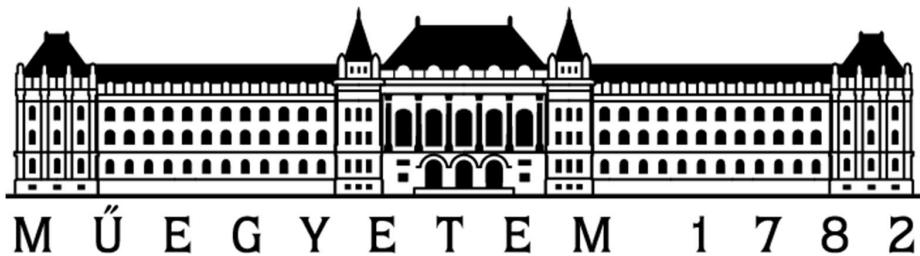


Heat Transfer and Fluid Flow Calculations of Industrial Shell Boilers and Evaluation of Operation Conditions

Saif-Aldain Aqel

2025

SAIF-ALDAIN AQEL
FINAL PROJECT



BUDAPEST UNIVERSITY OF TECHNOLOGY AND ECONOMICS
FACULTY OF MECHANICAL ENGINEERING
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Heat Transfer and Fluid Flow Calculations of
Industrial Shell Boilers and Evaluation of
Operating Conditions

Supervisor:
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Budapest, 2025



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FINAL PROJECT ASSIGNMENT

Publicly Available

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	Code of the Curriculum: 2NAAG0	Specialisation: Document ref. number:
	Curriculum: Bachelor of Science Degree Program in Mechanical Engineering	2NAAG0-PE GEEN:2026-1:2NAAG0:QTY3S6
	Final Project issued by: Energetikai Gépek és Rendszerek Tanszék	Final exam organised by: Áramlástan Tanszék
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Project Description	Title	Heat transfer and fluid flow calculations of industrial shell boilers and evaluation of operation conditions Nagyvízterű ipari kazánok hőátadási és folyadékáramlási számításai, valamint működési feltételek értékelése
	Details	1. Give an overview of application of shell boilers in industrial energy supply 2. Select a certain design of shell boilers for investigation and show its main data 3. Make combustion calculations considering gaseous and/or liquid fuel firing 4. Make heat transfer calculations for both fluegas and water-steam side 5. Make hydraulic calculations for both fluegas and water-steam side 6. Summarize all calculations and evaluate operation conditions of selected boiler 7. Make a sensitivity analysis of selected shell boiler on possible operation condition variations 8. Summarize all the results and evaluate them
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Final Exam	1 st subject (group)	2 nd subject (group)	3 rd subject (group)
	ZVEGEENBGHK Hőközlés	ZVEGEVGBX01 Áramlástechnikai gépek	ZVEGEENBGB Energetikai folyamatok és berendezések

Authentication	Handed out: 8 September 2025	Deadline: 12 December 2025
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Declarations

Declaration about the acceptability of the thesis

This thesis fulfills every formal and content requirements of the regulation of the Budapest University of Technology and Economics, moreover it fulfills the assignment of the final project. This thesis is suitable for a review and an open defense.

Budapest,



Dr. Lezsovits Ferenc

Declaration about the independent work

I, Saif-Aldain Ahmad Deeb Aqel (QTY3S6), hereby declare that the Thesis submitted for assessment and defense, exclusively contains the results of my own work assisted by my supervisor. Further to it, it is also stated that all other results taken from the technical literature or other sources are clearly identified and referred to according to copyright (footnotes/references are chapter and verse, and placed appropriately).

I accept that the scientific results presented in my Thesis can be utilized by the Department of the supervisor for further research or teaching purposes.

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Saif-Aldain Aqel

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Abstract

This thesis develops a three pass fire tube industrial shell boiler model, implemented in Python, the modelling framework integrates (i) detailed fuel-air combustion, (ii) six sequential gas side heat exchange stages representing furnace, tube banks, reversal chambers, and economizer, and (iii) a water/steam circuit governed by saturated boiling in the pressure parts and single phase heating in the economizer. The gas–water energy balance is solved using a one dimensional marching algorithm, which updates local heat transfer coefficients, wall temperatures, and segmental duties based on a full resistance network.

Combustion calculations provide the adiabatic flame temperature, the fully burnt flue gas composition, and the total heat release the natural gas fuel provides. Hydraulic losses are resolved concurrently using friction factor and minor loss correlations yielding complete gas/water pressure drop profiles. Boiler level performance metrics, obtained under different operation conditions and analyzed, demonstrating that efficiency exhibits a shallow optimum near the design excess air setting; that pressure mainly affects steam quantity rather than boiler efficiency; and that firing rate scales heat duties approximately linearly within the practical load range. The modelling framework provides a physics based tool suitable for analyzing industrial shell boiler behavior, supporting performance evaluation, operational optimization, and design exploration.

Nomenclature

Latin symbols

Symbol	Name	Units
A	Area	m^2
A_j	Gray-band weight	—
A_{bulk}	Bulk cross-flow area	m^2
$A_{\text{cold,flow}}$	Cold-side flow area	m^2
A_{flow}	Flow area	m^2
AFR	Air-fuel ratio	—
$A_{\text{hot,flow}}$	Hot-side flow area	m^2
B	Baffle spacing	m
C	Correlation coefficient	—
C_0	Bundle loss constant	—
D	Characteristic diameter	m
D_h	Hydraulic diameter	m
D_i	Inner diameter	m
D_o	Outer diameter	m
D_{shell}	Shell diameter	m
dx	Step length	m
f	Friction factor	—
F	View/enhancement factor	—
G	Mass flux	$\text{kg}, \text{m}^{-2}, \text{s}^{-1}$
Gz	Graetz number	—
h	Enthalpy / HTC	$\text{J}, \text{kg}^{-1} / \text{W}, \text{m}^{-2}, \text{K}^{-1}$
h_g	Gas-side HTC	$\text{W}, \text{m}^{-2}, \text{K}^{-1}$
HHV	Higher heating value	J, kg^{-1} (or $\text{J}, \text{mol}^{-1}$)
\dot{H}	Enthalpy rate	W
h_w	Water-side HTC	$\text{W}, \text{m}^{-2}, \text{K}^{-1}$
K	Loss/absorption coefficient	—
k	Thermal conductivity	$\text{W}, \text{m}^{-1}, \text{K}^{-1}$
K_j	Gray-band absorption	—
L	Length	m
L_b	Mean beam length	m
LHV	Lower heating value	J, kg^{-1} (or $\text{J}, \text{mol}^{-1}$)

Symbol	Name	Units
M	Molar mass	$\text{kg}, \text{mol}^{-1}$
M_{mix}	Mixture molar mass	$\text{kg}, \text{mol}^{-1}$
\dot{m}	Mass flow rate	kg, s^{-1}
M_w	Water molar mass	$\text{kg}, \text{mol}^{-1}$
n	Moles / exponent	mol (or -)
\dot{n}	Molar flow rate	$\text{mol}, \text{s}^{-1}$
N	Count	-
N_{rows}	Tube rows	-
Nu	Nusselt number	-
p	Pressure / partial pressure	Pa
P	Pressure	Pa
P_{LHV}	LHV firing rate	W
p_r	Reduced pressure	-
Pr	Prandtl number	-
Q	Heat rate	W
$q'(x)$	Linear heat flux	W, m^{-1}
q''	Heat flux	W, m^{-2}
Q_{in}	Heat input	W
Q_{useful}	Useful heat	W
R	Thermal resistance / bend radius	-
Re	Reynolds number	-
R_p	Roughness parameter	μm
R'	Resistance per length	$\text{K}, \text{W}^{-1}, \text{m}^{-1}$
S_L	Longitudinal pitch	m
S_T	Transverse pitch	m
T	Temperature	K
T_{ad}	Adiabatic flame temp.	K
T_{film}	Film temperature	K
T_{sat}	Saturation temperature	K
t	Wall thickness	m
τ_j	Optical thickness	-
UA	Overall conductance	W, K^{-1}
$UA'(x)$	Conductance per length	$\text{W}, \text{K}^{-1}, \text{m}^{-1}$
u_{max}	Velocity factor	-
V	Velocity	m, s^{-1}
w_i	Mass fraction	-
X	Mole fraction vector	-
x	Vapor quality	-
x	Axial coordinate	m
x_i	Mole fraction	-
X_{tt}	Martinelli parameter	-
y_i	Molar fraction	-
ζ	Loss coefficient	-

Greek symbols

Symbol	Name	Units
α	Exponent/constant	—
ΔP	Pressure drop	Pa
ΔT	Temperature difference	K
δ	Thickness	m
ε	Emissivity / roughness	—
η	Efficiency	—
κ	Thermal conductivity	W,m ⁻¹ ,K ⁻¹
λ	Excess air ratio	—
μ	Dynamic viscosity	Pa.s
ν	Stoichiometric/kinematic viscosity	mol/mol (or m ² ,s ⁻¹)
π	Pi	—
ρ	Density	kg,m ⁻³
σ	Stefan–Boltzmann constant	W,m ⁻² ,K ⁻⁴

Subscripts / indices / conventions

Index	Meaning	Units
ad	Adiabatic	—
conv	Convective	—
crit	Critical	—
eq	Equilibrium	—
fw	Feedwater	—
HX _j	HX stage	—
in	Inlet	—
nb	Nucleate boiling	—
out	Outlet	—
prod	Products	—
rad	Radiative	—
react	Reactants	—
ref	Reference	—
sens	Sensible	—
tot	Total	—

Abbreviations

Abbrev.	Meaning	Units
AFR	Air-fuel ratio	—
HHV	Higher heating value	—

Abbrev.	Meaning	Units
HP	Enthalpy–pressure mode	—
HTC	Heat-transfer coefficient	—
IAPWS-IF97	Water/steam properties standard	—
LHV	Lower heating value	—
NASA	Thermo data source	—

Chapter 1

Introduction

Industrial shell boilers remain one of the most widely deployed technologies for producing saturated steam and hot water in small to medium industrial plants. Their popularity arises from their compact construction, robust heat transfer surfaces, straightforward operation, and comparatively low installation and maintenance requirements. Typical applications span food and beverage processing, chemicals and pharmaceuticals, textiles, healthcare, and general manufacturing sectors where steady, reliable steam generation is essential for heating, processing, and auxiliary services.

Despite their apparent simplicity, the thermal behavior of shell boilers is governed by tightly coupled processes: multi stage radiative and convective heat transfer, natural circulation boiling inside the pressure parts, complex flue gas property variations, and geometry dependent hydraulic losses. Modern operation demands higher efficiency, reduced emissions, increased reliability, and improved control.

This thesis develops a physics based model for a three pass fire tube shell boiler that integrates combustion calculations, detailed flue gas thermophysical properties, multi stage heat transfer modelling, and hydraulic loss estimation. The model is implemented as a one dimensional marching solver applied to six sequential heat exchange stages;

$$\text{HX}_1 \rightarrow \text{HX}_2 \rightarrow \text{HX}_3 \rightarrow \text{HX}_4 \rightarrow \text{HX}_5 \rightarrow \text{HX}_6, \quad (1.1)$$

representing the furnace, reversal chambers, convective tube banks, and the economizer, see figure 1.1. On the water side, the boiler drum provides a saturated interface for nucleate boiling in the pressure parts, while the economizer section is treated as a single phase internal flow. Gas side properties are supplied by Cantera, enabling temperature dependent transport, specific heat, thermal conductivity, and radiative behavior to be modelled.

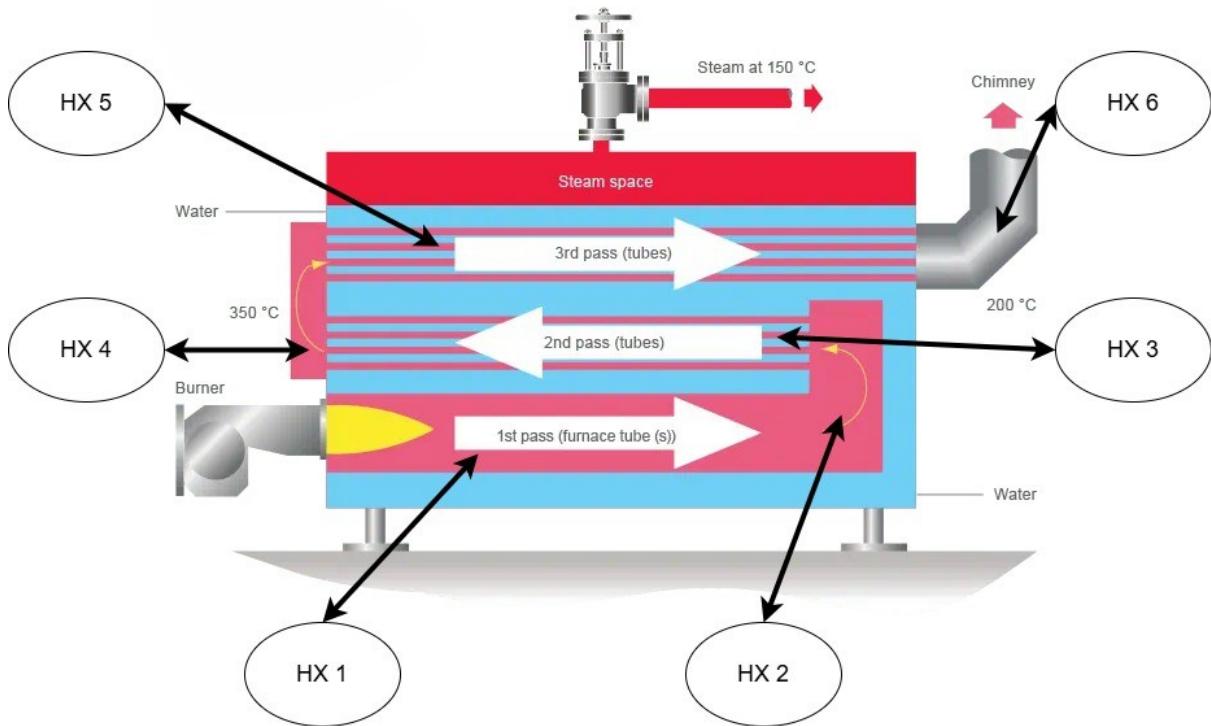


Figure 1.1: Shell boiler labeled stages (adapted from [13]).

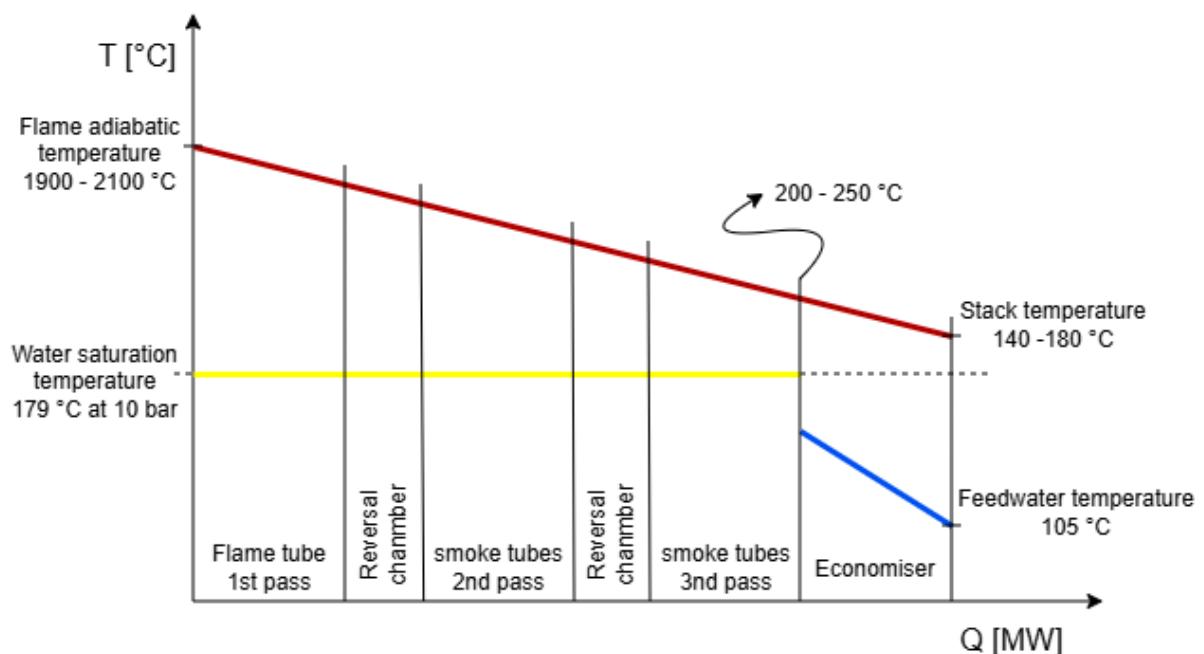


Figure 1.2: $T-Q$ diagram for the three pass boiler with economizer.

The overall objectives of the study are:

1. To construct a unified combustion-boiler model capable of predicting flue gas temperature, composition, adiabatic flame temperature, and total heat input based on fuel composition and excess air settings.

2. To resolve heat transfer processes along the boiler using stage specific geometries, convection correlations, and a spectral based gas radiation model.
3. To quantify hydraulic losses across each pass using friction factor relations and minor loss coefficients, yielding the total boiler gas side pressure drop.
4. To compute boiler level performance, including useful heat transfer, direct and indirect efficiencies, stack temperature, and stage wise duties.
5. To evaluate sensitivity of boiler performance to key operating parameters, excess air ratio, drum pressure, and fuel mass flow rate.

The numerical framework is structured such that the water/steam mass flow is determined iteratively from the global energy balance. For each operating condition, a fixed point loop between assumed efficiency and resulting steam flow is solved until convergence, ensuring consistency between combustion input, heat transfer output, and steam generation.

The remainder of this thesis is organized as follows. Chapter 2 identifies typical industrial applications of shell boilers and introduces key design features. Chapter 3 describes the boiler geometry and outlines the six heat transfer stages. Chapter 4 develops the combustion and flue gas model, including stoichiometry and adiabatic flame temperature prediction. Chapter 5 covers the heat transfer framework, combining convection and radiation on the gas side with pool boiling and single phase correlations on the water side. Chapter 6 presents the hydraulic model. Chapter 7 reports the resulting boiler performance, while Chapter 8 examines the sensitivity of the system to variations in λ , pressure, and firing rate. Chapter 9 concludes with a summary of findings.

Chapter 2

Industrial Application of Shell Boilers

Fire tube boilers- shell boilers

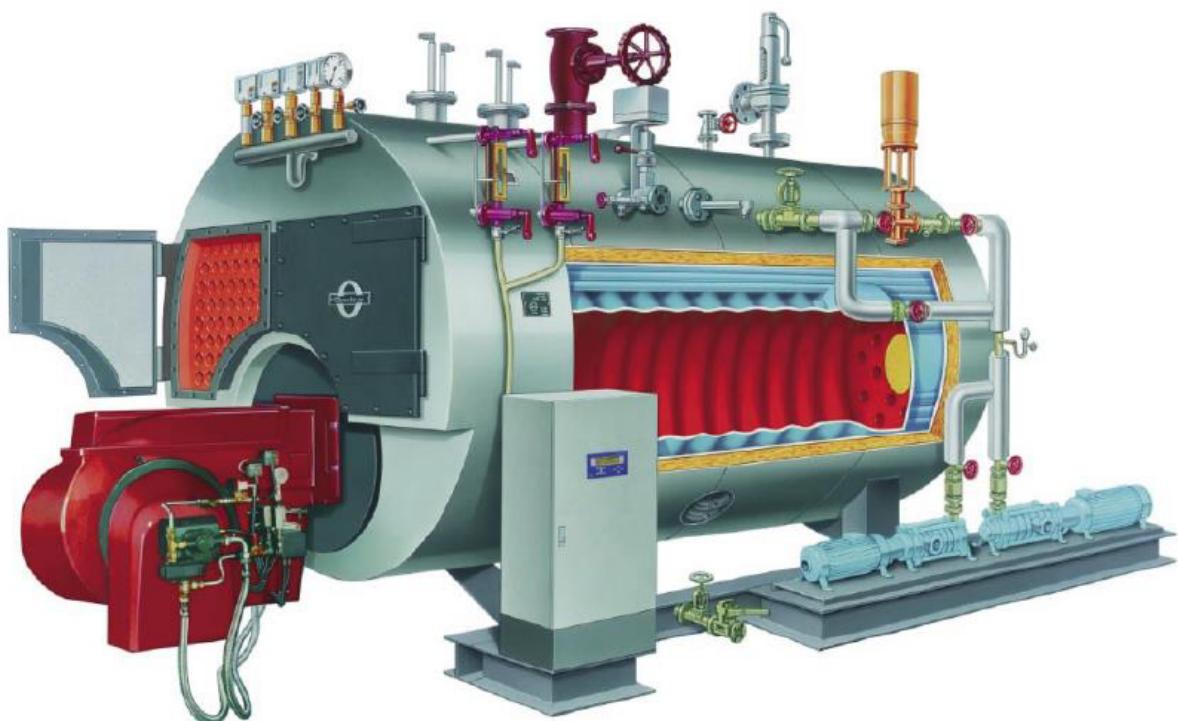


Figure 2.1: Example of a packaged fire tube shell boiler in industrial service (reproduced from [5]).

