Shell Boiler Simulation – Progress Draft

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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:

- Operating pressure range (typical):
  - Saturated steam: approximately 6–25 bar(a), occasionally up to 30 bar(a)
  - Hot-water service: typically up to 10–16 bar(a)
- 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 decentralised 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 efficient 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 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.

3 Geometry

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4 Industrial Application of Shell Boilers

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  - 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 decentralised 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.

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

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 $\mathrm{d}x$; all local quantities are defined per unit length.

- **Notation (per segment)**
- x – axial coordinate along the gas flow [m]
- $\mathrm{d}x$ – 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 [W/m² · 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 [W/K/m]

5.2 Local energy balance

For each differential segment of length $\mathrm{d}x$, 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:

$$\mathrm{d}Q(x) = q'(x)\,\mathrm{d}x$$

- Gas stream:

$$\mathrm{d}Q(x) = -\,\dot{m}_g\,\mathrm{d}h_g(x) \quad \Rightarrow \quad \frac{\mathrm{d}h_g}{\mathrm{d}x} = -\,\frac{q'(x)}{\dot{m}_g}$$

- Water stream:

$$\mathrm{d}Q(x) = +\,\dot{m}_w\,\mathrm{d}h_w(x) \quad \Rightarrow \quad \frac{\mathrm{d}h_w}{\mathrm{d}x} = +\frac{q'(x)}{\dot{m}_w}$$

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

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

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

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:

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

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

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 correlations: single-tube, tube-banks, economizer, radiation model

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:

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

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

5.5.1 Single-tube and reversal-chamber stages (HX_1, HX_2, HX_4)

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: $A = A_{\mathrm{hot,flow}}$ (from geometry builder)
- Velocity:

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

- Reynolds and Prandtl numbers:

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

  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 $\mathrm{Re} < 2300$, the code uses a Graetz correlation for thermally developing laminar flow:

$$\mathrm{Gz} = \mathrm{Re}\,\mathrm{Pr}\,\frac{D}{L}$$

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

(Incropera et al. 2011)

Turbulent flow (Gnielinski with Petukhov friction factor)
For $\mathrm{Re} \geq 2300$, the Gnielinski correlation is applied with a Petukhov friction factor:

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

(Munson et al. 2013)

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

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

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

(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 (HX_3, HX_5 – gas side)

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:

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

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

5.5.3 Economizer stage (HX_6 – gas crossflow over tubes)

The economizer `"economiser"` stage reverses the roles: gas flows outside the tubes in crossflow, 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: $A_{\mathrm{bulk}} = A_{\mathrm{hot,flow}}$
- Optional maximum/mean velocity factor:

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

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

- Reynolds and Prandtl numbers:

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

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

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

(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:

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

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

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

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

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

(Incropera et al. 2011)

5.5.4 Gas radiation model (H O/CO participation)

Radiative heat transfer from the flue gas to the furnace surfaces is explicitly accounted for by a participating-medium model for the H O/CO 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:

$$p_{\mathrm{H_2O}} = y_{\mathrm{H_2O}}\,P, \qquad p_{\mathrm{CO_2}} = y_{\mathrm{CO_2}}\,P$$

(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:

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

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

3. Effective optical thickness in each gray band:

$$p_{\mathrm{ratio}} = \frac{p_{\mathrm{H_2O}} + p_{\mathrm{CO_2}}}{P_{\mathrm{atm}}}$$

(Modest 2013)

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

(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:

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

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

(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:

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

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 correlations: internal flow and external crossflow over tube banks

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 Internal forced convection and flow boiling in the economiser (HX_6)

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

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

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

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 ($\mathrm{Re} < 2300$) For fully developed laminar internal flow in a circular tube:

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

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

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

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

(Incropera et al. 2011)

5.6.1.3 Turbulent regime ($\mathrm{Re} \geq 2300$) The Gnielinski correlation is used:

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

(Munson et al. 2013)

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

(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:

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

(Incropera et al. 2011)

5.6.2 External crossflow over tube banks (water side in HX_3 and HX_5)

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 $A *$ cold,flow supplied by the geometry builder.

