default to zero unless specified.

In `solve_stage`, the total per-stage loss coefficient K_{sum} is uniformly distributed across N steps:

$$K_{\text{per step}} = \frac{K_{\text{sum}}}{N}$$

The per-step minor loss is

$$\Delta P_{\text{minor}} = -K_{\text{per step}} \left(\frac{\rho V^2}{2} \right)$$

- Total gas-side drop:

$$\Delta P_{\text{total}} = \Delta P_{\text{fric}} + \Delta P_{\text{minor}}$$

Water-side pressure losses are intentionally not included in this model (all water movement is treated as once-through enthalpy update at constant pressure).

6.1 Gas-Side ΔP per Stage

During each call to `solve_stage`, the solver marches through all steps and accumulates:

- `dP_stage_fric`
- `dP_stage_minor`
- `dP_stage_total`

These appear in each stage row of `summary_rows` returned by `run_hx()`.

An example schema from `summary_from_profile()`:

```
"ΔP_stage_fric[Pa]": dP_fric,
"ΔP_stage_minor[Pa]": dP_minor,
"ΔP_stage_total[Pa]": dP_total,
```

Values are integrated over the entire stage length:

$$\Delta P_{\text{stage}} = \sum_{i=1}^N \Delta P(i)$$

6.2 Water-Side ΔP per Stage

The present solver does not compute water-side frictional or accelerational pressure losses.

From the code (`update_water_after_step`), pressure remains constant:

```
WaterStream(mass_flow=w.mass_flow, h=h_new, P=w.P)
```

Thus:

- Water-side ΔP per stage = 0 Pa
- Total water-side ΔP = 0 Pa

This assumption is consistent with pool-boiling and saturated-drum configurations where the water is not routed through high-velocity conduits.

6.3 Total Boiler ΔP and Stack Pressure

The boiler-level gas-side pressure drop is assembled in the TOTAL_BOILER row of summary_from_profile():

```
"ΔP_stage_fric[Pa]": dP_total_fric,  
"ΔP_stage_minor[Pa]": dP_total_minor,  
"ΔP_stage_total[Pa]": dP_total_total,
```

This yields:

- Total frictional drop:

$$\Delta P_{\text{fric,tot}} = \sum_{k=1}^6 \Delta P_{\text{fric},k}$$

- Total minor-loss drop:

$$\Delta P_{\text{minor,tot}} = \sum_{k=1}^6 \Delta P_{\text{minor},k}$$

- Overall boiler gas-side drop:

$$\Delta P_{\text{boiler}} = \Delta P_{\text{fric,tot}} + \Delta P_{\text{minor,tot}}$$

Stack exit pressure is simply the outlet gas pressure after stage 6:

gas_out.P

reported separately in the boiler summary.

6.4 Consolidated ΔP Table (from solver output)

A typical extracted table structure (values populated after running main.py):

Stage	Kind	ΔP_fric [Pa]	ΔP_minor [Pa]	ΔP_total [Pa]
HX_1	single_tube
HX_2	reversal_chamber
HX_3	tube_bank
HX_4	reversal_chamber
HX_5	tube_bank
HX_6	economiser	0	0	0
TOTAL	-	Σ	Σ	Σ

HX_6 (economiser) contributes zero ΔP by design (`_gas_dp_components` returns 0 for this stage).

The table is directly generated as part of `summary_rows` once `main.py` completes the mass-flow/efficiency iteration and writes final CSVs.

Chapter 7

Boiler Performance Results

This section summarizes the boiler-level performance obtained from the coupled combustion–heat-transfer simulation. All numerical values are extracted from the stage summary and boiler summary data produced by the post-processing step (fields `Q_stage [MW]`, `UA_stage [MW/K]`, `η_direct [-]`, `η_indirect [-]`, `Q_total_useful [MW]`, `Q_in_total [MW]`, `P_LHV [MW]`, `stack_temperature [°C]`, etc.).

7.1 Energy balance (Q_{in} , Q_{useful})

The total useful heat transferred from the flue gas to the water/steam side is obtained by integrating the local line heat flux $q'(x)$ over all stages:

$$Q_{\text{useful}} = \sum_{k=1}^6 Q_{\text{stage},k} = \sum_{k=1}^6 \int_{\text{stage } k} q'(x) \, dx$$

In the implementation this appears as the sum of `Q_stage [MW]` over all stages in `summary_rows`, with the boiler-level result reported in the `TOTAL_BOILER` row as `Q_total_useful [MW]`.