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 Standard 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

2.3 Advantages and Limitations

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.

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 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 reversal chamber.
 - Second pass: return of flue gas through banks of small-diameter fire-tubes back to the front reversal chamber 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: large diameter furnace tube running from burner front to rear reversal chamber.
 - Pass 2: First bank of smoke-tubes (typically reversing at the rear turnaround chamber).
 - Pass 3: Second bank of smoke-tubes.
 - 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: 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

Configuration

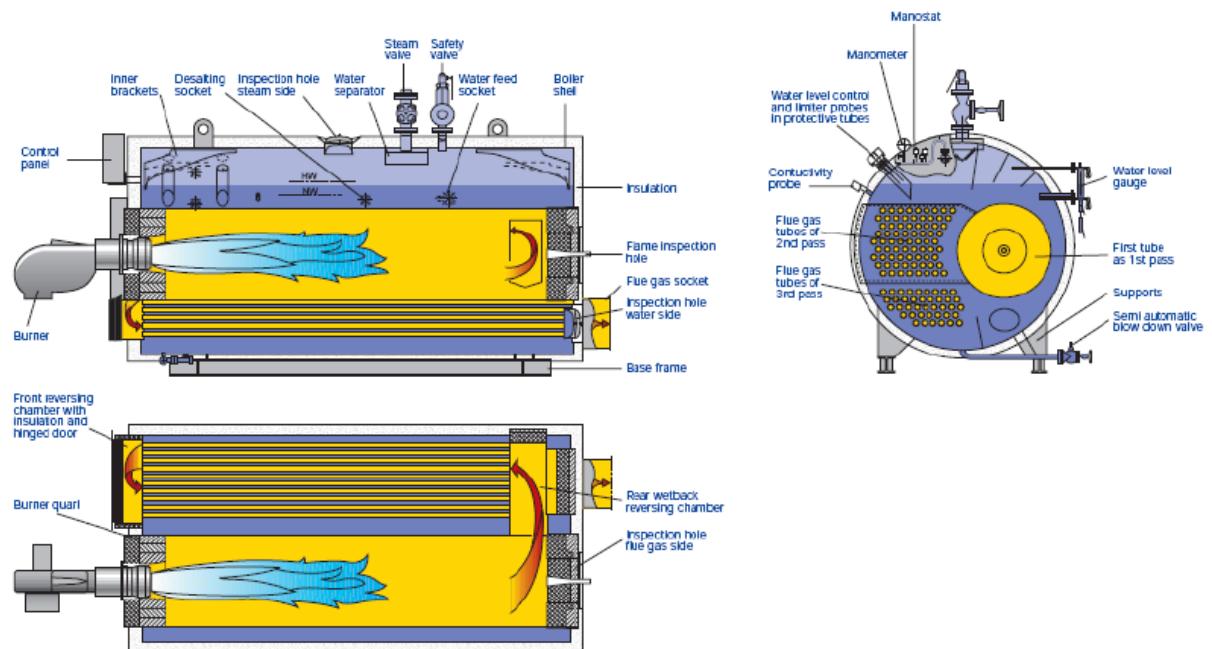


Figure 3.1: Example of shell boiler setup components (reproduced from [5]).

The simulated unit is a three pass fire tube shell boiler with six distinct gas side heat transfer stages and a single common steam drum on the water/steam side. Hot flue gas from the burner traverses a radiative furnace, two reversal chambers, two convective tube banks, and a final economizer before leaving to the stack.

3.1 Layout

The gas path is represented as:

$$\text{Burner} \rightarrow \text{HX}_1 \rightarrow \text{HX}_2 \rightarrow \text{HX}_3 \rightarrow \text{HX}_4 \rightarrow \text{HX}_5 \rightarrow \text{HX}_6 \rightarrow \text{stack} \quad (3.1)$$

with the following interpretation:

- HX_1 – Furnace (first pass)
Large, single furnace tube where combustion products enter directly from the burner and transfer heat mainly by radiation and high-temperature convection to the surrounding water/steam.
- HX_2 – First reversal chamber
Short cylindrical wet back chamber that turns the flow from the furnace outlet into the first convective tube bank (gas direction change = 180°).
- HX_3 – First convective tube bank (second pass) Bank of small diameter fire tubes arranged in a staggered pattern inside the shell, to boost convection; flue gas flows inside of the tubes, water/steam outside.
- HX_4 – Second reversal chamber Second turning chamber redirecting gas from the first to the second tube bank.
- HX_5 – Second convective tube bank (third pass) Second fire-tube bundle, representing the last in-boiler convective pass.
- HX_6 – Economizer Separate, downstream tube bank used to preheat feedwater in single-phase operation before entering the drum/boiler circuit, recovering heat, and boosting efficiency of the boiler.

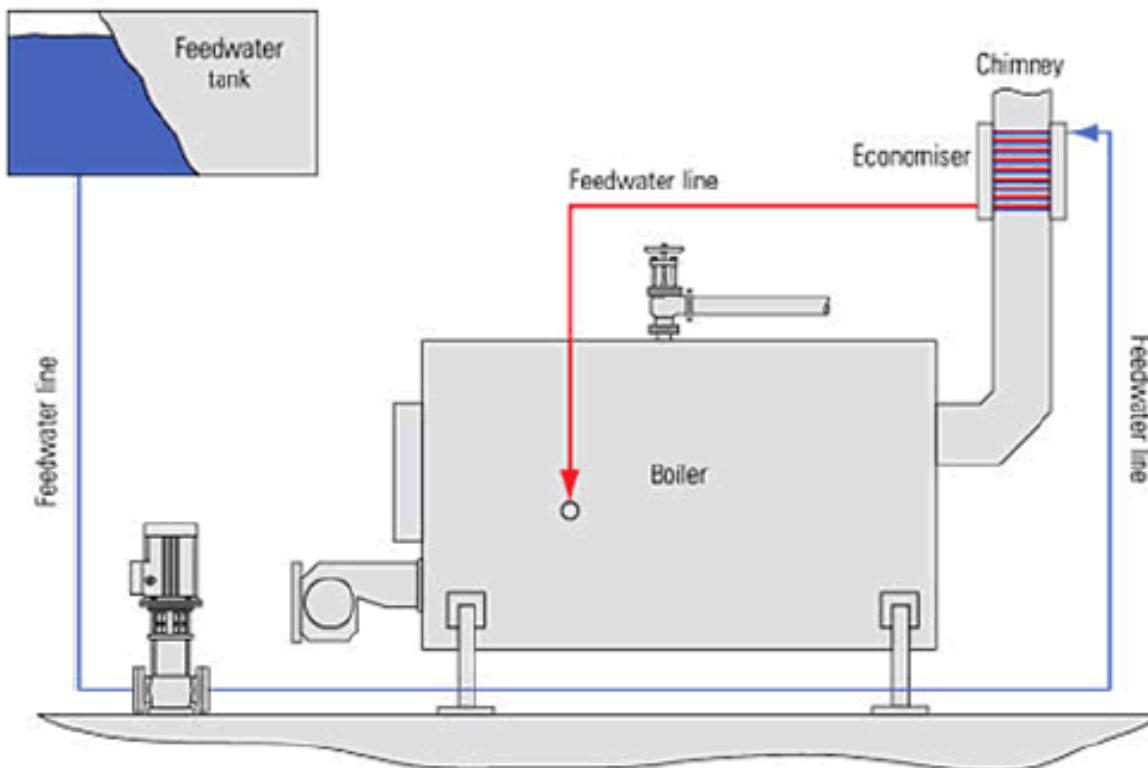


Figure 1: Economizer in Fire Tube Steam Boiler.

Figure 3.2: Three-pass shell boiler with rear-mounted economizer for feedwater pre-heating (reproduced from [12]).

3.2 Geometry and surface specification

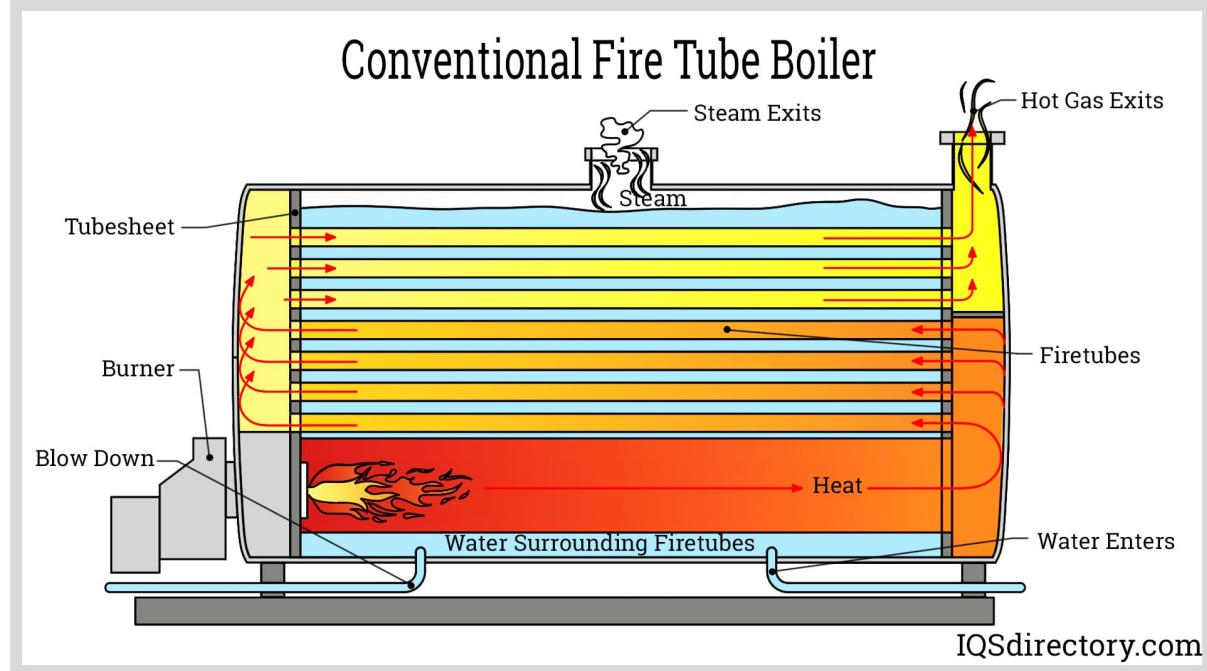


Figure 3.3: Detailed cross-section of the simulated boiler, showing drum, furnace, tube banks and reversal chambers (reproduced from [6]).

Drum

The boiler drum is modelled as a single horizontal cylindrical vessel without internal separators or circulation devices. It provides saturated liquid and vapour at drum pressure.

The inner diameter of the drum is $D_{i,\text{drum}} = 4.5 \text{ m}$ and the total length is $L_{\text{drum}} = 5.0 \text{ m}$

The drum wall is made of carbon steel with a uniform thickness of $t_{\text{drum}} = 0.05 \text{ m}$ and thermal conductivity $k_{\text{drum}} = 40 \text{ W m}^{-1}\text{K}^{-1}$

A fouling layer of thickness 0.1 mm and conductivity $0.2 \text{ W m}^{-1}\text{K}^{-1}$ is applied on the inner surface.

Pool boiling stages

All five pressure part stages located inside the drum are modelled under pool boiling conditions. These stages represent the furnace and convective passes before the economizer. Internal flow is one dimensional while external boiling occurs at drum saturation conditions.

All stages use steel walls with thermal conductivity $k_{\text{wall}} = 50 \text{ W m}^{-1}\text{K}^{-1}$, with internal roughness $\zeta_{\text{gas}} = 50 \mu\text{m}$, and outer roughness $\zeta_{\text{water}} = 20 \mu\text{m}$, while surface emissivity is 0.80.

Fouling resistance is included via a uniform fouling layer of thickness 0.1 mm and conductivity $0.2 \text{ W m}^{-1}\text{K}^{-1}$.

The main geometric parameters of the pool boiling stages are summarized in Table~3.1.

Table 3.1: Pool boiling pressure part geometry

Element Kind	D_i [m]	L [m]	Tube no.	Wall thickness [mm]	Roughness [μm]
HX1	single tube	1.40	5.276	1	20
HX2	reversal chamber	1.60	0.80	1	20
HX3	tube bank	0.076	4.975	118	2.9
HX4	reversal chamber	1.60	0.80	1	20
HX5	tube bank	0.076	5.620	100	2.9

The tube banks HX3 and HX5 are staggered arrangements with six tube rows. The transverse and longitudinal pitches are both $S_T = S_L = 0.11 \text{ m}$, respectively. Reversal chambers HX2 and HX4 include curvature effects through a bend radius of 0.8 m

Economizer

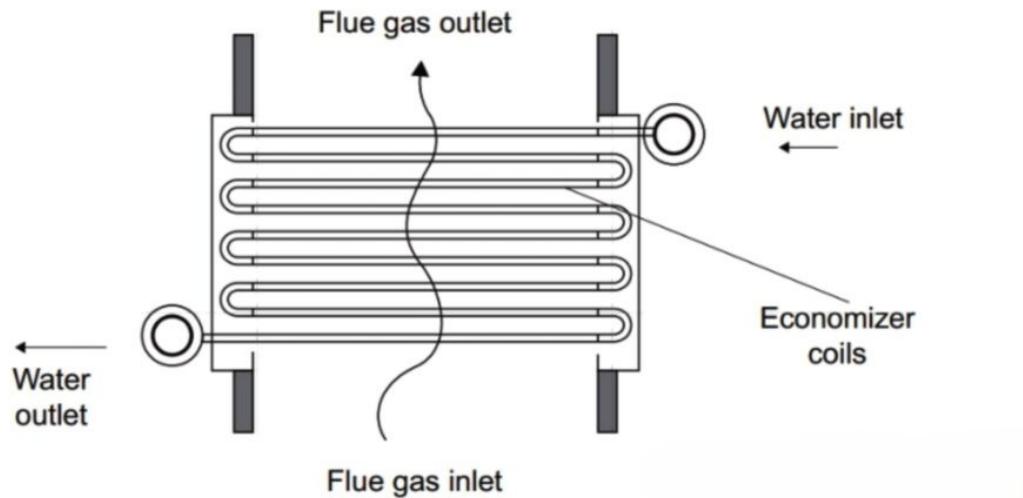


Figure 3.4: Cross-section of the economizer tube bundle HX_6 , showing gas-side cross-flow and water-side internal flow (reproduced from [7]).

The economizer is modelled as a shell and tube heat exchanger operating under single phase conditions on both sides. It is located downstream of the final pool boiling stage.

Flue gas flows on the shell side through a cylindrical duct of inner diameter $D_{\text{shell}} = 0.60 \text{ m}$. The tube side consists of 120 tubes of inner diameter $D_{i,\text{eco}} = 0.0250 \text{ m}$ with a tube length of $L_{\text{tube}} = 80 \text{ m}$.

The tube bundle is arranged in a staggered configuration. Transverse and longitudinal pitches are $S_T = 0.075 \text{ m}$ and $S_L = 0.08 \text{ m}$ respectively. Baffle spacing is 0.15 m with a baffle cut of 0.25 .

The economizer tubes are made of steel with wall thickness $t_{\text{eco}} = 2.6 \text{ mm}$ and thermal conductivity $k_{\text{eco}} = 50 \text{ W m}^{-1}\text{K}^{-1}$. Inner surface roughness is $20 \mu\text{m}$ and outer surface roughness is $50 \mu\text{m}$.

3.3 Assumptions and limitations

1. Combustion and flue gas
 - Ideal complete combustion, with fixed excess air,
 - Adiabatic flame temperature from equilibrium chemistry, using NASA polynomials.
 - Ideal gas mixture $p = \rho RT$, with transport properties $\mu(T)$ $k(T)$ $c_p(T)$ from polynomial data.
 - Steady state boiler operation, with fixed fuel air and feedwater.
 - Boiler efficiency computed on HHV or LHV basis, using standard energy balance equations.
2. Heat transfer
 - One dimensional steady heat transfer per stage.
 - Uniform wall conductivity and thickness, radial conduction only.
 - Gas side HTC from standard correlations properties **vary** with temperature pressure and composition.
 - Gas radiation via band averaged grey model for CO_2 and H_2O , no spectral resolution, and no soot formation.
 - Water side HTC uses IAPWS-IF97 properties, homogenized two phase model.
 - Drum at fixed pressure, and perfect steam water separation (no carryover).
3. Hydraulic and thermal performance
 - 1D, steady, single phase flow.
 - Constant mass flow along each stage.
 - Compressibility effects appear only through property variations $\rho(T, P)$ and $\mu(T, P)$ in Re and $\rho V^2/2$.

Chapter 4

Combustion Model

Determine combustion conditions inside the furnace (1st pass), resulting in a fully burnt flue gas stream, entering the heat transfer model at adiabatic temperature.

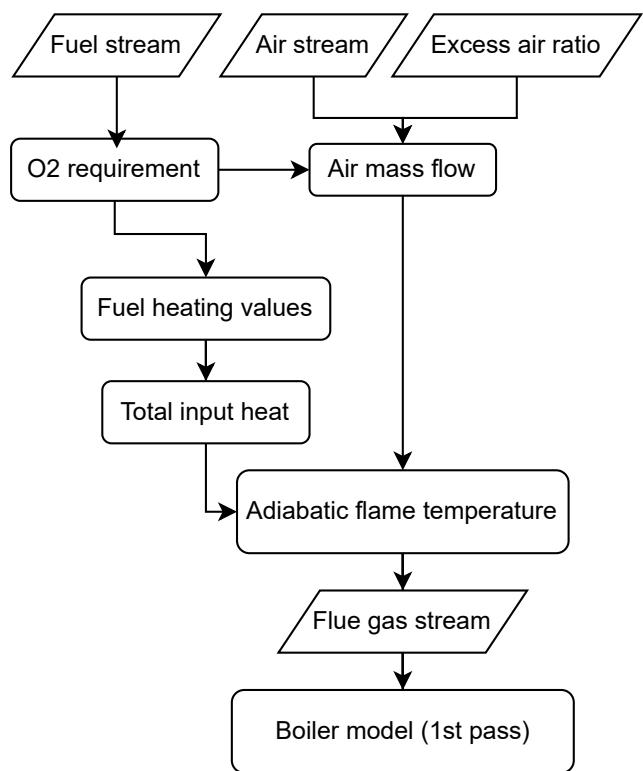


Figure 4.1: Combustion flow

4.1 Fuel and Air

4.1.1 Fuel Stream

The boiler is fired with a natural-gas-type fuel defined in the simulation input (config/fuel.yaml).

The fuel is supplied at $300K$ and $1.013 \times 10^5 Pa$ with a mass flow rate of $0.1kg/s$. Its composition is specified by user on a mass fraction.

Table 4.1: Fuel composition in mass fractions. [4]

Component	Formula	Mass fraction $w_i [-]$
Methane	CH_4	0.8548
Ethane	C_2H_6	0.0622
Propane	C_3H_8	0.0207
n-Butane	C_4H_{10}	0.00518
Hydrogen sulfide	H_2S	0.000104
Nitrogen	N_2	0.0414
Carbon dioxide	CO_2	0.0155
Water vapour	H_2O	0.00
Argon	Ar	0.00

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

$$x_i = \frac{\frac{w_i}{M_i}}{\sum_j \frac{w_j}{M_j}} \quad (4.1)$$

which is provided by the function `to_mol` in `combustion/mass_mole.py`, where M_i is the molar mass of species i from `molar_masses` in `common/constants.py`.

4.1.2 Air Stream

Combustion air is represented as a separate `GasStream` object, analogous to the fuel stream, with:

- temperature $T_{air} = 300 K$,
- pressure $P_{air} = 1.013 \times 10^5 Pa$,
- mass flow rate determined internally from the specified excess air ratio λ ,
- composition:

Table 4.2: Air composition in mass fractions. [8]

Component	Formula	Mass fraction w_i [-]
Oxygen	O ₂	0.233
Nitrogen	N ₂	0.755
Argon	Ar	0.013
Carbon dioxide	CO ₂	0.00006

The mass fractions satisfy $\sum_i w_i = 1$ and are converted internally to mole fractions whenever stoichiometric or thermophysical properties are required.