5.6.2.1 Geometry inputs from `GeometryBuilder`

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

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

- Reynolds and Prandtl numbers:

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

5.6.2.2 Zukauskas banded correlation

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

Coefficient selection:

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

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

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

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

(Incropera et al. 2011)

The external HTC is then:

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

5.6.3 Treatment of boiling: pool boiling in HX_1–HX_5, flow boiling in HX_6

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 stages HX_1–HX_5 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:

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

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

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

  (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:

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

  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 HX_6: internal single-phase and Chen-type flow boiling

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:

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

   $$\begin{aligned} h_{\text{nb}} &= h_{\text{Cooper}}(p, q''), \\ h_w &= F\, h_{\text{lo}} + S\, h_{\text{nb}}. \end{aligned}$$

   (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:

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

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.

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::summary_from_profile`.

The model divides gas-side pressure losses into:

- **Frictional losses**:
  Computed by Colebrook–White (turbulent), laminar 64/Re, and a linear transitional blend for
  (2300 < 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 (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.

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]`, `_direct[-]`, `_indirect[-]`, `Q_total_useful[MW]`, `Q_in_total[MW]`, `P_LHV[MW]`, `stack_temperature[°C]`, etc.).

7.1 Energy balance ($Q_{\mathbf{in}}$, $Q_{\mathbf{useful}}$)

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:

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

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):

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

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):

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

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

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

- `_direct[-]` $\rightarrow \eta_{\mathrm{direct}}$
- `_indirect[-]` $\rightarrow \eta_{\mathrm{indirect}}$

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

- Direct (LHV) efficiency: $\eta_{\mathrm{direct}} =$ `[ _direct · 100]` %
- Indirect efficiency: $\eta_{\mathrm{indirect}} =$ `[ _indirect · 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:

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

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

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

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

$$\left|\dot{m}_{\mathrm{w}}^{(n)} - \dot{m}_{\mathrm{w}}^{(n-1)}\right| < 10^{-3}\,\mathrm{kg/s}$$

The final converged values to be reported are:

- Converged feedwater/steam mass flow:

$$\dot{m}_{\mathrm{w}} = \texttt{[m\_w, kg/s]}$$

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

$$N_\mathrm{iter} = \texttt{[N]}$$

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_in_T[°C]`, `gas_out_T[°C]`
- Water inlet/outlet temperatures: `water_in_T[°C]`, `water_out_T[°C]`
- Gas-side pressure drops: `ΔP_stage_fric[Pa]`, `ΔP_stage_minor[Pa]`, `ΔP_stage_total[Pa]`
- Decomposition of duty into convection and radiation: `Q_conv_stage[MW]`, `Q_rad_stage[MW]`

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

Kind	$T_{g,\mathrm{in}}$ [°C]	$T_{g,\mathrm{out}}$ [°C]	$T_{w,\mathrm{in}}$ [°C]	$T_{w,\mathrm{out}}$ [°C]	Q_stage [MW]	UA_stage [MW/K]	ΔP_stage [Pa]
single tube	[·]	[·]	[·]	[·]	[·]	[·]	[·]
reversal ch.	[·]	[·]	[·]	[·]	[·]	[·]	[·]
tube bank	[·]	[·]	[·]	[·]	[·]	[·]	[·]
reversal ch.	[·]	[·]	[·]	[·]	[·]	[·]	[·]
tube bank	[·]	[·]	[·]	[·]	[·]	[·]	[·]
economiser	[·]	[·]	[·]	[·]	[·]	[·]	[·]

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

$$\phi_{\mathrm{rad},k} = \frac{Q_{\mathrm{rad},k}}{Q_{\mathrm{stage},k}} = \frac{\texttt{Q\_rad\_stage[MW]}}{\texttt{Q\_stage[MW]}}$$

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_in_total[MW]
Useful heat to water/steam	Q_{useful}	Q_total_useful[MW]
Direct efficiency (LHV basis)	η_{direct}	_direct[-]
Indirect efficiency	η_{indirect}	_indirect[-]
Stack gas temperature	T_{stack}	stack_temperature[°C]
Gas-side friction loss	ΔP_{fric}	ΔP_stage_fric[Pa]
Gas-side minor losses	$\Delta P_{\mathrm{minor}}$	ΔP_stage_minor[Pa]
Total gas-side pressure drop	ΔP_{tot}	ΔP_stage_total[Pa]
Total convective heat transfer	Q_{conv}	Q_conv_stage[MW]
Total radiative heat transfer	Q_{rad}	Q_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.

8 Sensitivity Analysis

placeholder

9 Conclusion

placeholder

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