The total input heat from combustion Q_{in} is taken from the combustion module as the rate of heat release from complete fuel burnout (field `Q_in_total [MW]` in the `TOTAL_BOILER` row):

$$Q_{\text{in}} = Q_{\text{in},\text{total}}$$

For reference, the firing rate on an LHV basis is also reported as `P_LHV [MW]`, obtained from the fuel lower heating value and the fuel mass flow rate.

A concise numerical statement (to be filled from the CSV):

- $Q_{\text{in}} = Q_{\text{in},\text{total}} = [\text{Q_in_total MW}]$
- $Q_{\text{useful}} = Q_{\text{total},\text{useful}} = [\text{Q_total_useful MW}]$

where the bracketed placeholders are to be replaced by the corresponding values from the TOTAL_BOILER row.

7.2 Efficiencies (direct and indirect)

Two boiler efficiencies are reported:

- Direct efficiency (LHV basis)

Direct efficiency is defined as the ratio of useful heat transferred to the firing rate based on fuel LHV:

$$\eta_{\text{direct}} = \frac{Q_{\text{useful}}}{P_{\text{LHV}}}$$

where P_{LHV} is the firing capacity (field P_LHV [MW]).

- Indirect efficiency (heat-balance basis)

Indirect efficiency is defined as the ratio of useful heat to the total heat released by combustion:

$$\eta_{\text{indirect}} = \frac{Q_{\text{useful}}}{Q_{\text{in}}}$$

In the post-processing, these appear as the boiler-level fields in the TOTAL_BOILER row:

- $\eta_{\text{direct}} [-] \rightarrow \eta_{\text{direct}}$
- $\eta_{\text{indirect}} [-] \rightarrow \eta_{\text{indirect}}$

Text to be instantiated in the final report (numbers from CSV):

- Direct (LHV) efficiency: $\eta_{\text{direct}} = [\eta_{\text{direct}} \cdot 100] \%$
- Indirect efficiency: $\eta_{\text{indirect}} = [\eta_{\text{indirect}} \cdot 100] \%$

7.3 Steam generation rate and mass-flow convergence

The water/steam mass flow rate is not prescribed but obtained iteratively from an assumed overall boiler efficiency and the combustion heat input. At each iteration n the code:

1. Assumes an efficiency $\eta^{(n)}$.
2. Computes the target useful duty:

$$Q_{\text{target}}^{(n)} = \eta^{(n)} Q_{\text{in}}$$

3. Determines the required water mass flow $\dot{m}_w^{(n)}$ from the enthalpy rise between feedwater and saturated steam at drum pressure:

$$\dot{m}_w^{(n)} = \frac{Q_{\text{target}}^{(n)}}{h_{\text{steam}}(P_{\text{drum}}) - h_{\text{fw}}}$$

4. Runs the full multi-stage heat-exchanger model with $\dot{m}_w^{(n)}$ and reads back the resulting indirect efficiency $\eta_{\text{indirect}}^{(n)}$ from the TOTAL_BOILER row.
5. Sets the next efficiency guess $\eta^{(n+1)} = \eta_{\text{indirect}}^{(n)}$ and repeats until the mass-flow change is below the specified tolerance:

$$|\dot{m}_w^{(n)} - \dot{m}_w^{(n-1)}| < 10^{-3} \text{ kg/s}$$

The final converged values to be reported are:

- Converged feedwater/steam mass flow:

$$\dot{m}_w = [\text{m_w}, \text{ kg/s}]$$

- Number of outer iterations to achieve $|\Delta\dot{m}_w| < 10^{-3} \text{ kg/s}$:

$$N_{\text{iter}} = [\text{N}]$$

In the narrative, this subsection should state that the mass-flow/efficiency fixed point converged and that the final efficiency used in the performance summary is the converged η_{indirect} .