4.1.3 Stoichiometric Oxygen requirement

Evaluated the stoichiometric oxygen requirement via `stoich_O2_required_per_mol_fuel` in `combustion/flue.py`. The algorithm is:

1. Use per mole of species stoichiometric O₂ factors $\nu_{O_{2,i}}$ from `o2_per_mol` in `common/constants.py`:

Table 4.3: Combustion reactions and stoichiometric factors

Species	Global reaction (complete combustion)	$\nu_{O_{2,i}}$ [mol O ₂ / mol species]
CH ₄	CH ₄ + 2 O ₂ → CO ₂ + 2 H ₂ O	2.0
C ₂ H ₆	C ₂ H ₆ + 3.5 O ₂ → 2 CO ₂ + 3 H ₂ O	3.5
C ₃ H ₈	C ₃ H ₈ + 5 O ₂ → 3 CO ₂ + 4 H ₂ O	5.0
C ₄ H ₁₀	C ₄ H ₁₀ + 6.5 O ₂ → 4 CO ₂ + 5 H ₂ O	6.5
H ₂ S	H ₂ S + 1 O ₂ → SO ₂ + H ₂ O	1.0
N ₂ , CO ₂ , H ₂ O	Inert/fully oxidized → no additional O ₂	0.0

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

$$\nu_{O_2, \text{stoich}} = \sum_i x_i \nu_{O_2,i} \quad (4.2)$$

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

3. 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

$$n_{\text{fuel, total}} = \sum_i \frac{w_i}{M_i} \quad (4.3)$$

Thus the stoichiometric O₂ requirement per unit fuel mass is

$$n_{O_2,\text{stoich}}^{(m)} = \nu_{O_2,\text{stoich}} n_{\text{fuel},\text{total}} \quad (4.4)$$

Converting to mass of O₂ per kg of fuel:

$$\dot{m}_{O_2,\text{stoich}} = n_{O_2,\text{stoich}}^{(m)} M_{O_2} \quad (4.5)$$

4.1.4 Air-fuel ratio and excess air λ

The simulation specifies an excess air ratio $\lambda = 1.05$ in config/operation.yaml. This value enters the calculation through air_flow_rates(air, fuel, excess) in combustion/flue.py.

Actual O₂ supplied

Using:

$$\dot{n}_{O_2,\text{actual}} = \lambda \dot{n}_{O_2,\text{stoich}} = \lambda \nu_{O_2,\text{stoich}} \dot{n}_{\text{fuel}} \quad (4.6)$$

Air required

Air O₂ mole fraction (from air.yaml): $x_{O_2,\text{air}}$

Air molar flow, given by air_flow_rates():

$$\dot{n}_{\text{air}} = \frac{\dot{n}_{O_2,\text{actual}}}{x_{O_2,\text{air}}} \quad (4.7)$$

The air molar mass (mixture weighted) is:

$$M_{\text{air}} = \sum_i x_i M_i \quad (4.8)$$

Therefore the air mass flow rate:

$$\dot{m}_{\text{air}} = \dot{n}_{\text{air}} M_{\text{air}} \quad (4.9)$$

Air-fuel ratio

Mass based air fuel ratio:

$$\text{AFR} = \frac{\dot{m}_{\text{air}}}{\dot{m}_f} \quad (4.10)$$

4.2 Heating values and firing rate

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, air)` and then used by `total_input_heat()`.

4.2.1 HHV and LHV

For each fuel species, complete combustion is considered:

- $\text{CH}_4 + 2 \text{O}_2 \rightarrow \text{CO}_2 + 2 \text{H}_2\text{O}$
- $\text{C}_2\text{H}_6 + 3.5 \text{O}_2 \rightarrow 2 \text{CO}_2 + 3 \text{H}_2\text{O}$

The implementation also supports heavier hydrocarbons (C_3H_8 , C_4H_{10}) and sulphur species (H_2S), which are handled using stoichiometric oxygen requirements.

Builds complete-combustion products assuming all water remains in the vapour phase. The lower heating value (LHV) is obtained directly from the gas-phase products.

The higher heating value (HHV) is obtained by adding the latent heat of condensation of the water formed.

Latent heat of water

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

```
latent_H2O = WaterProps.h_g(P_ref) - WaterProps.h_f(P_ref)
```

where:

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

Reference thermodynamic data

All reactant and product enthalpies are obtained from the Cantera thermodynamic database via the mechanism file `config/flue_cantera.yaml`.

Mixture molar enthalpies are evaluated at the reference state $T_{\text{ref}} = 298.15 \text{ K}$ and $P_{\text{ref}} = 101,325 \text{ Pa}$ using Cantera's species NASA polynomial fits.

Methodology

The mixture molar heating values are computed directly from the molar enthalpy difference between reactants and products at the reference state:

$$\text{LHV}_{\text{mol}} = h_{\text{react}}(T_{\text{ref}}, P_{\text{ref}}) - h_{\text{prod}}(T_{\text{ref}}, P_{\text{ref}}) \quad (4.11)$$

The higher heating value is then obtained as

$$\text{HHV}_{\text{mol}} = \text{LHV}_{\text{mol}} + n_{\text{H}_2\text{O}} (h_g - h_f) M_{\text{H}_2\text{O}} \quad (4.12)$$

After obtaining the mixture molar heating values, conversion to mass basis uses

$$\text{HHV}_{\text{mix}} = \frac{\text{HHV}_{\text{mol}}}{M_{\text{mix}}}, \quad \text{LHV}_{\text{mix}} = \frac{\text{LHV}_{\text{mol}}}{M_{\text{mix}}}, \quad (4.13)$$

The firing rate corresponding to a fuel mass flow \dot{m}_f then follows directly:

$$P_{\text{HHV}} = \dot{m}_f \text{HHV}_{\text{mix}}, \quad P_{\text{LHV}} = \dot{m}_f \text{LHV}_{\text{mix}}. \quad (4.14)$$

4.2.2 Total heat input

The function `total_input_heat()` combines chemical and sensible contributions: where `sensible_heat()` uses:

$$Q_{\text{sens}} = \dot{m} [h(T, P, Y) - h(T_{\text{ref}}, P, Y)] \quad (4.15)$$

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

$$Q_{\text{in}} = P_{\text{LHV}} + Q_{\text{sens,fuel}} + Q_{\text{sens,air}} \approx P_{\text{LHV}} \quad (4.16)$$

4.3 Flame and flue gas

The combustion model must provide two closely related but conceptually distinct outputs:

1. The adiabatic flame temperature T_{ad} and equilibrium combustion state, which define the thermodynamic upper limit of the combustion process.
2. A practical flue-gas stream to be used as the hot-side working fluid in the boiler heat-transfer and pressure-drop calculations.

These two objectives place conflicting requirements on the combustion model. Accurate prediction of T_{ad} requires a full chemical-equilibrium treatment including high-temperature dissociation. In contrast, boiler heat-transfer and hydraulics require a chemically frozen reduced product set with stable thermophysical properties.

For this reason, the model deliberately computes two distinct flue-gas representations from the same reactant energy balance:

- an equilibrium flue gas used solely to determine T_{ad} and equilibrium composition, and
- a fully burnt boiler flue gas used as the working fluid throughout the boiler model.

Both streams are derived from the same inlet conditions and satisfy the same adiabatic, constant-pressure energy balance, but they differ in their chemical treatment and intended use.

4.3.1 Methodology

Fuel and air are assumed to mix perfectly and react adiabatically at constant pressure P , equal to the inlet pressure. Heat losses and shaft work are neglected.

The total inlet enthalpy rate of the unmixed reactants is

$$\dot{H}_{\text{react}} = \dot{m}_{\text{air}} h_{\text{air}}(T_{\text{air}}, P, \mathbf{x}_{\text{air}}) + \dot{m}_{\text{fuel}} h_{\text{fuel}}(T_{\text{fuel}}, P, \mathbf{x}_{\text{fuel}}) \quad (4.17)$$

with total mass flow

$$\dot{m}_{\text{tot}} = \dot{m}_{\text{air}} + \dot{m}_{\text{fuel}}. \quad (4.18)$$

The target specific enthalpy of the reacting mixture is therefore

$$h_{\text{target}} = \frac{\dot{H}_{\text{react}}}{\dot{m}_{\text{tot}}}. \quad (4.19)$$

The overall reactant composition is constructed from the molar flow rates of each species in the fuel and air streams.

Reactant species molar flow rates are obtained by converting inlet mass fractions to mole fractions and scaling by the corresponding total molar flow rates:

$$\dot{n}_i^{(\text{air})}, \quad \dot{n}_i^{(\text{fuel})}. \quad (4.20)$$

The total molar flow rate of species i is

$$\dot{n}_i = \dot{n}_i^{(\text{air})} + \dot{n}_i^{(\text{fuel})}, \quad (4.21)$$

and the overall reactant mole fractions are

$$X_{i,\text{react}} = \frac{\dot{n}_i}{\sum_j \dot{n}_j}. \quad (4.22)$$

This reactant mixture, together with h_{target} and pressure P , defines the common thermodynamic basis for both flue-gas representations described below.

4.3.2 Equilibrium flame state and adiabatic flame temperature

The equilibrium flame state is computed using Cantera by enforcing chemical equilibrium at constant enthalpy and pressure:

$$\begin{aligned} h_{\text{products}}(T_{\text{ad}}, P, \mathbf{X}_{\text{eq}}) &= h_{\text{target}}, \\ P_{\text{out}} &= P, \end{aligned} \quad (4.23)$$

where \mathbf{X}_{eq} satisfies chemical equilibrium at (T_{ad}, P) .

The reacting mixture is initialized at $T = 300$ K, pressure P , and composition $\mathbf{X}_{\text{react}}$, and Cantera's HP equilibrium solver is used to determine the equilibrium temperature and species composition.

The resulting equilibrium flue gas:

- includes all species permitted by the chemical mechanism, including dissociation products,
- defines the adiabatic flame temperature T_{ad} ,
- is used exclusively for combustion diagnostics and performance assessment.

This stream is not used in downstream boiler calculations.

4.3.3 Boiler flue gas

For boiler heat-transfer and pressure-drop calculations, a second flue-gas stream is constructed assuming complete combustion without dissociation.

Complete oxidation is implemented explicitly for a fixed fuel species set (CH_4 , C_2H_6 , C_3H_8 , C_4H_{10} , H_2S), accounting for any CO_2 , H_2O , N_2 , and Ar present in the inlet streams, and assuming excess-air operation ($\lambda \geq 1$). The resulting product set is limited to stable species such as CO_2 , H_2O , N_2 , O_2 , Ar, and SO_2 .

The boiler flue-gas temperature T_{flue} is obtained from an adiabatic, constant-pressure energy balance:

$$h_{\text{products}}(T_{\text{flue}}, P, \mathbf{Y}_{\text{burnt}}) = h_{\text{target}}. \quad (4.24)$$

This fully burnt, chemically frozen flue gas:

- satisfies the same overall energy balance as the equilibrium flame state,
- has a reduced, stable species set suitable for property evaluation,
- is used as the hot-side working fluid in all boiler heat-transfer and pressure-drop calculations.

Chapter 5

Heat Transfer Model

This model simulates heat transfer from hot flue gas to the water/steam mixture in the drum, flue gas entering first pass, is specified by the results of the combustion model, and water entering the economizer, specified by user at 105°C temperature with the mass flow to be calculated iteratively until convergence of water in and steam produced.

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 [$W/m^2 \cdot K$]
- 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 [$W/K/m$]

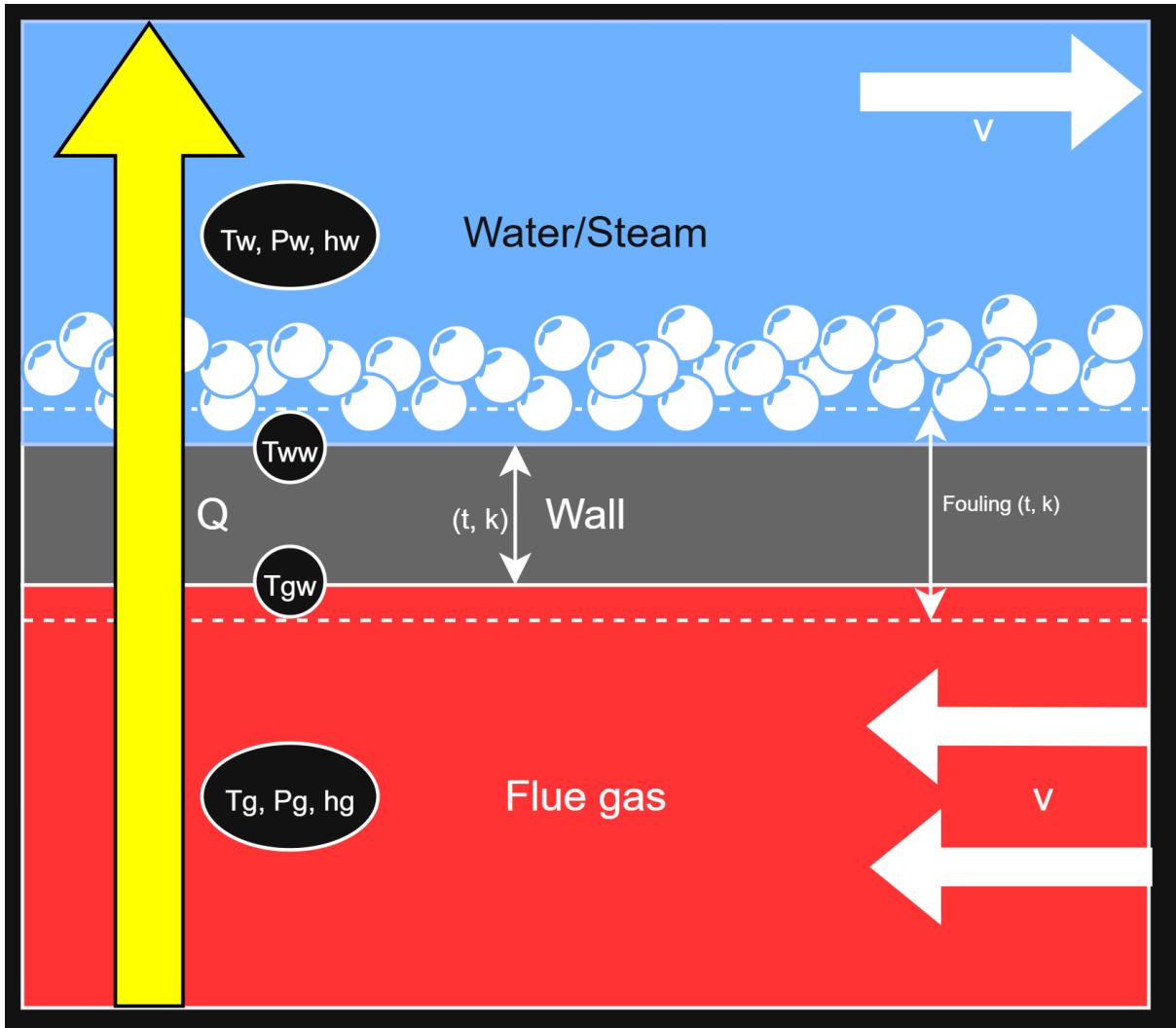


Figure 5.1: Cross section of heat transfer network from gas to water/steam

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:

$$q'(x) = UA'(x) [T_g(x) - T_w(x)] \quad (5.1)$$

- Relation to the segment duty:

$$dQ(x) = q'(x) dx \quad (5.2)$$

- Gas stream:

$$dQ(x) = -\dot{m}_g dh_g(x) \Rightarrow \frac{dh_g}{dx} = -\frac{q'(x)}{\dot{m}_g} \quad (5.3)$$

- Water stream:

$$dQ(x) = +\dot{m}_w dh_w(x) \Rightarrow \frac{dh_w}{dx} = +\frac{q'(x)}{\dot{m}_w} \quad (5.4)$$

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

$$Q_{\text{step}} = q'(x) \Delta x \quad (5.5)$$

$$\Delta h_g = -\frac{Q_{\text{step}}}{\dot{m}_g}, \quad \Delta h_w = +\frac{Q_{\text{step}}}{\dot{m}_w} \quad (5.6)$$

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:

$$R'_g = \frac{1}{h_g(x) P_g} \quad (5.7)$$

- Gas side fouling:

$$R'_{fg} = R'_{fi}(P_g) \quad (\text{from specified fouling thickness and conductivity}) \quad (5.8)$$

- Tube wall:

$$R'_w = \frac{\ln(D_o/D_i)}{2\pi k_w} \quad (5.9)$$

- Water side fouling:

$$R'_{fc} = R'_{fo}(P_w) \quad (5.10)$$

- Water side convection:

$$R'_c = \frac{1}{h_w(x) P_w} \quad (5.11)$$

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:

$$\frac{1}{UA'(x)} = R'_g + R'_{fg} + R'_w + R'_{fc} + R'_c \quad (5.12)$$

or equivalently,

$$UA'(x) = \left[\frac{1}{h_g P_g} + R'_{fg} + R'_w + R'_{fc} + \frac{1}{h_w P_w} \right]^{-1} \quad (5.13)$$

The linear heat flux then follows directly:

$$q'(x) = UA'(x) [T_g(x) - T_w(x)] \quad (5.14)$$

5.4 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:

$$T_{gw} = T_g - \frac{q'}{h_{g,\text{tot}} P_g} \quad (5.15)$$

$$T_{ww} = T_w + \frac{q'}{h_w P_w} \quad (5.16)$$

The wall conduction temperature drop is:

$$\Delta T_{\text{wall}} = T_{gw} - T_{ww} \quad (5.17)$$

which is also equal to:

$$\Delta T_{\text{wall}} = q' [R'_{fg} + R'_w + R'_{fc}] \quad (5.18)$$

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.

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.

5.5 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 :

$$Q_{\text{stage},j} = \int_0^{L_j} q'(x) dx \approx \sum_i q'_i \Delta x_i \quad (5.19)$$

$$(UA)_j = \int_0^{L_j} UA'(x) dx \approx \sum_i UA'_i \Delta x_i \quad (5.20)$$

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

$$Q_{\text{useful}} = \sum_{j=1}^6 Q_{\text{stage},j} \quad (5.21)$$

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

5.6 Heat Transfer Coefficient

5.6.1 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:

$$h_{g,\text{tot}} = h_{g,\text{conv}} + h_{g,\text{rad}} \quad (5.22)$$

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`.

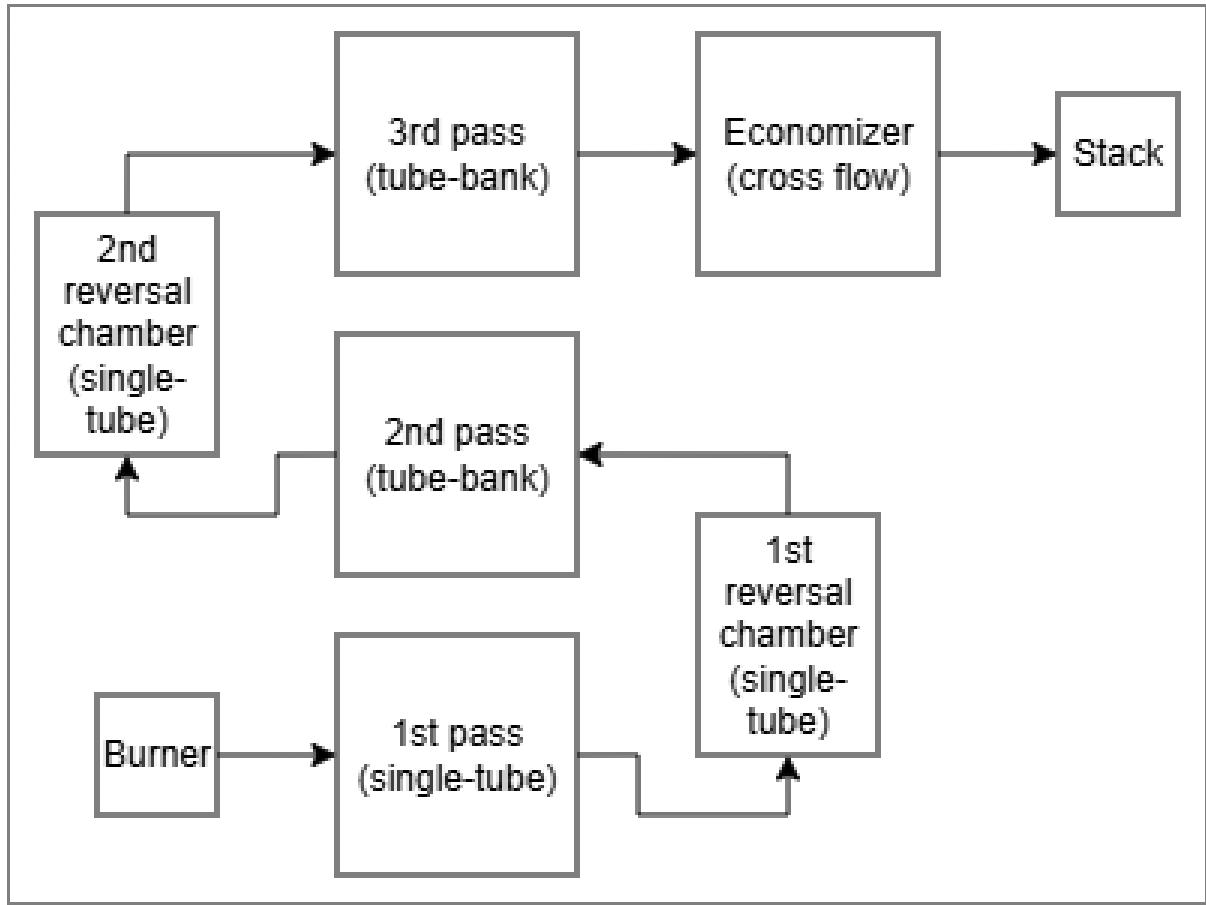


Figure 5.2: Path of flue gas through the 6 stages

5.6.1.1 Internal flow

Stages of kind `single_tube`, `reversal_chamber`, and `tube_bank` corresponding to furnace (first pass), both reversal chambers, and both tube banks are treated as internal forced convection in a circular duct. The characteristic quantities are:

- Diameter: D (supplied by `stages.yaml`)
- Length: L (supplied by `stages.yaml`)
- Tubes number: n (supplied by `stages.yaml` for tube banks)
- Flow area: $A = \frac{1}{4}\pi n D^2$ (calculated by geometry builder)
- Velocity:

$$V = \frac{\dot{m}_g}{\rho_g A} \quad (5.23)$$

- Reynolds and Prandtl numbers:

$$\text{Re} = \frac{\rho_g V D}{\mu_g}, \quad \text{Pr} = \frac{c_{p,g} \mu_g}{k_g} \quad (5.24)$$

Local gas properties $\rho_g, \mu_g, k_g, c_{p,g}$ are obtained from the Cantera mixture via the functions defined in `common\props.py`, at the local gas temperature and pressure. [9]

Laminar/developing flow (Graetz-type) For $\text{Re} < 2300$, uses a Graetz correlation for thermally developing laminar flow:

$$Gz = \text{Re} \Pr \frac{D}{L} \quad (5.25)$$

$$\text{Nu} = 3.66 + \frac{0.0668 Gz}{1 + 0.04 Gz^{2/3}} \quad (5.26)$$

[3]

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

$$f = (0.79 \ln \text{Re} - 1.64)^{-2} \quad (5.27)$$

[11]

$$\text{Nu} = \frac{\frac{f}{8}(\text{Re} - 1000) \Pr}{1 + 12.7 \sqrt{\frac{f}{8}} (\Pr^{2/3} - 1)} \quad (5.28)$$

[3] The local convective heat-transfer coefficient is then:

$$h_{g,\text{conv}} = \frac{\text{Nu} k_g}{D} \quad (5.29)$$

[3]

5.6.1.2 Cross flow

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 cross flow over a tube bank.

Key geometry quantities (from GeometryBuilder for the economizer):

- Tube outer diameter: $D = D_o$
- Gas side cross flow area: $A_{\text{bulk}} = A_{\text{hot,flow}}$
- Optional maximum/mean velocity factor:

$$V_{\text{bulk}} = \frac{\dot{m}_g}{\rho_g A_{\text{bulk}}}, \quad V = u_{\max} V_{\text{bulk}} \quad (5.30)$$

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

- Reynolds and Prandtl numbers:

$$\text{Re} = \frac{\rho_g V D}{\mu_g}, \quad \text{Pr} = \frac{c_{p,g} \mu_g}{k_g} \quad (5.31)$$

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

$$\text{Nu} = C \text{Re}^m \text{Pr}^n \quad (5.32)$$

[3]

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:

$$n = \begin{cases} 0.36, & \text{Pr} \leq 10 \\ 0.25, & \text{Pr} > 10 \end{cases} \quad (5.33)$$

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

$$\text{Nu} = 0.3 + \frac{0.62 \text{Re}^{1/2} \text{Pr}^{1/3}}{\left[1 + (0.4/\text{Pr})^{2/3}\right]^{1/4}} \left[1 + \left(\frac{\text{Re}}{282000}\right)^{5/8}\right]^{4/5} \quad (5.34)$$

[3] The gas-side convective HTC in the economizer is then:

$$h_{g,\text{conv}}^{(\text{HX6})} = \frac{\text{Nu} k_g}{D_o} \quad (5.35)$$

[3]

5.6.1.3 Radiation model

Radiative heat transfer from the flue gas to the furnace surfaces is explicitly accounted for by a participating medium model for the H_2O/CO_2 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:

$$p_{H_2O} = y_{H_2O} P, \quad p_{CO_2} = y_{CO_2} P \quad (5.36)$$

[10] 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:

$$L_b = \begin{cases} L_{\text{rad,override}}, & \text{if specified in the stage} \\ 0.9 D_{h,\text{gas}}, & \text{otherwise} \end{cases} \quad (5.37)$$

[10] with $D_{h,\text{gas}}$ the gas-side hydraulic diameter.

3. Effective optical thickness in each gray band:

$$p_{\text{ratio}} = \frac{p_{\text{H}_2\text{O}} + p_{\text{CO}_2}}{P_{\text{atm}}} \quad (5.38)$$

[10]

$$\tau_j = K_j \left(\frac{T}{1000 \text{ K}} \right)^{T_{\text{exp}}} p_{\text{ratio}} L_b \quad (5.39)$$

[10]

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:

$$\varepsilon_g = 1 - \sum_{j=1}^4 A_j \exp(-\tau_j) \quad (5.40)$$

[10] with ε_g constrained to $[0, 1]$.

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

$$T_{\text{film}} = \frac{T_g + T_{gw}}{2} \quad (5.41)$$

$$h_{g,\text{rad}} = 4 \sigma F \varepsilon_g T_{\text{film}}^3 \quad (5.42)$$

[10]

where:

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

5.6.2 Water side

Water side heat transfer is computed with geometry dependent correlations using local water properties from IAPWS97 (WaterProps), with stage specific geometry from the GeometryBuilder. The solver always works with a single effective water side heat transfer coefficient $h_w(x)$ per marching step, which may represent:

- pure pool boiling at a saturated surface,
- single phase forced convection.

In the implementation this logic is encapsulated in `water_htc`, which returns (h_w) for each step.

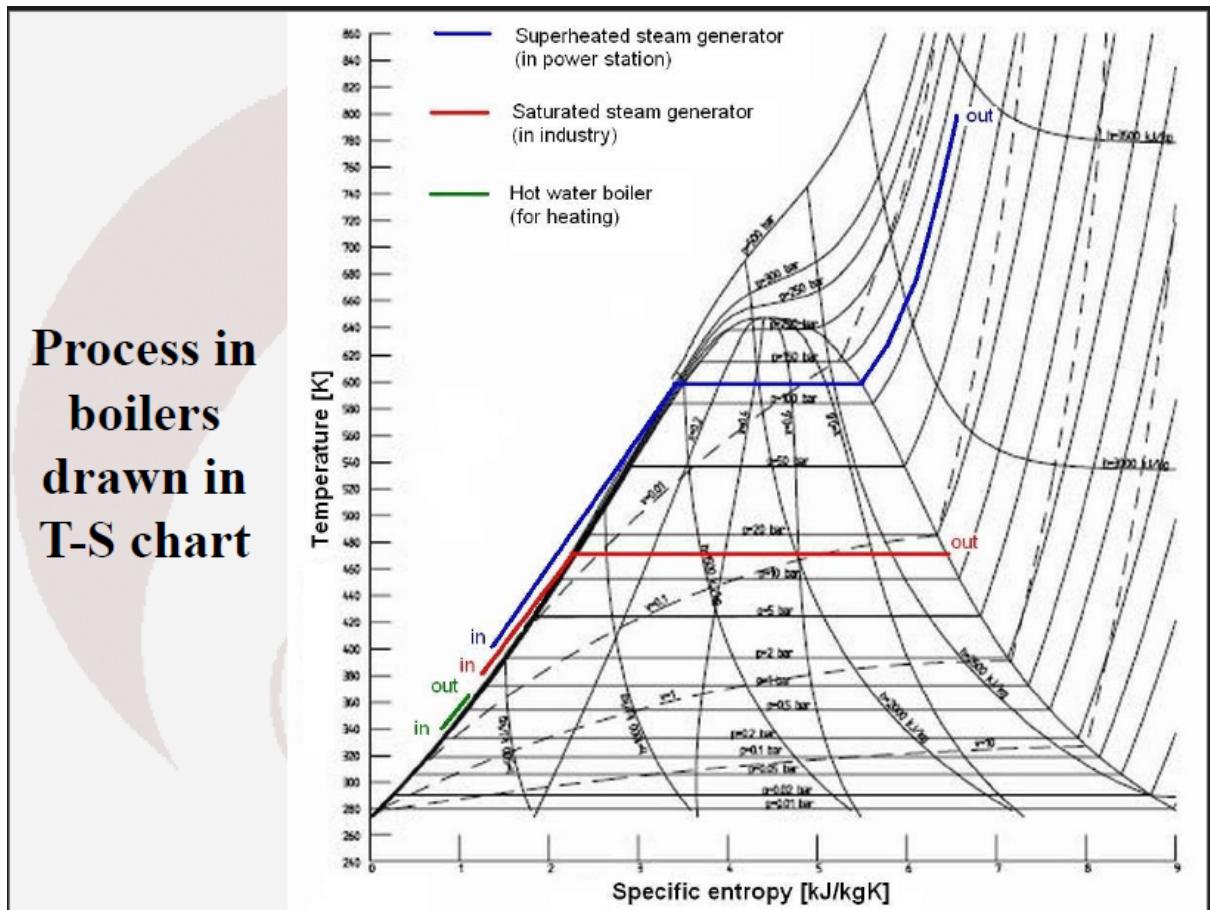


Figure 5.3: Temperature–entropy (T – s) representation of the feedwater heating and evaporation process across economiser and boiler at the operating pressure (reproduced from [5]).

The six stages of the boiler are divided, from the water-side point of view, into:

- HX_1 – HX_5 : pool-boiling stages
(`pool_boiling = true` in the stage specification)
- HX_6 : economizer stage
(`pool_boiling = false`)

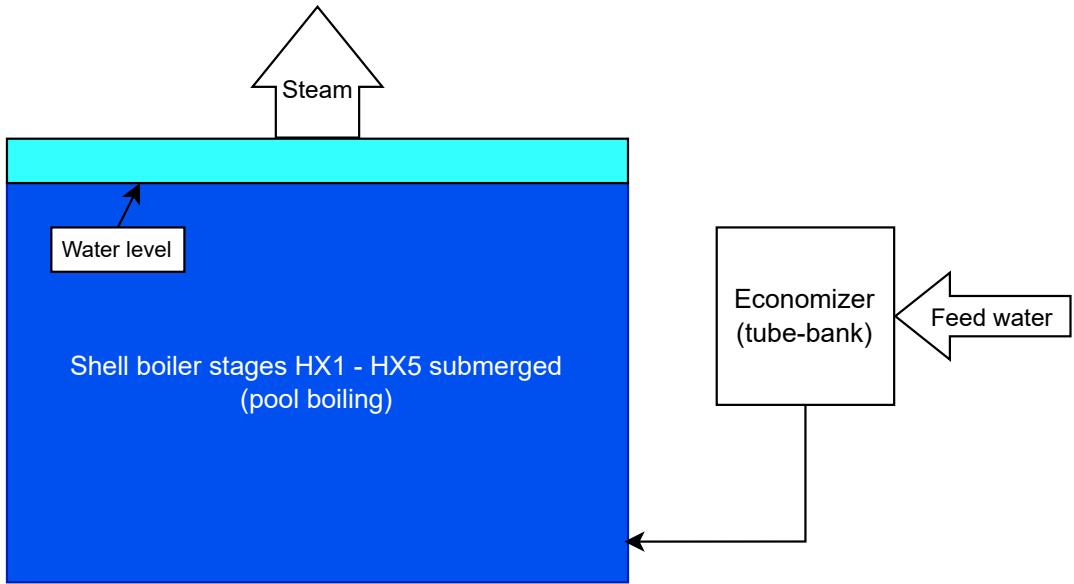


Figure 5.4: Path of water/steam through the 6 stages

5.6.2.1 Internal Flow

In the economiser stage (HX_6), feedwater flows inside tubes and is heated by flue gas in external crossflow.

The water remains in the single-phase liquid region throughout this section, and the water-side heat transfer coefficient is therefore computed using forced convection correlations for internal flow.

Stages of kind `single_tube`, `reversal_chamber`, and `tube_bank` corresponding to furnace (first pass), both reversal chambers, and both tube banks are treated as internal forced convection in a circular duct. The characteristic quantities are:

- Diameter: D (supplied by `stages.yaml`)
- Length: L (supplied by `stages.yaml`)
- Tubes number: n (supplied by `stages.yaml` for tube banks)
- Flow area: $A = \frac{1}{4}\pi n D^2$ (calculated by geometry builder)
- Velocity:

$$V = \frac{\dot{m}_g}{\rho_g A} \quad (5.43)$$

- Reynolds and Prandtl numbers:

$$\text{Re} = \frac{\rho_g V D}{\mu_g}, \quad \text{Pr} = \frac{c_{p,g} \mu_g}{k_g} \quad (5.44)$$

Local gas properties $\rho_g, \mu_g, k_g, c_{p,g}$ are obtained from the Cantera mixture via the functions defined in `common\props.py`, at the local gas temperature and pressure. [9]

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

$$Gz = \text{Re} \Pr \frac{D}{L} \quad (5.45)$$

$$\text{Nu} = 3.66 + \frac{0.0668 Gz}{1 + 0.04 Gz^{2/3}} \quad (5.46)$$

[3]

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

$$f = (0.79 \ln \text{Re} - 1.64)^{-2} \quad (5.47)$$

[11]

$$\text{Nu} = \frac{\frac{f}{8}(\text{Re} - 1000) \Pr}{1 + 12.7 \sqrt{\frac{f}{8}} (\Pr^{2/3} - 1)} \quad (5.48)$$

[3]

A viscosity correction is applied:

$$\text{Nu}_w \leftarrow \text{Nu}_w \left(\frac{\mu_b}{\mu_w} \right)^{0.11}. \quad (5.49)$$

[3]

The local convective heat-transfer coefficient is then:

$$h_{g,\text{conv}} = \frac{\text{Nu} k_g}{D} \quad (5.50)$$

[3]

5.6.2.2 Pool Boiling

The main boiler heating surfaces (HX_1 – HX_5) are modelled as pool boiling surfaces immersed in saturated water at the local pressure.

These sections represent the furnace walls, passes, and reversal chambers, where heat transfer is governed primarily by nucleate boiling rather than by a well-defined bulk liquid velocity.

For these stages, the bulk water temperature entering the wall energy balance is fixed at the saturation temperature:

$$T_w = T_{\text{sat}}(p_w). \quad (5.51)$$

The water-side heat transfer coefficient is computed using the Cooper correlation for nucleate pool boiling:

$$h_{\text{nb}} = 55 p_r^{0.12} R_p^{-0.55} M_w^{-0.5} (q'')^{0.67}, \quad (5.52)$$

[1]

where

$$p_r = \frac{p}{p_{\text{crit}}}, \quad (5.53)$$

R_p is the surface roughness in μm , M_w is the molecular weight of water, and q'' is the local heat flux.

The resulting coefficient is used directly:

$$h_w = h_{\text{nb}}. \quad (5.54)$$

This approach reflects the natural circulation character of the boiler, where boiling heat transfer is dominated by surface conditions and heat flux rather than by forced convection effects.

Chapter 6

Hydraulic Model

Hydraulic behavior 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`.

The model divides pressure losses into:

- Frictional losses
- Minor losses (inlet, outlet, bends, etc.)
- Total pressure drop (sum of the above)

6.1 Frictional losses

Gas and water sides

The per step frictional pressure drop follows a standard 1D Darcy formulation:

$$\Delta P_{\text{fric}} = -f \frac{\Delta x}{D_h} \left(\frac{\rho V^2}{2} \right) \quad (6.1)$$

[15]

Here:

- f is the Darcy friction factor,
- D_h is the relevant side hydraulic diameter ($D_h = \text{hot_Dh}$ for gas, $D_h = \text{cold_Dh}$ for water),
- ρ and V are local density and velocity on the relevant side,
- Δx is the current marching step length.

The friction factor is computed from Reynolds number and relative roughness via `_friction_factor`:

- Laminar ($\text{Re} < 2300$):

$$f = \frac{64}{\text{Re}} \quad (6.2)$$

[15]

- Transitional ($2300 \leq \text{Re} < 4000$): linear blend between laminar and turbulent values:

$$f = (1 - w)f_{\text{lam}} + wf_{\text{turb}}, \quad w = \frac{\text{Re} - 2300}{4000 - 2300} \quad (6.3)$$

[2]

- Turbulent ($\text{Re} \geq 4000$): Colebrook–White is solved iteratively, seeded by the Swamee–Jain explicit approximation.

Swamee–Jain seed (used as the initial guess):

$$f_{\text{SJ}} = \frac{0.25}{\left[\log_{10} \left(\frac{\varepsilon/D_h}{3.7} + \frac{5.74}{\text{Re}^{0.9}} \right) \right]^2} \quad (6.4)$$

[14]

Colebrook–White equation solved iteratively in the code:

$$\frac{1}{\sqrt{f}} = -2 \log_{10} \left(\frac{\varepsilon/D_h}{3.7} + \frac{2.51}{\text{Re}\sqrt{f}} \right) \quad (6.5)$$

[15]

The iteration is performed on $1/\sqrt{f}$ until convergence.

Local velocity and Reynolds number are evaluated using the side flow area A and properties:

$$V = \frac{\dot{m}}{\rho A}, \quad \text{Re} = \frac{\rho V D_h}{\mu} \quad (6.6)$$

Frictional losses are only applied for the economizer water side branch in `_water_dp_components`; for other stage kinds the current model sets $\Delta P_{\text{fric}} = 0$.

6.2 Gas side pressure drop in the economizer

The economizer gas side hydraulics differ fundamentally from all other modeled stages.

While other stages assume internal flow and apply a Darcy–Weisbach formulation, the economizer models external crossflow over a tube bank, and gas side pressure losses

are therefore computed using a bundle loss (drag-based) formulation rather than a wall-friction model.

Crossflow bundle formulation

The gas flows across a bank of tubes arranged either inline or staggered. A characteristic velocity is defined using a bulk velocity corrected by a geometry-dependent maximum-velocity factor:

$$V_{\text{bulk}} = \frac{\dot{m}}{\rho A_{\text{hot}}}, \quad V_{\text{char}} = u_{\max} V_{\text{bulk}} \quad (6.7)$$

where:

- A_{hot} = hot_flow_A is the free crossflow area,
- u_{\max} = umax_factor accounts for flow acceleration between tubes.

The Reynolds number is formed using the tube outer diameter:

$$\text{Re}_D = \frac{\rho V_{\text{char}} D_o}{\mu} \quad (6.8)$$

Bundle loss coefficient

The pressure loss per tube row is expressed via a dimensionless bundle loss coefficient:

$$\zeta_{\text{row}} = C_0 \text{Re}_D^m \Phi_{\text{geom}} \quad (6.9)$$

where:

- C_0 and m depend on tube arrangement (inline or staggered),
- Φ_{geom} accounts for pitch ratios:

$$\Phi_{\text{geom}} = \left(\frac{S_T/D_o}{1.5} \right)^{-0.2} \left(\frac{S_L/D_o}{1.5} \right)^{-0.2} \quad (6.10)$$

with transverse pitch S_T and longitudinal pitch S_L .

The total bundle loss coefficient is then:

$$\zeta_{\text{bundle}} = N_{\text{rows}} \zeta_{\text{row}} \quad (6.11)$$

where N_{rows} is the number of tube rows in the flow direction.

Distributed pressure loss

The dynamic pressure is evaluated using the characteristic velocity:

$$q = \frac{\rho V_{\text{char}}^2}{2} \quad (6.12)$$

The total bundle pressure drop is:

$$\Delta P_{\text{bundle}} = -\zeta_{\text{bundle}} q \quad (6.13)$$

This loss is distributed uniformly along the economizer length L across the marching steps:

$$\Delta P_{\text{fric,step}} = \Delta P_{\text{bundle}} \frac{\Delta x}{L} \quad (6.14)$$

where Δx is the local marching step length.