7.4 Stage-level performance

Stage-level performance is summarized from the per-stage rows (`stage_name` ≠ "TOTAL_BOILER") in the summary table returned by the post-processor. For each stage k the following quantities are available:

- Heat duty: Q_{stage} [MW]
- Overall conductance: UA_{stage} [MW/K]
- Gas inlet/outlet temperatures: $gas_{\text{in_T}}$ [$^{\circ}\text{C}$], $gas_{\text{out_T}}$ [$^{\circ}\text{C}$]
- Water inlet/outlet temperatures: $water_{\text{in_T}}$ [$^{\circ}\text{C}$], $water_{\text{out_T}}$ [$^{\circ}\text{C}$]
- Gas-side pressure drops: $\Delta P_{\text{stage_fric}}$ [Pa], $\Delta P_{\text{stage_minor}}$ [Pa], $\Delta P_{\text{stage_total}}$ [Pa]
- Decomposition of duty into convection and radiation: $Q_{\text{conv_stage}}$ [MW], $Q_{\text{rad_stage}}$ [MW]

A compact table layout for the report (values to be filled from the CSV) is:

Kind	$T_{g,\text{in}}$ [$^{\circ}\text{C}$]	$T_{g,\text{out}}$ [$^{\circ}\text{C}$]	$T_{w,\text{in}}$ [$^{\circ}\text{C}$]	$T_{w,\text{out}}$ [$^{\circ}\text{C}$]	Q_{stage} [MW]	UA_{stage} [MW/K]	ΔP_{stage} [Pa]
single	[·]	[·]	[·]	[·]	[·]	[·]	[·]
tube							
reversal	[·]	[·]	[·]	[·]	[·]	[·]	[·]
ch.							
tube	[·]	[·]	[·]	[·]	[·]	[·]	[·]
bank							

Kind	$T_{g,\text{in}}$ [°C]	$T_{g,\text{out}}$ [°C]	$T_{w,\text{in}}$ [°C]	$T_{w,\text{out}}$ [°C]	Q_{stage} [MW]	UA_{stage} [MW/K]	ΔP_{stage} [Pa]
reversal[·]	[·]	[·]	[·]	[·]	[·]	[·]	[·]
ch.							
tube bank	[·]	[·]	[·]	[·]	[·]	[·]	[·]
economiser	[·]	[·]	[·]	[·]	[·]	[·]	[·]

If desired, an additional column can be added to show the fraction of radiative heat transfer in each stage:

$$\phi_{\text{rad},k} = \frac{Q_{\text{rad},k}}{Q_{\text{stage},k}} = \frac{Q_{\text{rad_stage}} [\text{MW}]}{Q_{\text{stage}} [\text{MW}]}$$

This highlights the dominance of radiation in the furnace/reversal stages and convection in the tube banks and economiser.

7.5 Overall boiler summary

The overall boiler performance is finally summarized using the TOTAL_BOILER row of the summary table. A suggested boiler summary table is:

Quantity	Symbol	Value
Fuel firing (LHV basis)	P_{LHV}	P_{LHV} [MW]
Total heat input (combustion)	Q_{in}	$Q_{\text{in_total}}$ [MW]
Useful heat to water/steam	Q_{useful}	$Q_{\text{total_useful}}$ [MW]
Direct efficiency (LHV basis)	η_{direct}	η_{direct} [-]
Indirect efficiency	η_{indirect}	η_{indirect} [-]
Stack gas temperature	T_{stack}	stack_temperature [°C]
Gas-side friction loss	ΔP_{fric}	$\Delta P_{\text{stage_fric}}$ [Pa]
Gas-side minor losses	ΔP_{minor}	$\Delta P_{\text{stage_minor}}$ [Pa]
Total gas-side pressure drop	ΔP_{tot}	$\Delta P_{\text{stage_total}}$ [Pa]
Total convective heat transfer	Q_{conv}	$Q_{\text{conv_stage}}$ [MW]
Total radiative heat transfer	Q_{rad}	$Q_{\text{rad_stage}}$ [MW]

In the narrative text, the key messages of this subsection should be:

- The final converged steam production rate and overall efficiency.
- The relative contributions of convective and radiative heat transfer.
- The resulting stack temperature and global gas-side pressure drop across the boiler.

These boiler-level results provide the basis for the sensitivity analysis in Section 8 and for comparing alternative design or operating scenarios.

Chapter 8

Sensitivity Analysis

placeholder

Chapter 9

Conclusion

placeholder

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