6.3 Minor losses

Minor losses are applied using per-stage catalogue K values and the standard dynamic-pressure formulation:

$$\Delta P_{\text{minor}} = -K_{\text{minor}} \left(\frac{\rho V^2}{2} \right) \quad (6.15)$$

[2]

The total minor-loss coefficient K_{minor} is assembled differently for gas and water sides, but applied through the same formulation.

Coefficient assembly

Gas side.

For each stage, the total loss coefficient is assembled from geometry and user inputs:

$$K_{\text{minor}} = K_{\text{contraction}} + K_{\text{expansion}} + K_{\text{bend}} \quad (6.16)$$

Where:

- $K_{\text{contraction}}$: accounts for sudden expansion of flow area (e.g. $\text{HX}_2 \rightarrow \text{HX}_3$), default = 0.5.
- $K_{\text{expansion}}$ (Borda–Carnot): losses caused by sudden expansion of flow area (e.g. $\text{HX}_1 \rightarrow \text{HX}_2$), default = 1.
- K_{bend} : losses due to gas flow rotation in reversal chambers, default = 0.

The bend loss is distributed uniformly across the n marching steps:

$$K_{\text{bend,per-step}} = \frac{K_{\text{cold,bend}}}{n} \quad (6.17)$$

The per-step assembled coefficient is:

$$K_{\text{minor}} = K_{\text{bend,per-step}} + \mathbb{1}_{i=0} K_{\text{cold,inlet}} + \mathbb{1}_{i=n-1} K_{\text{cold,outlet}} \quad (6.18)$$

Application

For both gas and water sides, the minor-loss pressure drop is computed using the local dynamic pressure:

$$V = \frac{\dot{m}}{\rho A}, \quad q = \frac{\rho V^2}{2}, \quad \Delta P_{\text{minor}} = -K_{\text{minor}} q \quad (6.19)$$

where A is the relevant side flow area ($A = \text{cold_flow_A}$ for water, gas side area otherwise).

6.4 Total pressure drop

For each step, the total side pressure change is the sum of frictional and minor components:

$$\Delta P_{\text{total}} = \Delta P_{\text{fric}} + \Delta P_{\text{minor}} \quad (6.20)$$

[15]

This is what `pressure_drop_gas/water` return and what is applied to the streams in `update_gas/water_after_step`.

6.5 Coupling of ΔP into the energy solver

Gas/water pressure is updated step-wise using the same ΔP model:

$$P_{i+1} = P_i + \Delta P_{\text{total}}(P_i, T_i, \dots) \quad (6.21)$$

After each step:

1. The local gas/water state (T_i, P_i , composition) is used to evaluate ρ, μ, k , and c_p .
2. The friction factor and dynamic pressure are computed from these properties.
3. ΔP_{fric} and ΔP_{minor} are formed.
4. The updated pressure P_{i+1} is used for the next step.

In this way, compressibility enters through the pressure dependence of $\rho(T, P)$ and $\mu(T, P)$ and their effect on V , Re , and f .

Chapter 7

Performance

This section summarizes the boiler level performance obtained from the coupled combustion heat transfer simulation. All numerical values are extracted from the stages summary and boiler summary data produced by the post-processing step `heat/postproc.py`.

7.1 Solution procedure

For any given operating conditions, the main solver `run_boiler_case()` performs an outer fixed point iteration, on boiler efficiency, and water mass flow:

1. The combustion sub-model called by `Combustor.run()`, returns:
 - the lower heating value based firing rate P_{LHV} ,
 - the total combustion heat release Q_{in} ,
 - the adiabatic flame temperature T_{ad} ,
 - the fully burnt flue-gas stream at burner exit.
2. Given a current efficiency guess $\eta^{(n)}$ and the combustion result, the corresponding feedwater/steam mass flow $\dot{m}_w^{(n)}$ is computed by `_water_mass_from_efficiency()` as

$$h_{\text{in}} = h_{\text{fw}}(P_{\text{fw}}), \quad h_{\text{steam}} = h_g(P_{\text{fw}}), \quad (7.1)$$

$$\Delta h = h_{\text{steam}} - h_{\text{in}}, \quad (7.2)$$

$$Q_{\text{target}}^{(n)} = \eta^{(n)} Q_{\text{in}}, \quad (7.3)$$

$$\dot{m}_w^{(n)} = \frac{Q_{\text{target}}^{(n)}}{\Delta h}. \quad (7.4)$$

3. A WaterStream with mass flow $\dot{m}_w^{(n)}$ is created and passed, together with the combustion flue gas GasStream and the drum/stage definitions, to the multi stage heat exchanger solver `run_hx()`.
4. `run_hx()` returns per stage and boiler level summary tables.
5. The new efficiency estimate is set to the indirect efficiency,

$$\eta^{(n+1)} := \eta_{\text{indirect}}^{(n)}, \quad (7.5)$$

And the procedure is repeated until the change in water mass flow between iterations is below the specified tolerance

$$|\dot{m}_w^{(n)} - \dot{m}_w^{(n-1)}| < 10^{-3} \text{ kg/s}, \quad (7.6)$$

or a maximum number of iterations is reached.

At convergence, returning:

- converged water/steam mass flow $\dot{m}_{w,\text{base}}$,
- converged indirect efficiency $\eta_{\text{indirect,base}}$,

together with the corresponding boiler summary quantities (stack temperature, total pressure drop, etc.). These and more are exported to CSV as `boiler_summary.csv` and `stages_summary.csv`.

7.2 Energy balance

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:

$$Q_{\text{useful}} = \sum_{k=1}^6 Q_{\text{stage},k} = \sum_{k=1}^6 \int_q' (x) dx \quad (7.7)$$

The total input heat from combustion Q_{in} is taken from the combustion module as the rate of heat release from complete fuel burnout:

7.3 Efficiency

Efficiency indicates how well the boiler converts the heat released from fuel into useful steam or hot water. Two boiler efficiencies are reported:

- Direct efficiency (LHV):

$$\eta_{\text{direct}} = \frac{Q_{\text{useful}}}{P_{\text{LHV}}} \quad (7.8)$$

- Indirect efficiency:

$$\eta_{\text{indirect}} = 1 - \frac{Q_{\text{losses}}}{Q_{\text{in}}} \quad (7.9)$$

The direct and indirect methods together provide a complete view of boiler efficiency, with the direct method quantifying useful heat output and the indirect method identifying heat losses. Their combined use supports accurate performance evaluation and targeted efficiency improvements.

Chapter 8

Performance Analysis

The purpose of this chapter is to evaluate the thermal and hydraulic performance of the developed fire tube shell boiler model under representative operating conditions and systematic parameter variations. The analysis aims to quantify how key controllable and design relevant parameters influence boiler efficiency, steam production, heat transfer distribution, and pressure losses.

8.1 Control case

The control case defines the nominal operating condition of the boiler and serves as the reference point for all subsequent parametric studies. It represents typical industrial operation, enabling direct comparison with published industrial boiler performance data. Defined by:

- Fuel mass flow: $\dot{m}_{\text{fuel}} = 0.1 \text{ kg s}^{-1}$
- Excess air ratio: $\lambda = 1.05$
- Drum pressure: $P_{\text{drum}} = 10 \text{ bar}$
- Fouling factor : $f = 1 \text{ [-]}$

All parameters not under investigation are held fixed at their control values during each parametric sweep.

Table 8.1: Control case performance.

control	control
Fuel Mass Flow[Kg/S]	0.1
Air Flow[Kg/S]	1.69
Excess Air Ratio[-]	1.05
Feedwater Flow[Kg/S]	1.89
Steam Capacity[T/H]	6.81
η_{direct} [-]	0.95
η_{indirect} [-]	0.95
Stack Loss Fraction[-]	0.05
Q_Flue_Out[Mw]	0.25
conductance [MW/K]	0.01

control	control
input heat [MW]	4.68
useful heat [MW]	4.42
Q_Balance_Error[Mw]	-0
Pressure Drop Fric Total[Kpa]	-8.35
Pressure Drop Minor Total[Kpa]	-4.09
Pressure Drop Total[Kpa]	-12.45
Water Pressure Drop Fric Total[Kpa]	-0.06
Water Pressure Drop Minor Total[Kpa]	-0
Water Pressure Drop Total[Kpa]	-0.06
Lhv [Mj/Kg]	46.73
firing rate [MW]	4.67
adiabatic temperature [°C]	1981.5
Stack Temperature[°C]	152.38
Feedwater Pressure[Kpa]	1000.06
Drum Pressure[Kpa]	1000

The performance (notably $\eta_{\text{direct}} = 0.95$ on an LHV basis and $T_{\text{stack}} = 152.4^{\circ}\text{C}$) was compared against published reference values for gas-fired fire tube boilers with economizer [], and found to be within expected tolerance ranges.

8.1.1 Stage-wise heat transfer and hydraulics

Stage-wise analysis is used to understand how heat transfer mechanisms and hydraulic behavior evolve along the gas path, and to verify whether parameter variations (excess air, fuel flow, drum pressure) introduce any regime changes between stages.

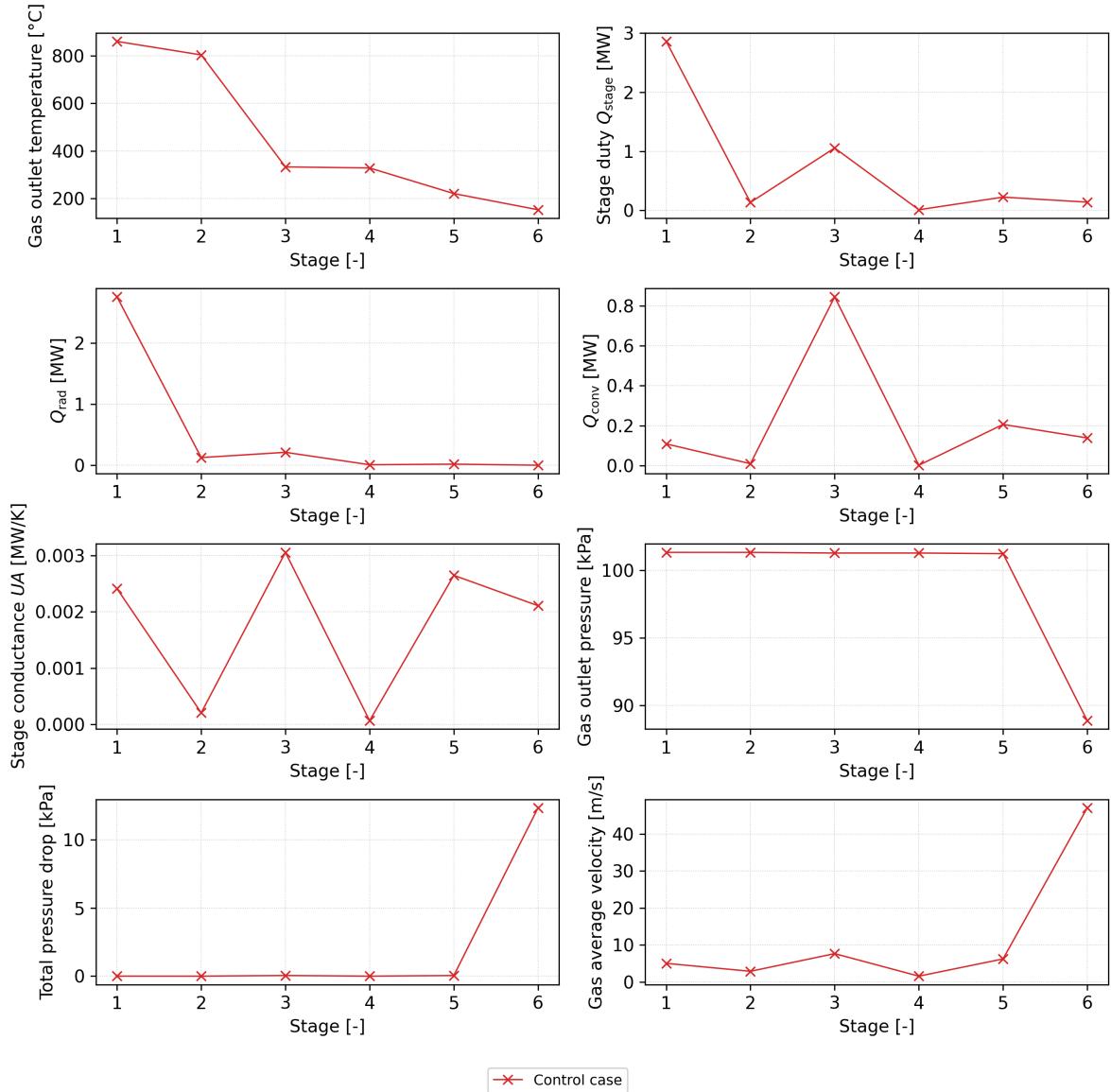


Figure 8.1: Stage wise heat transfer and hydraulic profiles

Across all runs the stage pattern stays the same: gas temperature drops from HX 1 to HX 6, stage heat duty is highest in the first stages and decreases downstream, and early stages are driven mainly by radiative transfer while later stages are relatively more convective.

Excess air primarily weakens and redistributes heat transfer by lowering upstream gas temperatures, reducing early-stage duties, shifting recovery downstream, and increasing gas velocity and total pressure drop. Fuel flow scales the entire system: higher fuel rates raise gas temperatures, stage duties, and both radiative and convective contributions, with the largest absolute impact in the furnace and first tube bank, while also increasing pressure losses. Drum pressure has a comparatively minor effect on gas-side behavior, mainly influencing downstream heat recovery through water-side conditions. Table: Control case stages summary.

stage KPI	HX_1	HX_2	HX_3	HX_4	HX_5	HX_6
Kind	Furnace	reversal	tube_bank	reversal	tube_bank	economizer
Gas In Pressure[Kpa]	101.33	101.32	101.32	101.27	101.27	101.23
Gas In Temp[°C]	1981.25	860.87	804.14	332.78	328.16	220.51
Gas In Enthalpy[Kj/Kg]	2612.29	1014.02	938.90	349.39	343.96	219.06
Gas Out Pressure[Kpa]	101.32	101.32	101.27	101.27	101.23	88.88
Gas Out Temp[°C]	860.87	804.14	332.78	328.16	220.51	152.38
Gas Out Enthalpy[Kj/Kg]	1014.02	938.90	349.39	343.96	219.06	141.69
Water In Temp[°C]	179.89	179.89	179.89	179.89	179.89	104.80
Water In Enthalpy[Kj/Kg]	762.68	762.68	762.68	762.68	762.68	440.00
Water In Pressure[Kpa]	1000.00	1000.00	1000.00	1000.00	1000.00	1000.06
Water Out Temp[°C]	179.89	179.89	179.89	179.89	179.89	122.09
Water Out Enthalpy[Kj/Kg]	762.68	762.68	762.68	762.68	762.68	513.21
Water Out Pressure[Kpa]	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00
Gas Avg Velocity[M/S]	5.04	2.90	7.67	1.58	6.24	47.04
Water Avg Velocity[M/S]						0.03
Pressure Drop Fric[Kpa]	-0.00	-0.00	-0.03	-0.00	-0.03	-8.30
Pressure Drop Minor[Kpa]	-0.00	-0.00	-0.02	-0.00	-0.02	-4.05
Pressure Drop Total[Kpa]	-0.00	-0.00	-0.05	-0.00	-0.05	-12.35
Water Pressure Drop Fric[Kpa]						-0.06
Water Pressure Drop Minor[Kpa]						-0.00
Water Pressure Drop Total[Kpa]						-0.06
Q Conv[Mw]	0.11	0.01	0.84	0.00	0.21	0.14
Q Rad[Mw]	2.75	0.13	0.21	0.01	0.02	0.00
Q Total[Mw]	2.86	0.13	1.06	0.01	0.22	0.14
conductance [MW/K]	0.00	0.00	0.00	0.00	0.00	0.00
Steam Capacity[T/H]	4.55	0.21	1.68	0.02	0.36	

8.2 Results and parametric analysis

8.2.1 Influence of excess air factor

The excess air factor λ quantifies the ratio of supplied combustion air to the theoretical stoichiometric requirement. It directly affects combustion completeness, flue gas mass flow rate, adiabatic flame temperature, and stack losses, making it a key operational control parameter in industrial boilers. This parameter is investigated to assess the trade-off between combustion stability and thermal efficiency. The excess air ratio is varied over the range

$$\lambda = [1.00, 1.05, 1.10, 1.15, 1.20, 1.30] [-], \quad (8.1)$$

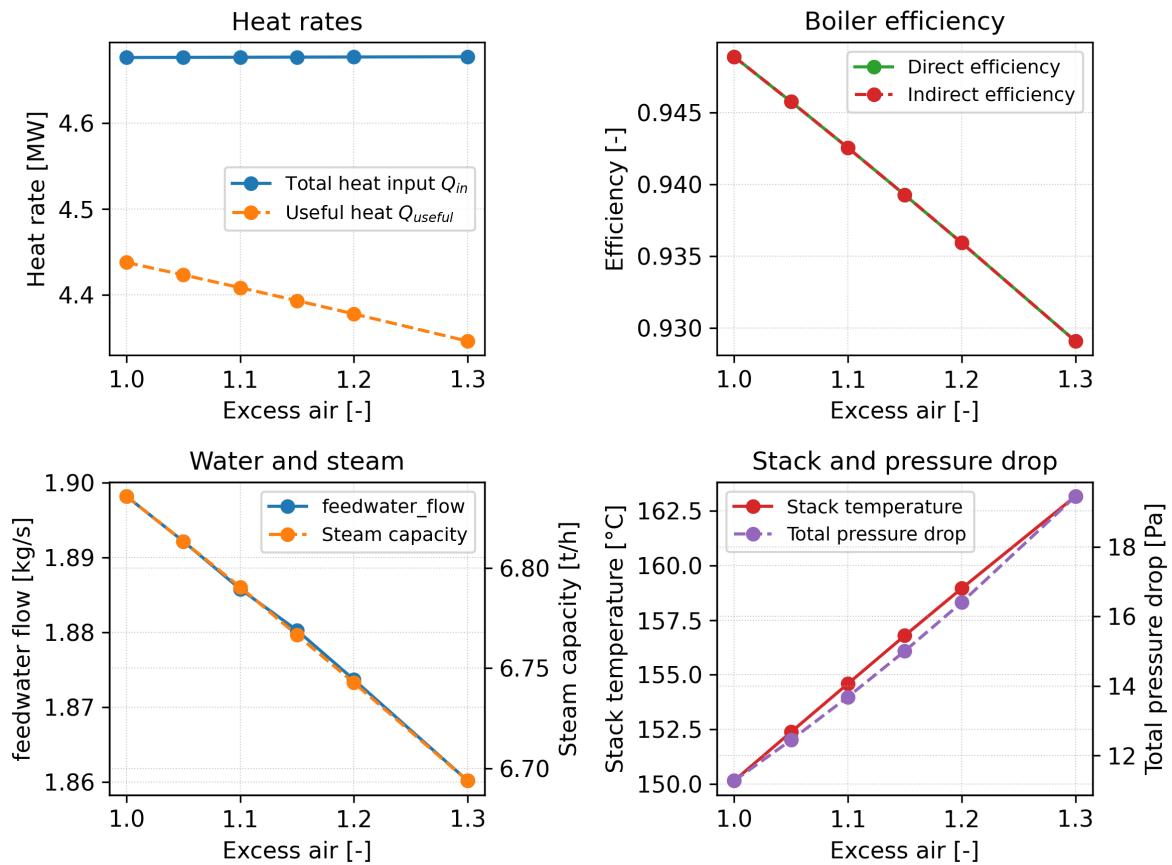


Figure 8.2: Boiler performance as a function of excess air factor

Increasing the excess air ratio increases flue-gas mass flow and sensible stack losses. As a result, boiler efficiency exhibits a maximum near the control value $\lambda = 1.05$, beyond which additional air primarily raises stack temperature and pressure losses without improving useful heat transfer.

Table 8.2: Excess air performance analysis.

excess air [-]	1.00	1.05	1.10	1.15	1.20	1.30
Fuel Mass Flow[Kg/S]	0.1	0.1	0.1	0.1	0.1	0.1
Air Flow[Kg/S]	1.61	1.69	1.77	1.85	1.93	2.09
Excess Air Ratio[-]	1	1.05	1.1	1.15	1.2	1.3
Feedwater Flow[Kg/S]	1.9	1.89	1.89	1.88	1.87	1.86
Steam Capacity[T/H]	6.84	6.81	6.79	6.77	6.74	6.69
η_{direct} [-]	0.95	0.95	0.94	0.94	0.94	0.93
η_{indirect} [-]	0.95	0.95	0.94	0.94	0.94	0.93
Stack Loss Fraction[-]	0.05	0.05	0.06	0.06	0.06	0.07
Q_Flue_Out[Mw]	0.24	0.25	0.27	0.28	0.3	0.33
conductance [MW/K]	0.01	0.01	0.01	0.01	0.01	0.01
input heat [MW]	4.68	4.68	4.68	4.68	4.68	4.68
useful heat [MW]	4.44	4.42	4.41	4.39	4.38	4.35
Q_Balance_Error[Mw]	-0	-0	-0	-0	-0	-0

excess air [-]	1.00	1.05	1.10	1.15	1.20	1.30
Pressure Drop Fric Total[Kpa]	-7.58	-8.35	-9.17	-10.05	-10.97	-12.97
Pressure Drop Minor Total[Kpa]	-3.7	-4.09	-4.51	-4.96	-5.44	-6.48
Pressure Drop Total[Kpa]	-11.28	-12.45	-13.69	-15.01	-16.4	-19.46
Water Pressure Drop Fric	-0.06	-0.06	-0.06	-0.06	-0.06	-0.05
Total[Kpa]						
Water Pressure Drop Minor	-0	-0	-0	-0	-0	-0
Total[Kpa]						
Water Pressure Drop Total[Kpa]	-0.06	-0.06	-0.06	-0.06	-0.06	-0.06
Lhv [Mj/Kg]	46.73	46.73	46.73	46.73	46.73	46.73
firing rate [MW]	4.67	4.67	4.67	4.67	4.67	4.67
adiabatic temperature [°C]	2052.36	1981.5	1915.54	1854.03	1796.53	1692.05
Stack Temperature[°C]	150.16	152.38	154.59	156.79	158.95	163.16
Feedwater Pressure[Kpa]	1000.06	1000.06	1000.06	1000.06	1000.06	1000.06
Drum Pressure[Kpa]	1000	1000	1000	1000	1000	1000

8.2.2 Influence of fuel mass flow

The fuel mass flow rate \dot{m}_{fuel} determines the firing rate of the boiler and therefore governs the total thermal input, flue gas temperature level, and achievable steam production capacity. It is a primary load-setting parameter in boiler operation and is investigated to evaluate how the system scales with increasing and decreasing demand. The fuel mass flow is varied according to

$$\dot{m}_{\text{fuel}} = [0.025, 0.050, 0.075, 0.10, 0.125] \frac{\text{kg}}{\text{s}}, = [25, 50, 75, 100, 125] \% \quad (8.2)$$

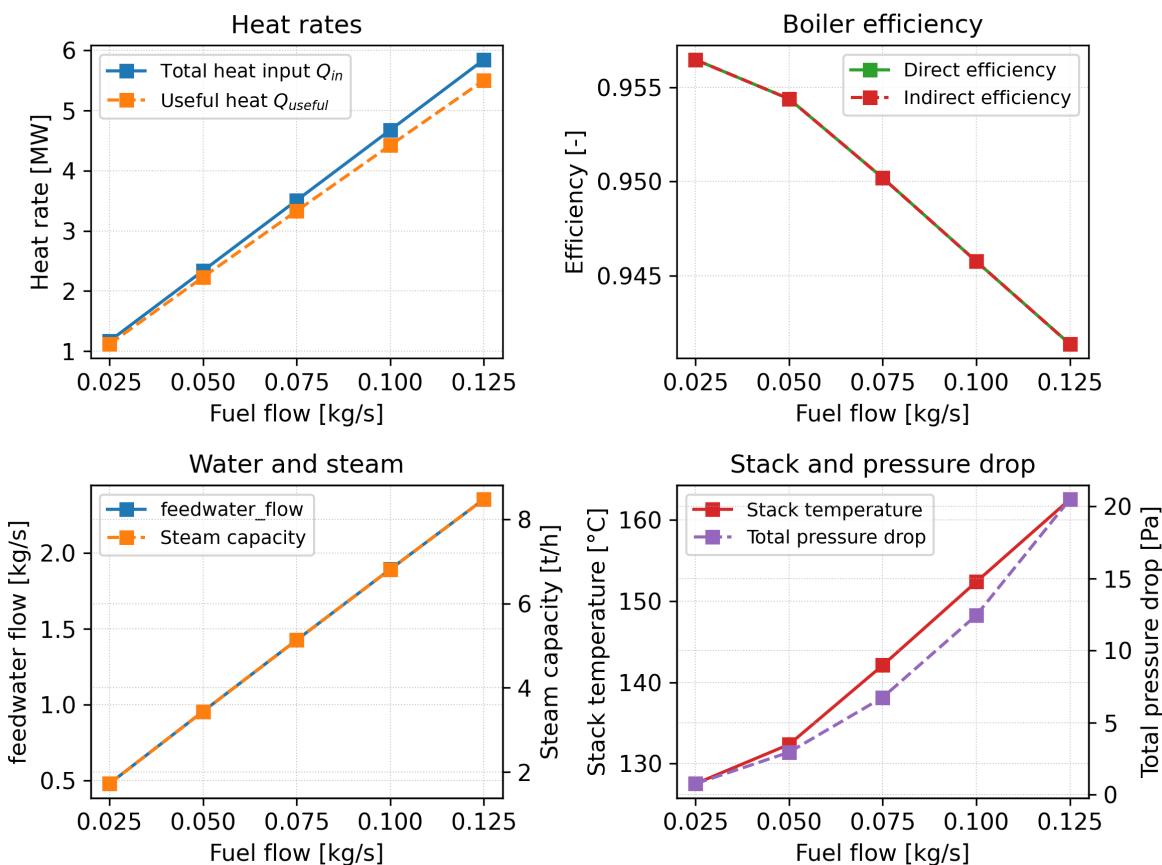


Figure 8.3: Boiler performance as a function of fuel mass flow

Steam capacity increases approximately linearly with fuel input, indicating that the available heat transfer surface is sufficient to absorb the additional duty. As the firing rate approaches the nominal design value, deviations from linearity become apparent, reflecting increasing limitations in heat transfer effectiveness rather than fuel input.

Table 8.3: Fuel flow performance analysis.

fuel flow [kg/s]	0.02	0.05	0.08	0.10	0.12
Fuel Mass Flow[Kg/S]	0.02	0.05	0.08	0.1	0.12
Air Flow[Kg/S]	0.42	0.85	1.27	1.69	2.11
Excess Air Ratio[-]	1.05	1.05	1.05	1.05	1.05
Feedwater Flow[Kg/S]	0.48	0.95	1.43	1.89	2.35
Steam Capacity[T/H]	1.72	3.44	5.13	6.81	8.48
η_{direct} [-]	0.96	0.95	0.95	0.95	0.94
η_{indirect} [-]	0.96	0.95	0.95	0.95	0.94
Stack Loss Fraction[-]	0.04	0.05	0.05	0.05	0.06
Q_Flue_Out[Mw]	0.05	0.11	0.17	0.25	0.34
conductance [MW/K]	0	0.01	0.01	0.01	0.01
input heat [MW]	1.17	2.34	3.51	4.68	5.85
useful heat [MW]	1.12	2.23	3.33	4.42	5.5
Q_Balance_Error[Mw]	-0	-0	-0	-0	-0
Pressure Drop Fric Total[Kpa]	-0.54	-2.02	-4.57	-8.35	-13.65
Pressure Drop Minor Total[Kpa]	-0.23	-0.93	-2.18	-4.09	-6.84
Pressure Drop Total[Kpa]	-0.77	-2.95	-6.75	-12.45	-20.49
Water Pressure Drop Fric Total[Kpa]	-0.01	-0.02	-0.03	-0.06	-0.11
Water Pressure Drop Minor	-0	-0	-0	-0	-0
Total[Kpa]					
Water Pressure Drop Total[Kpa]	-0.01	-0.02	-0.03	-0.06	-0.11
Lhv [Mj/Kg]	46.73	46.73	46.73	46.73	46.73
firing rate [MW]	1.17	2.34	3.5	4.67	5.84
adiabatic temperature [°C]	1981.5	1981.5	1981.5	1981.5	1981.5
Stack Temperature[°C]	127.53	132.36	142.11	152.38	162.54
Feedwater Pressure[Kpa]	1000.01	1000.02	1000.03	1000.06	1000.11
Drum Pressure[Kpa]	1000	1000	1000	1000	1000

8.2.3 Influence of drum pressure

The drum pressure P_{drum} determines the saturation temperature and latent heat of vaporization of water, thereby influencing steam generation characteristics and the available temperature driving force for heat transfer. This parameter is investigated to quantify how changes in operating pressure affect boiler efficiency, steam capacity, and stack temperature. The drum pressure is varied over the range

$$P_{\text{drum}} = [4.0, 10.0, 16.0] \text{ bar}, \quad (8.3)$$

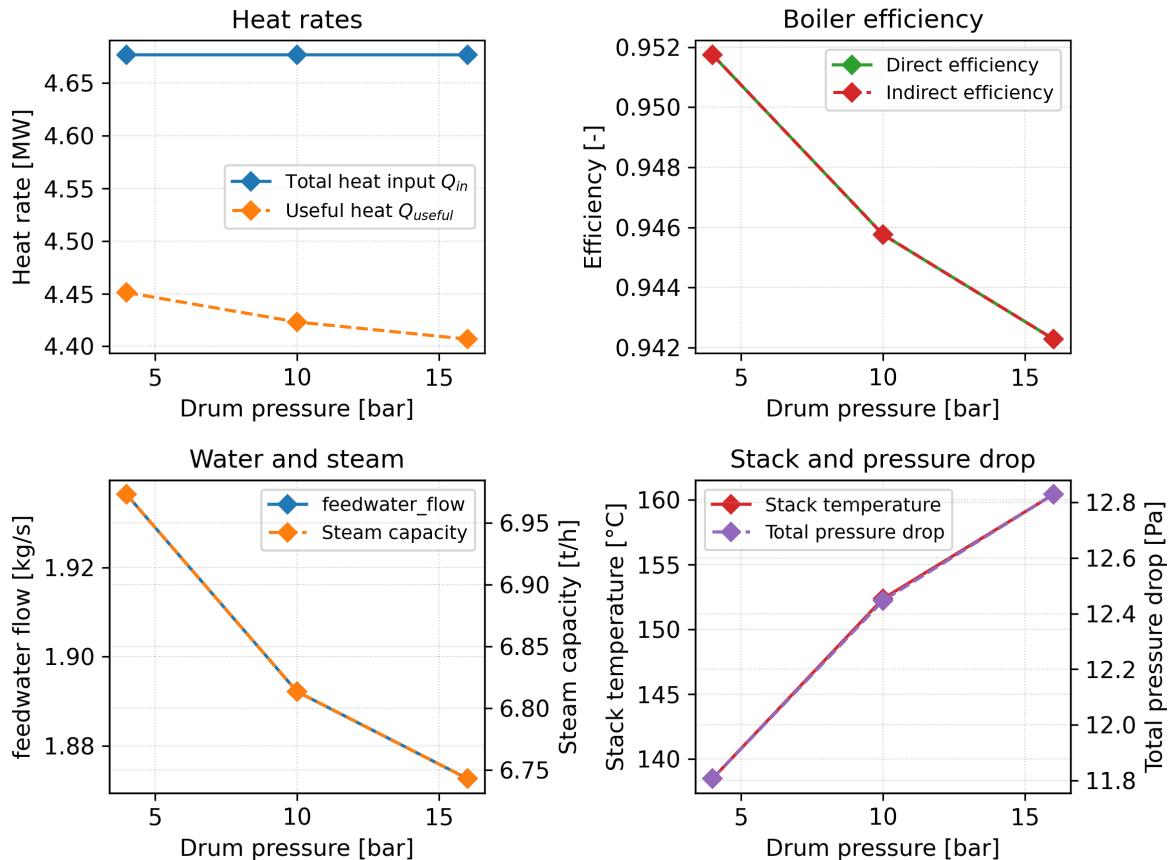


Figure 8.4: Boiler performance as a function of drum pressure

Increasing the drum pressure, allows a larger steam mass flow to be generated for the same absorbed thermal duty. The direct efficiency decreases, since higher water and steam temperatures reduce the available driving temperature difference on the gas side. Consistent with this, the stack temperature increases, indicating a diminished potential for further heat recovery.

Table 8.4: Drum pressure performance analysis.

drum pressure [bar]	4.00	10.00	16.00
Fuel Mass Flow[Kg/S]	0.1	0.1	0.1

drum pressure [bar]	4.00	10.00	16.00
Air Flow[Kg/S]	1.69	1.69	1.69
Excess Air Ratio[-]	1.05	1.05	1.05
Feedwater Flow[Kg/S]	1.94	1.89	1.87
Steam Capacity[T/H]	6.97	6.81	6.74
η_{direct} [-]	0.95	0.95	0.94
η_{indirect} [-]	0.95	0.95	0.94
Stack Loss Fraction[-]	0.05	0.05	0.06
Q_Flue_Out[Mw]	0.23	0.25	0.27
conductance [MW/K]	0.01	0.01	0.01
input heat [MW]	4.68	4.68	4.68
useful heat [MW]	4.45	4.42	4.41
Q_Balance_Error[Mw]	-0	-0	-0
Pressure Drop Fric Total[Kpa]	-7.91	-8.35	-8.62
Pressure Drop Minor Total[Kpa]	-3.9	-4.09	-4.21
Pressure Drop Total[Kpa]	-11.81	-12.45	-12.83
Water Pressure Drop Fric Total[Kpa]	-0.06	-0.06	-0.06
Water Pressure Drop Minor Total[Kpa]	-0	-0	-0
Water Pressure Drop Total[Kpa]	-0.06	-0.06	-0.06
Lhv [Mj/Kg]	46.73	46.73	46.73
firing rate [MW]	4.67	4.67	4.67
adiabatic temperature [°C]	1981.5	1981.5	1981.5
Stack Temperature[°C]	138.49	152.38	160.44
Feedwater Pressure[Kpa]	400.06	1000.06	1600.06
Drum Pressure[Kpa]	400	1000	1600

8.2.4 Influence of fouling

The fouling factor f represents the degradation of effective heat transfer performance caused by deposits on gas-side and water-side heat exchange surfaces during operation, as dimensionless fouling thickness multiplier. Fouling increases thermal resistance, reduces overall heat transfer coefficients, and can significantly impact efficiency and stack losses over time. This parameter is investigated to assess the sensitivity of boiler performance to surface degradation. The fouling factor is varied as

$$f = [0.5\times, 1\times, 2\times, 5\times, 10\times]. \quad (8.4)$$

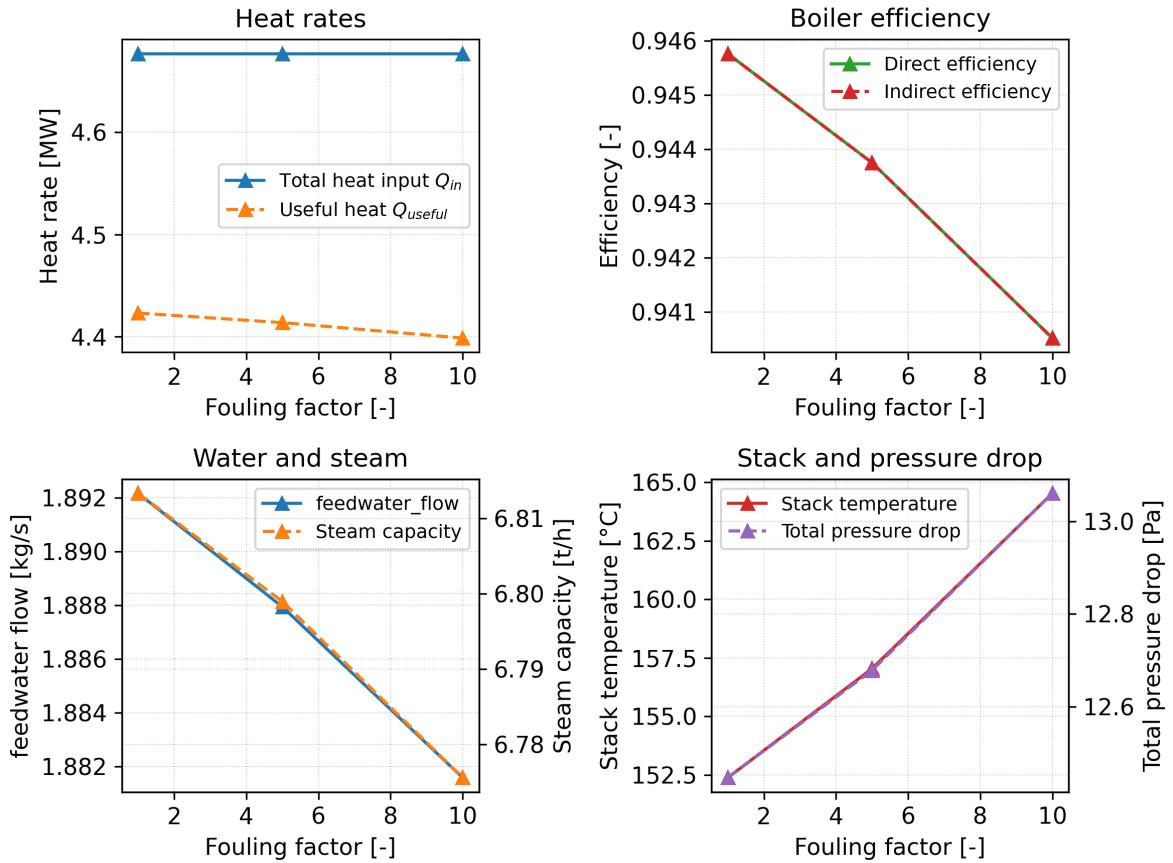


Figure 8.5: Boiler performance as a function of fouling factor

The effect of fouling is distributed across all stages, but its impact is most pronounced in the downstream convective sections where heat transfer is already limited by smaller temperature differences. As fouling increases, these sections lose effectiveness first.

While the boiler can continue to operate under fouled conditions, the results highlight the importance of maintaining clean heat transfer surfaces to ensure higher efficiency.

Table 8.5: Fouling performance analysis.

fouling [-]	1.00	5.00	10.00
Fuel Mass Flow[Kg/S]	0.1	0.1	0.1
Air Flow[Kg/S]	1.69	1.69	1.69
Excess Air Ratio[-]	1.05	1.05	1.05
Feedwater Flow[Kg/S]	1.89	1.89	1.88
Steam Capacity[T/H]	6.81	6.8	6.78
η_{direct} [-]	0.95	0.94	0.94
η_{indirect} [-]	0.95	0.94	0.94
Stack Loss Fraction[-]	0.05	0.06	0.06
Q_Flue_Out[Mw]	0.25	0.26	0.28
conductance [MW/K]	0.01	0.01	0.01
input heat [MW]	4.68	4.68	4.68
useful heat [MW]	4.42	4.41	4.4
Q_Balance_Error[Mw]	-0	-0	-0
Pressure Drop Fric Total[Kpa]	-8.35	-8.51	-8.77
Pressure Drop Minor Total[Kpa]	-4.09	-4.17	-4.29
Pressure Drop Total[Kpa]	-12.45	-12.68	-13.06
Water Pressure Drop Fric Total[Kpa]	-0.06	-0.06	-0.06
Water Pressure Drop Minor Total[Kpa]	-0	-0	-0
Water Pressure Drop Total[Kpa]	-0.06	-0.06	-0.06
Lhv [Mj/Kg]	46.73	46.73	46.73
firing rate [MW]	4.67	4.67	4.67
adiabatic temperature [°C]	1981.5	1981.5	1981.5
Stack Temperature[°C]	152.38	157.04	164.53
Feedwater Pressure[Kpa]	1000.06	1000.06	1000.06
Drum Pressure[Kpa]	1000	1000	1000

8.3 Conclusions from performance analysis

This section summarizes the main findings of the parametric performance analysis and highlights the relative influence of key operating parameters on boiler behavior and efficiency.

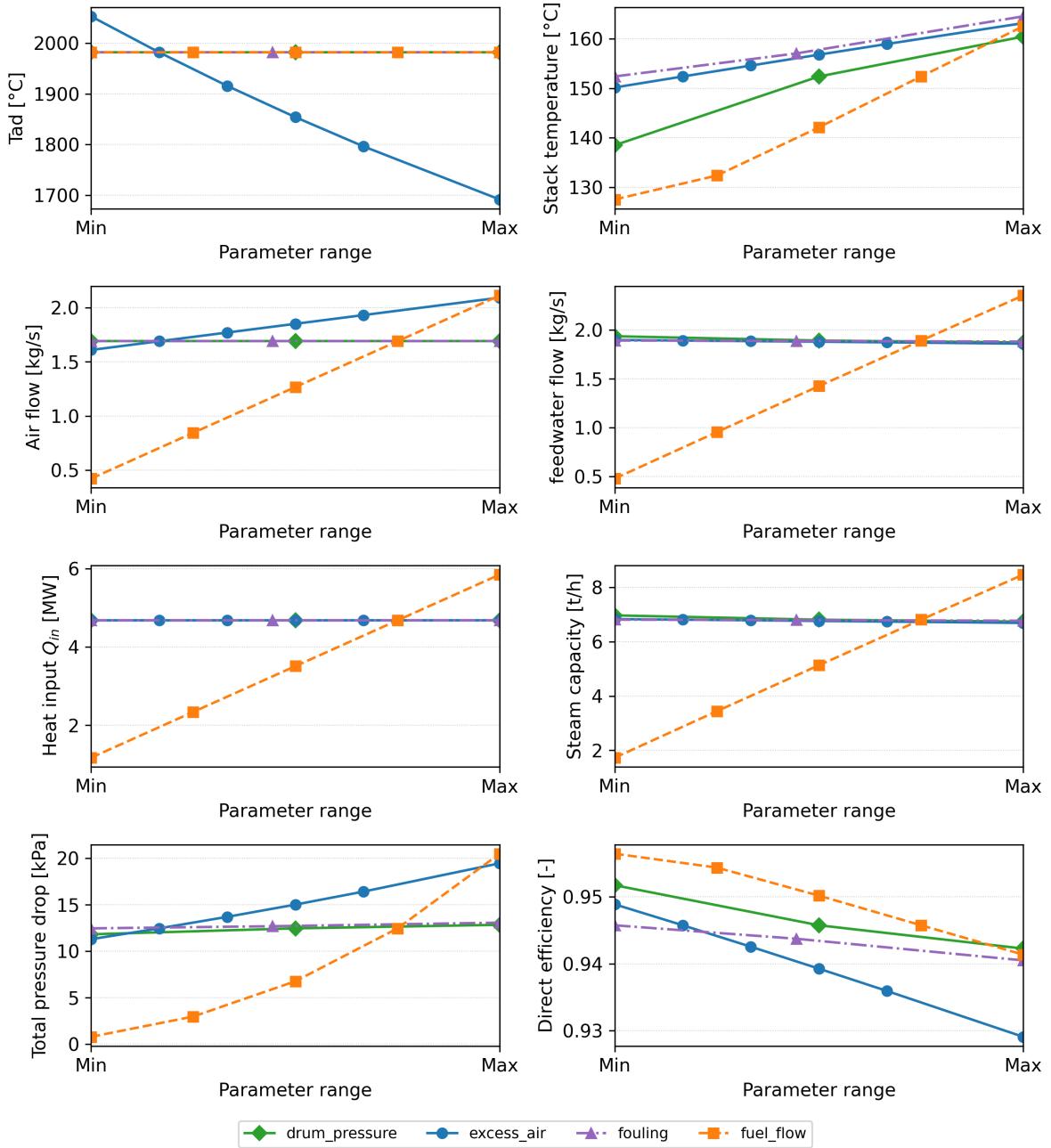


Figure 8.6: Overview of key boiler performance indicators for all parameter groups

Overall, the results show that fuel flow is the dominant factor affecting boiler performance. Increasing fuel flow strongly increases heat input, steam production, stack temperature, pressure drop, and leads to a noticeable reduction in direct efficiency at higher values. In contrast, changes in excess air, drum pressure, and fouling mainly cause smaller, secondary shifts, primarily influencing stack temperature and efficiency, but leave most other boiler variables relatively unchanged.

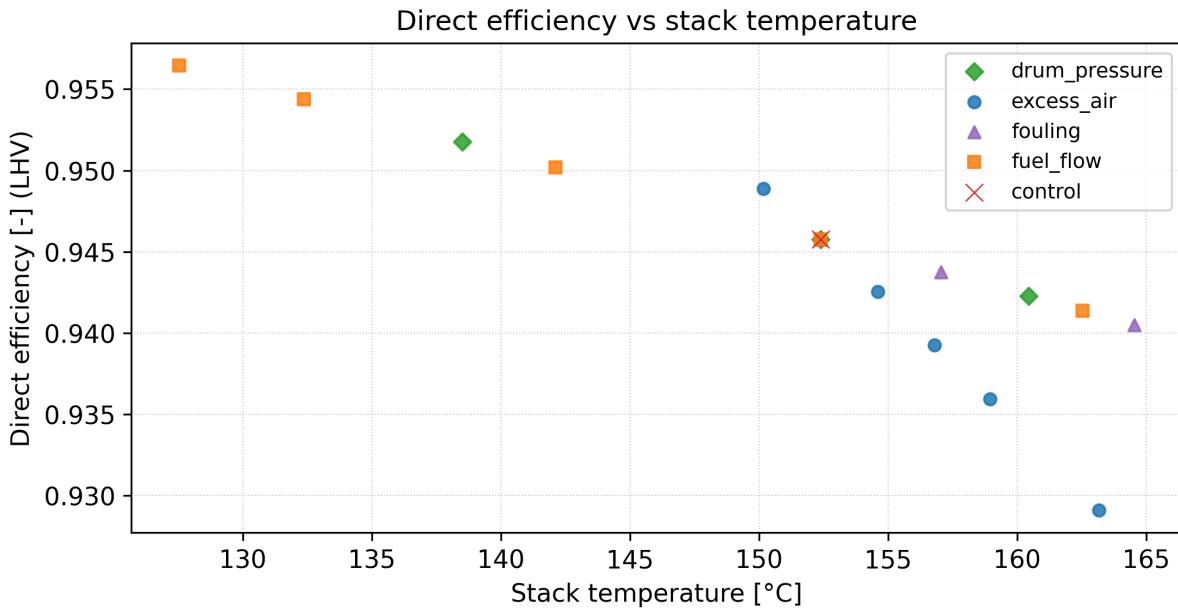


Figure 8.7: Scatter diagram showing stack temperature and direct efficiency

The parametric analysis demonstrates that the developed boiler model captures physically consistent trends across a wide range of operating conditions.

The excess air ratio is identified as the most influential parameter affecting boiler efficiency, primarily through its control of flue-gas mass flow, adiabatic flame temperature, and stack losses. An efficiency optimum is observed near the nominal excess air setting, consistent with industrial practice.

Fuel mass flow primarily scales the thermal duty and steam production rate, with efficiency remaining nearly constant over the investigated range. This indicates that, within practical limits, the available heat transfer surface is sufficient to accommodate load variations without significant degradation in performance.

Drum pressure mainly influences steam generation through changes in latent heat and saturation temperature, while its effect on overall efficiency is secondary. Higher pressures reduce the temperature driving force for heat transfer, resulting in elevated stack temperatures.

Fouling degrades heat transfer effectiveness across all stages, with the strongest impact observed in downstream convective sections. The results highlight the importance of maintaining clean heat transfer surfaces to preserve efficiency and minimize stack losses.

Overall, the analysis confirms that the coupled combustion–heat transfer–hydraulic framework provides a robust tool for evaluating operational trade-offs and identifying efficiency-critical parameters in industrial fire tube shell boilers.

Chapter 9

Summary

This thesis presented a physics based modelling framework for a three pass fire tube industrial shell boiler, integrating combustion, heat transfer, and hydraulic behavior within a single tool. The model was implemented in Python and structured around a one dimensional marching solver that resolves gas side and water/steam side processes consistently along the boiler flow path.

The developed framework couples three main sub models:

- A detailed fuel air combustion model.
- Heat transfer is resolved across six sequential gas side stages.
- Gas side pressure losses are computed concurrently with heat transfer, Water side pressure losses are evaluated for the economizer circuit.

The performance analysis demonstrates that boiler efficiency is most sensitive to the excess air ratio, which directly controls flue gas mass flow, adiabatic flame temperature, and stack losses. The firing rate primarily governs the absolute thermal duty and steam production. Drum pressure mainly influences steam quantity through its effect on latent heat and saturation temperature, while having only a secondary impact on overall thermal efficiency; higher pressures reduce the available temperature driving force, elevating stack temperatures.

Across all cases, the coupled model captures the interplay between combustion conditions, heat transfer effectiveness, and hydraulic constraints, providing a physically consistent basis for assessing operational trade offs and identifying efficiency critical control parameters in industrial fire tube boilers.

Appendix A

config and input

The following tables show all variables given by the user to the program.

Air Properties (*config/air.yaml*)

Table A.1: Air parameters.

Quantity / Species	Symbol	Value	Units
Temperature	T	300.0	K
Pressure	P	101325	Pa
Oxygen (molar fraction)	x_{O_2}	0.23067	(–)
Nitrogen (molar fraction)	x_{N_2}	0.755866	(–)
Argon (molar fraction)	x_{Ar}	0.01287	(–)
Carbon dioxide (molar fraction)	x_{CO_2}	0.000594	(–)
Water vapour (molar fraction)	x_{H_2O}	0.0	(–)

Drum Geometry and Wall Properties (*config/drum.yaml*)

Table A.2: Drum parameters.

Quantity	Symbol	Value	Units
Inner diameter	D_{drum}	4.5	m
Length	L_{drum}	5.0	m
Wall thickness	δ_{wall}	0.05	m
Wall thermal conductivity	k_{wall}	40	$W m^{-1} K^{-1}$
Inner surface roughness	ε	5	μm
Inner surface emissivity	ε_r	0.80	(–)

Quantity	Symbol	Value	Units
Fouling thickness	δ_f	1.0×10^{-4}	m
Fouling conductivity	k_f	0.2	$\text{W m}^{-1} \text{K}^{-1}$

Fuel Properties (*config/fuel.yaml*)

Table A.3: Fuel parameters.

Quantity / Species	Symbol	Value	Units
Temperature	T	300.0	K
Pressure	P	101325	Pa
Mass flow rate	\dot{m}_{fuel}	0.1	kg s^{-1}
Methane (molar fraction)	CH_4	0.849546	(—)
Ethane (molar fraction)	C_2H_6	0.061889	(—)
Propane (molar fraction)	C_3H_8	0.020597	(—)
Butane (molar fraction)	C_4H_{10}	0.005154	(—)
Hydrogen sulfide (molar fraction)	H_2S	0.000103	(—)
Nitrogen (molar fraction)	N_2	0.041293	(—)
Carbon dioxide (molar fraction)	CO_2	0.016418	(—)
Water (molar fraction)	H_2O	0.005	(—)
Argon (molar fraction)	Ar	0.0	(—)

Operating Conditions (*config/operation.yaml*)

Table A.4: Operation parameters.

Quantity	Symbol	Value	Units
Excess air ratio	λ	1.05	(—)
Drum pressure	P_{drum}	10	bar

Heat Exchange Stages (*config/stages.yaml*)

Table A.5: Stages parameters.

Quantity	Symbol	HX-1	HX-2	HX-3	HX-4	HX-5	HX-6	Units
Inner diameter	D_i	1.4	1.6	0.076	1.6	0.076	0.0250	m
Inner / tube length	L_i, L	5.276	0.8	4.975	0.8	5.620	80	m
Wall thickness	δ	0.02	0.02	0.02	0.02	0.02	0.02	m
Thermal conductivity	k	50	50	50	50	50	50	$\text{W m}^{-1} \text{K}^{-1}$
Curvature radius	R	—	0.8	—	0.8	—	—	m
Number of tubes	N	—	—	118	—	100	120	(—)
Number of rows	N_{rows}	—	—	6	—	6	26	(—)
Transverse pitch	S_T	—	—	0.11	—	0.11	0.075	m
Longitudinal pitch	S_L	—	—	0.11	—	0.11	0.08	m
Baffle spacing	B	—	—	0.45	—	0.45	0.15	m
Baffle cut	c	—	—	0.25	—	0.25	0.25	(—)
Bundle clearance	—	—	—	0.010	—	0.010	0.010	m
Shell inner diameter	D_{shell}	—	—	—	—	—	0.6	m
Hot inlet loss	$K_{\text{hot,in}}$	0.5	—	0.5	—	0.5	0.5	(—)
Hot outlet loss	$K_{\text{hot,out}}$	0.0	—	1.0	—	1.0	1.0	(—)
Hot bend loss	$K_{\text{hot,bend}}$	0.0	0.3	—	0.3	—	—	(—)
Cold inlet loss	$K_{\text{cold,in}}$	0.0	—	—	—	—	0.5	(—)
Cold outlet loss	$K_{\text{cold,out}}$	0.0	—	—	—	—	1.0	(—)
Cold bend loss	$K_{\text{cold,bend}}$	0.0	—	—	—	—	0.3	(—)

Water Properties (*config/water.yaml*)

Table A.6: Water parameters.

Quantity	Symbol	Value	Units
Specific enthalpy	h	4.40×10^5	J kg^{-1}
Composition	$x_{\text{H}_2\text{O}}$	1.0	(–)

Appendix B

Results Summary

B.1 Boiler Results

The following pages show the full results tables, for boiler key performance indices, including the control case and all other iterations.

Appendix: Boiler KPIs – All Runs

KPI columns 1/4

run	param_group	param_value	fuel mass flow [kg/s]	air flow [kg/s]	excess air ratio [-]	feedwater flow [kg/s]	steam capacity [t/h]	eta direct [-]	eta indirect [-]
default_case	control		0.1	1.69026	1.05	1.89217	6.81335	0.945761	0.945761
drum_pressure_4.0bar	drum_pressure	4	0.1	1.69026	1.05	1.93638	6.97293	0.951746	0.951746
drum_pressure_10.0bar	drum_pressure	10	0.1	1.69026	1.05	1.89217	6.81335	0.945761	0.945761
drum_pressure_16.0bar	drum_pressure	16	0.1	1.69026	1.05	1.87266	6.74283	0.942282	0.942282
excess_air_1.0	excess_air	1	0.1	1.60977	1	1.89818	6.83583	0.948896	0.948896
excess_air_1.05	excess_air	1.05	0.1	1.69026	1.05	1.89217	6.81335	0.945761	0.945761
excess_air_1.1	excess_air	1.1	0.1	1.77075	1.1	1.8858	6.7905	0.942557	0.942557
excess_air_1.15	excess_air	1.15	0.1	1.85124	1.15	1.88027	6.76653	0.939278	0.939278
excess_air_1.2	excess_air	1.2	0.1	1.93173	1.2	1.87368	6.7427	0.935943	0.935943
excess_air_1.3	excess_air	1.3	0.1	2.0927	1.3	1.86019	6.69377	0.929098	0.929098
fouling_1	fouling	1	0.1	1.69026	1.05	1.89217	6.81335	0.945761	0.945761
fouling_5	fouling	5	0.1	1.69026	1.05	1.88795	6.79898	0.94375	0.94375
fouling_10	fouling	10	0.1	1.69026	1.05	1.88158	6.77559	0.940513	0.940513
fuel_flow_0.025kgs	fuel_flow	0.025	0.025	0.422565	1.05	0.477867	1.7229	0.956457	0.956457
fuel_flow_0.05kgs	fuel_flow	0.05	0.05	0.845131	1.05	0.954431	3.43788	0.95438	0.95438
fuel_flow_0.075kgs	fuel_flow	0.075	0.075	1.2677	1.05	1.42556	5.13406	0.950189	0.950189
fuel_flow_0.1kgs	fuel_flow	0.1	0.1	1.69026	1.05	1.89217	6.81335	0.945761	0.945761
fuel_flow_0.125kgs	fuel_flow	0.125	0.125	2.11283	1.05	2.35408	8.47728	0.941374	0.941374

KPI columns 2/4

run	param_group	param_value	Stack loss fraction [-]	Q_flue_out [MW]	UA [MW/K]	Q_in total [MW]	Q_useful [MW]	Q_balance_error [MW]	pressure drop friction total [kPa]
default_case	control		0.0542386	0.25366	0.0105003	4.67675	4.42309	-0.000120622	-8.35417
drum_pressure_4.0bar	drum_pressure	4	0.0482544	0.225674	0.0103183	4.67675	4.45108	-0.000120623	-7.90743
drum_pressure_10.0bar	drum_pressure	10	0.0542386	0.25366	0.0105003	4.67675	4.42309	-0.000120622	-8.35417
drum_pressure_16.0bar	drum_pressure	16	0.0577177	0.269931	0.0106355	4.67675	4.40682	-0.000120622	-8.62182
excess_air_1.0	excess_air	1	0.0511038	0.238992	0.0103366	4.6766	4.43761	-0.000120313	-7.58097
excess_air_1.05	excess_air	1.05	0.0542386	0.25366	0.0105003	4.67675	4.42309	-0.000120622	-8.35417
excess_air_1.1	excess_air	1.1	0.057443	0.268655	0.0106391	4.6769	4.40824	-0.000120904	-9.17493
excess_air_1.15	excess_air	1.15	0.0607221	0.284	0.0107812	4.67705	4.39305	-0.000121165	-10.0454
excess_air_1.2	excess_air	1.2	0.0640575	0.29961	0.0109219	4.6772	4.37759	-0.000121404	-10.9667
excess_air_1.3	excess_air	1.3	0.0709018	0.331643	0.0111794	4.6775	4.34586	-0.000121822	-12.9711
fouling_1	fouling	1	0.0542386	0.25366	0.0105003	4.67675	4.42309	-0.000120622	-8.35417
fouling_5	fouling	5	0.0562497	0.263066	0.0100044	4.67675	4.41368	-0.000120628	-8.51203
fouling_10	fouling	10	0.0594867	0.278204	0.00940156	4.67675	4.39855	-0.000120609	-8.77456
fuel_flow_0.025kgs	fuel_flow	0.025	0.0435434	0.0509104	0.00374832	1.16919	1.11828	-3.01561e-05	-0.542363
fuel_flow_0.05kgs	fuel_flow	0.05	0.0456202	0.106677	0.00662273	2.33837	2.2317	-6.03094e-05	-2.02449
fuel_flow_0.075kgs	fuel_flow	0.075	0.0498112	0.174716	0.00868244	3.50756	3.33285	-9.04667e-05	-4.57141
fuel_flow_0.1kgs	fuel_flow	0.1	0.0542386	0.25366	0.0105003	4.67675	4.42309	-0.000120622	-8.35417
fuel_flow_0.125kgs	fuel_flow	0.125	0.0586258	0.342723	0.0121564	5.84594	5.50321	-0.000150773	-13.6466

KPI columns 3/4

run	param_group	param_value	pressure drop minor total [kPa]	pressure drop total [kPa]	water pressure drop fric total [kPa]	water pressure drop minor total [kPa]	water pressure drop total [kPa]	LHV [kJ/kg]	P-LHV [MW]
default_case	control	-4.09237	-12.4465	-0.0559112	-0.000981025	-0.0568922	46731	4.6731	
drum_pressure_4.0bar	drum_pressure	4	-3.89966	-11.8071	-0.0583874	-0.00102521	-0.0594126	46731	4.6731
drum_pressure_10.0bar	drum_pressure	10	-4.09237	-12.4465	-0.0559112	-0.000981025	-0.0568922	46731	4.6731
drum_pressure_16.0bar	drum_pressure	16	-4.20651	-12.8283	-0.0550437	-0.000962062	-0.0560058	46731	4.6731
excess_air_1.0	excess_air	1	-3.6978	-11.2788	-0.0561612	-0.000986843	-0.0571481	46731	4.6731
excess_air_1.05	excess_air	1.05	-4.09237	-12.4465	-0.0559112	-0.000981025	-0.0568922	46731	4.6731
excess_air_1.1	excess_air	1.1	-4.51307	-13.688	-0.0556276	-0.000974849	-0.0566025	46731	4.6731
excess_air_1.15	excess_air	1.15	-4.96132	-15.0067	-0.0554122	-0.000969562	-0.0563817	46731	4.6731
excess_air_1.2	excess_air	1.2	-5.43822	-16.405	-0.0551056	-0.000963195	-0.0560688	46731	4.6731
excess_air_1.3	excess_air	1.3	-6.48472	-19.4558	-0.0544629	-0.000950212	-0.0554131	46731	4.6731
fouling_1	fouling	1	-4.09237	-12.4465	-0.0559112	-0.000981025	-0.0568922	46731	4.6731
fouling_5	fouling	5	-4.16622	-12.6782	-0.0564279	-0.000977851	-0.0574058	46731	4.6731
fouling_10	fouling	10	-4.28569	-13.0603	-0.0573099	-0.00097325	-0.0582832	46731	4.6731
fuel_flow_0.025kgs	fuel_flow	0.025	-0.225954	-0.768317	-0.00855037	-6.25129e-05	-0.00861288	46731	1.16827
fuel_flow_0.05kgs	fuel_flow	0.05	-0.92787	-2.95236	-0.0170261	-0.000249509	-0.0172756	46731	2.33655
fuel_flow_0.075kgs	fuel_flow	0.075	-2.18072	-6.75214	-0.0272303	-0.000556733	-0.0277871	46731	3.50482
fuel_flow_0.1kgs	fuel_flow	0.1	-4.09237	-12.4465	-0.0559112	-0.000981025	-0.0568922	46731	4.6731
fuel_flow_0.125kgs	fuel_flow	0.125	-6.84049	-20.4871	-0.107079	-0.00151877	-0.108598	46731	5.84137

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run	param_group	param_value	Tad [°C]	stack temperature [°C]	feedwater pressure [kPa]	drum pressure [kPa]
default_case	control		1981.5	152.384	1000.06	1000
drum_pressure_4.0bar	drum_pressure	4	1981.5	138.492	400.059	400
drum_pressure_10.0bar	drum_pressure	10	1981.5	152.384	1000.06	1000
drum_pressure_16.0bar	drum_pressure	16	1981.5	160.44	1600.06	1600
excess_air_1.0	excess_air	1	2052.36	150.157	1000.06	1000
excess_air_1.05	excess_air	1.05	1981.5	152.384	1000.06	1000
excess_air_1.1	excess_air	1.1	1915.54	154.591	1000.06	1000
excess_air_1.15	excess_air	1.15	1854.03	156.792	1000.06	1000
excess_air_1.2	excess_air	1.2	1796.53	158.95	1000.06	1000
excess_air_1.3	excess_air	1.3	1692.05	163.161	1000.06	1000
fouling_1	fouling	1	1981.5	152.384	1000.06	1000
fouling_5	fouling	5	1981.5	157.043	1000.06	1000
fouling_10	fouling	10	1981.5	164.531	1000.06	1000
fuel_flow_0.025kgs	fuel_flow	0.025	1981.5	127.526	1000.01	1000
fuel_flow_0.05kgs	fuel_flow	0.05	1981.5	132.364	1000.02	1000
fuel_flow_0.075kgs	fuel_flow	0.075	1981.5	142.11	1000.03	1000
fuel_flow_0.1kgs	fuel_flow	0.1	1981.5	152.384	1000.06	1000
fuel_flow_0.125kgs	fuel_flow	0.125	1981.5	162.541	1000.11	1000

B.2 Stages Results

The following pages show the full results tables, for boiler stages, including the control case and all other iterations.

Appendix: Stages Summary – All Runs

Columns slice 1/4

run	param_group	param_value	stage	kind	gas in pressure [kPa]	gas in temp [°C]	gas in enthalpy [kJ/kg]	gas out pressure [kPa]	gas out temp [°C]	gas out enthalpy [kJ/kg]	water in temp [°C]
default_case	control		HX_1	single_tube	101.325	1981.25	2612.29	101.322	860.869	1014.02	179.886
default_case	control		HX_2	reversal_chamber	101.322	860.869	1014.02	101.322	804.137	938.904	179.886
default_case	control		HX_3	tube_bank	101.322	804.137	938.904	101.274	332.777	349.389	179.886
default_case	control		HX_4	reversal_chamber	101.274	332.777	349.389	101.274	328.165	343.961	179.886
default_case	control		HX_5	tube_bank	101.274	328.165	343.961	101.228	220.508	219.062	179.886
default_case	control		HX_6	economiser	101.228	220.508	219.062	88.8785	152.384	141.687	104.795
drum_pressure_4.0bar	drum_pressure	4	HX_1	single_tube	101.325	1981.25	2612.29	101.322	864.013	1018.2	143.613
drum_pressure_4.0bar	drum_pressure	4	HX_2	reversal_chamber	101.322	864.013	1018.2	101.322	806.98	942.651	143.613
drum_pressure_4.0bar	drum_pressure	4	HX_3	tube_bank	101.322	806.98	942.651	101.275	310.843	323.634	143.613
drum_pressure_4.0bar	drum_pressure	4	HX_4	reversal_chamber	101.275	310.843	323.634	101.275	306.425	318.465	143.613
drum_pressure_4.0bar	drum_pressure	4	HX_5	tube_bank	101.275	306.425	318.465	101.231	189.555	183.755	143.613
drum_pressure_4.0bar	drum_pressure	4	HX_6	economiser	101.231	189.555	183.755	89.5179	138.492	126.054	104.901
drum_pressure_10.0bar	drum_pressure	10	HX_1	single_tube	101.325	1981.25	2612.29	101.322	860.869	1014.02	179.886
drum_pressure_10.0bar	drum_pressure	10	HX_2	reversal_chamber	101.322	860.869	1014.02	101.322	804.137	938.904	179.886
drum_pressure_10.0bar	drum_pressure	10	HX_3	tube_bank	101.322	804.137	938.904	101.274	332.777	349.389	179.886
drum_pressure_10.0bar	drum_pressure	10	HX_4	reversal_chamber	101.274	332.777	349.389	101.274	328.165	343.961	179.886
drum_pressure_10.0bar	drum_pressure	10	HX_5	tube_bank	101.274	328.165	343.961	101.228	220.508	219.062	179.886
drum_pressure_10.0bar	drum_pressure	10	HX_6	economiser	101.228	220.508	219.062	88.8785	152.384	141.687	104.795
drum_pressure_16.0bar	drum_pressure	16	HX_1	single_tube	101.325	1981.25	2612.29	101.322	859.482	1012.17	201.378
drum_pressure_16.0bar	drum_pressure	16	HX_2	reversal_chamber	101.322	859.482	1012.17	101.322	802.962	937.357	201.378
drum_pressure_16.0bar	drum_pressure	16	HX_3	tube_bank	101.322	802.962	937.357	101.274	346.03	365.02	201.378
drum_pressure_16.0bar	drum_pressure	16	HX_4	reversal_chamber	101.274	346.03	365.02	101.273	341.316	359.454	201.378
drum_pressure_16.0bar	drum_pressure	16	HX_5	tube_bank	101.273	341.316	359.454	101.225	239.007	240.286	201.378
drum_pressure_16.0bar	drum_pressure	16	HX_6	economiser	101.225	239.007	240.286	88.4967	160.44	150.775	104.69
excess_air_1.0	excess_air	1	HX_1	single_tube	101.325	2052.16	2735.17	101.323	848.134	1002.25	179.886
excess_air_1.0	excess_air	1	HX_2	reversal_chamber	101.323	848.134	1002.25	101.322	791.07	926.426	179.886
excess_air_1.0	excess_air	1	HX_3	tube_bank	101.322	791.07	926.426	101.279	326.567	343.657	179.886
excess_air_1.0	excess_air	1	HX_4	reversal_chamber	101.279	326.567	343.657	101.279	322.002	338.268	179.886
excess_air_1.0	excess_air	1	HX_5	tube_bank	101.279	322.002	338.268	101.236	218.196	217.375	179.886
excess_air_1.0	excess_air	1	HX_6	economiser	101.236	218.196	217.375	90.0462	150.157	139.778	104.795
excess_air_1.05	excess_air	1.05	HX_1	single_tube	101.325	1981.25	2612.29	101.322	860.869	1014.02	179.886
excess_air_1.05	excess_air	1.05	HX_2	reversal_chamber	101.322	860.869	1014.02	101.322	804.137	938.904	179.886
excess_air_1.05	excess_air	1.05	HX_3	tube_bank	101.322	804.137	938.904	101.274	332.777	349.389	179.886
excess_air_1.05	excess_air	1.05	HX_4	reversal_chamber	101.274	332.777	349.389	101.274	328.165	343.961	179.886

run	param_group	param_value	stage	kind	gas in pressure [kpa]	gas in temp [°C]	gas in enthalpy [kJ/kg]	gas out pressure [kpa]	gas out temp [°C]	gas out enthalpy [kJ/kg]	water in temp [°C]
excess_air_1.05	excess_air	1.05	HX_5	tube_bank	101.274	328.165	343.961	101.228	220.508	219.062	179.886
excess_air_1.05	excess_air	1.05	HX_6	economiser	101.228	220.508	219.062	88.8785	152.384	141.687	104.795
excess_air_1.1	excess_air	1.1	HX_1	single_tube	101.325	1915.3	2499.98	101.322	872.375	1024.46	179.886
excess_air_1.1	excess_air	1.1	HX_2	reversal_chamber	101.322	872.375	1024.46	101.322	816.115	950.217	179.886
excess_air_1.1	excess_air	1.1	HX_3	tube_bank	101.322	816.115	950.217	101.269	338.75	354.922	179.886
excess_air_1.1	excess_air	1.1	HX_4	reversal_chamber	101.269	338.75	354.922	101.269	334.099	349.465	179.886
excess_air_1.1	excess_air	1.1	HX_5	tube_bank	101.269	334.099	349.465	101.218	222.78	220.763	179.886
excess_air_1.1	excess_air	1.1	HX_6	economiser	101.218	222.78	220.763	87.637	154.591	143.606	104.795
excess_air_1.15	excess_air	1.15	HX_1	single_tube	101.325	1853.8	2396.93	101.322	882.662	1033.56	179.886
excess_air_1.15	excess_air	1.15	HX_2	reversal_chamber	101.322	882.662	1033.56	101.322	827.011	960.352	179.886
excess_air_1.15	excess_air	1.15	HX_3	tube_bank	101.322	827.011	960.352	101.264	344.477	360.239	179.886
excess_air_1.15	excess_air	1.15	HX_4	reversal_chamber	101.264	344.477	360.239	101.264	339.795	354.762	179.886
excess_air_1.15	excess_air	1.15	HX_5	tube_bank	101.264	339.795	354.762	101.209	225.006	222.465	179.886
excess_air_1.15	excess_air	1.15	HX_6	economiser	101.209	225.006	222.465	86.3183	156.792	145.547	104.795
excess_air_1.2	excess_air	1.2	HX_1	single_tube	101.325	1796.3	2302.05	101.322	891.745	1041.32	179.886
excess_air_1.2	excess_air	1.2	HX_2	reversal_chamber	101.322	891.745	1041.32	101.322	836.83	969.305	179.886
excess_air_1.2	excess_air	1.2	HX_3	tube_bank	101.322	836.83	969.305	101.259	349.949	365.327	179.886
excess_air_1.2	excess_air	1.2	HX_4	reversal_chamber	101.259	349.949	365.327	101.259	345.245	359.837	179.886
excess_air_1.2	excess_air	1.2	HX_5	tube_bank	101.259	345.245	359.837	101.199	227.179	224.156	179.886
excess_air_1.2	excess_air	1.2	HX_6	economiser	101.199	227.179	224.156	84.92	158.95	147.464	104.795
excess_air_1.3	excess_air	1.3	HX_1	single_tube	101.325	1691.83	2133.18	101.322	906.389	1052.91	179.886
excess_air_1.3	excess_air	1.3	HX_2	reversal_chamber	101.322	906.389	1052.91	101.321	853.299	983.692	179.886
excess_air_1.3	excess_air	1.3	HX_3	tube_bank	101.321	853.299	983.692	101.248	360.105	374.762	179.886
excess_air_1.3	excess_air	1.3	HX_4	reversal_chamber	101.248	360.105	374.762	101.248	355.382	369.274	179.886
excess_air_1.3	excess_air	1.3	HX_5	tube_bank	101.248	355.382	369.274	101.178	231.351	227.466	179.886
excess_air_1.3	excess_air	1.3	HX_6	economiser	101.178	231.351	227.466	81.8692	163.161	151.247	104.795
fouling_1	fouling	1	HX_1	single_tube	101.325	1981.25	2612.29	101.322	860.869	1014.02	179.886
fouling_1	fouling	1	HX_2	reversal_chamber	101.322	860.869	1014.02	101.322	804.137	938.904	179.886
fouling_1	fouling	1	HX_3	tube_bank	101.322	804.137	938.904	101.274	332.777	349.389	179.886
fouling_1	fouling	1	HX_4	reversal_chamber	101.274	332.777	349.389	101.274	328.165	343.961	179.886
fouling_1	fouling	1	HX_5	tube_bank	101.274	328.165	343.961	101.228	220.508	219.062	179.886
fouling_1	fouling	1	HX_6	economiser	101.228	220.508	219.062	88.8785	152.384	141.687	104.795
fouling_5	fouling	5	HX_1	single_tube	101.325	1981.25	2612.29	101.322	966.415	1155.73	179.886
fouling_5	fouling	5	HX_2	reversal_chamber	101.322	966.415	1155.73	101.322	898.305	1064	179.886
fouling_5	fouling	5	HX_3	tube_bank	101.322	898.305	1064	101.27	366.218	388.937	179.886
fouling_5	fouling	5	HX_4	reversal_chamber	101.27	366.218	388.937	101.27	360.464	382.107	179.886
fouling_5	fouling	5	HX_5	tube_bank	101.27	360.464	382.107	101.222	233.355	233.792	179.886
fouling_5	fouling	5	HX_6	economiser	101.222	233.355	233.792	88.6468	157.043	146.941	104.795
fouling_10	fouling	10	HX_1	single_tube	101.325	1981.25	2612.29	101.322	1133.97	1385.46	179.886
fouling_10	fouling	10	HX_2	reversal_chamber	101.322	1133.97	1385.46	101.322	1053.16	1273.97	179.886

run	param_group	param_value	stage	kind	gas in pressure [kPa]	gas in temp [°C]	gas in enthalpy [kJ/kg]	gas out pressure [kPa]	gas out temp [°C]	gas out enthalpy [kJ/kg]	water in temp [°C]
fouling_10	fouling	10	HX_3	tube_bank	101.322	1053.16	1273.97	101.264	418.238	451.157	179.886
fouling_10	fouling	10	HX_4	reversal_chamber	101.264	418.238	451.157	101.264	410.57	441.932	179.886
fouling_10	fouling	10	HX_5	tube_bank	101.264	410.57	441.932	101.212	254.084	257.656	179.886
fouling_10	fouling	10	HX_6	economiser	101.212	254.084	257.656	88.2647	164.531	155.396	104.795
fuel_flow_0.025kgs	fuel_flow	0.025	HX_1	single_tube	101.325	1981.25	2612.29	101.325	450.07	489.657	179.886
fuel_flow_0.025kgs	fuel_flow	0.025	HX_2	reversal_chamber	101.325	450.07	489.657	101.325	414.551	446.718	179.886
fuel_flow_0.025kgs	fuel_flow	0.025	HX_3	tube_bank	101.325	414.551	446.718	101.323	230.779	230.835	179.886
fuel_flow_0.025kgs	fuel_flow	0.025	HX_4	reversal_chamber	101.323	230.779	230.835	101.323	226.841	226.317	179.886
fuel_flow_0.025kgs	fuel_flow	0.025	HX_5	tube_bank	101.323	226.841	226.317	101.32	188.405	182.448	179.886
fuel_flow_0.025kgs	fuel_flow	0.025	HX_6	economiser	101.32	188.405	182.448	100.557	127.526	113.748	104.795
fuel_flow_0.05kgs	fuel_flow	0.05	HX_1	single_tube	101.325	1981.25	2612.29	101.324	634.566	719.186	179.886
fuel_flow_0.05kgs	fuel_flow	0.05	HX_2	reversal_chamber	101.324	634.566	719.186	101.324	587.494	659.61	179.886
fuel_flow_0.05kgs	fuel_flow	0.05	HX_3	tube_bank	101.324	587.494	659.61	101.314	263.768	268.847	179.886
fuel_flow_0.05kgs	fuel_flow	0.05	HX_4	reversal_chamber	101.314	263.768	268.847	101.313	259.913	264.389	179.886
fuel_flow_0.05kgs	fuel_flow	0.05	HX_5	tube_bank	101.313	259.913	264.389	101.302	197.47	192.759	179.886
fuel_flow_0.05kgs	fuel_flow	0.05	HX_6	economiser	101.302	197.47	192.759	98.3726	132.364	119.173	104.795
fuel_flow_0.075kgs	fuel_flow	0.075	HX_1	single_tube	101.325	1981.25	2612.29	101.324	762.539	884.323	179.886
fuel_flow_0.075kgs	fuel_flow	0.075	HX_2	reversal_chamber	101.324	762.539	884.323	101.323	709.458	815.295	179.886
fuel_flow_0.075kgs	fuel_flow	0.075	HX_3	tube_bank	101.323	709.458	815.295	101.297	300.027	310.989	179.886
fuel_flow_0.075kgs	fuel_flow	0.075	HX_4	reversal_chamber	101.297	300.027	310.989	101.297	295.755	306.003	179.886
fuel_flow_0.075kgs	fuel_flow	0.075	HX_5	tube_bank	101.297	295.755	306.003	101.271	208.897	205.787	179.886
fuel_flow_0.075kgs	fuel_flow	0.075	HX_6	economiser	101.271	208.897	205.787	94.5729	142.11	130.121	104.795
fuel_flow_0.1kgs	fuel_flow	0.1	HX_1	single_tube	101.325	1981.25	2612.29	101.322	860.869	1014.02	179.886
fuel_flow_0.1kgs	fuel_flow	0.1	HX_2	reversal_chamber	101.322	860.869	1014.02	101.322	804.137	938.904	179.886
fuel_flow_0.1kgs	fuel_flow	0.1	HX_3	tube_bank	101.322	804.137	938.904	101.274	332.777	349.389	179.886
fuel_flow_0.1kgs	fuel_flow	0.1	HX_4	reversal_chamber	101.274	332.777	349.389	101.274	328.165	343.961	179.886
fuel_flow_0.1kgs	fuel_flow	0.1	HX_5	tube_bank	101.274	328.165	343.961	101.228	220.508	219.062	179.886
fuel_flow_0.1kgs	fuel_flow	0.1	HX_6	economiser	101.228	220.508	219.062	88.8785	152.384	141.687	104.795
fuel_flow_0.125kgs	fuel_flow	0.125	HX_1	single_tube	101.325	1981.25	2612.29	101.321	940.504	1120.71	179.886
fuel_flow_0.125kgs	fuel_flow	0.125	HX_2	reversal_chamber	101.321	940.504	1120.71	101.32	881.485	1041.5	179.886
fuel_flow_0.125kgs	fuel_flow	0.125	HX_3	tube_bank	101.32	881.485	1041.5	101.243	362.532	384.561	179.886
fuel_flow_0.125kgs	fuel_flow	0.125	HX_4	reversal_chamber	101.243	362.532	384.561	101.243	357.636	378.755	179.886
fuel_flow_0.125kgs	fuel_flow	0.125	HX_5	tube_bank	101.243	357.636	378.755	101.17	231.942	232.169	179.886
fuel_flow_0.125kgs	fuel_flow	0.125	HX_6	economiser	101.17	231.942	232.169	80.8379	162.541	153.148	104.795

Columns slice 2/4

run	param_group	param_value	stage	kind	water_in_enthalpy [kJ/kg]	water_in_pressure [kpa]	water_out_temp [°C]	water_out_enthalpy [kJ/kg]	water_out_pressure [kpa]	gas_avg_velocity [m/s]	water_avg_velocity [m/s]
default_case	control		HX_1	single_tube	762.683	1000	179.886	762.683	1000	5.04104	
default_case	control		HX_2	reversal_chamber	762.683	1000	179.886	762.683	1000	2.89824	
default_case	control		HX_3	tube_bank	762.683	1000	179.886	762.683	1000	7.66849	
default_case	control		HX_4	reversal_chamber	762.683	1000	179.886	762.683	1000	1.58457	
default_case	control		HX_5	tube_bank	762.683	1000	179.886	762.683	1000	6.23595	
default_case	control		HX_6	economiser	440	1000.06	122.087	513.209	1000	47.0379	0.0339143
drum_pressure_4.0bar	drum_pressure	4	HX_1	single_tube	604.723	400	143.613	604.723	400	5.04975	
drum_pressure_4.0bar	drum_pressure	4	HX_2	reversal_chamber	604.723	400	143.613	604.723	400	2.90601	
drum_pressure_4.0bar	drum_pressure	4	HX_3	tube_bank	604.723	400	143.613	604.723	400	7.5499	
drum_pressure_4.0bar	drum_pressure	4	HX_4	reversal_chamber	604.723	400	143.613	604.723	400	1.52724	
drum_pressure_4.0bar	drum_pressure	4	HX_5	tube_bank	604.723	400	143.613	604.723	400	5.92022	
drum_pressure_4.0bar	drum_pressure	4	HX_6	economiser	440	400.059	117.507	493.347	400	44.677	0.0346423
drum_pressure_10.0bar	drum_pressure	10	HX_1	single_tube	762.683	1000	179.886	762.683	1000	5.04104	
drum_pressure_10.0bar	drum_pressure	10	HX_2	reversal_chamber	762.683	1000	179.886	762.683	1000	2.89824	
drum_pressure_10.0bar	drum_pressure	10	HX_3	tube_bank	762.683	1000	179.886	762.683	1000	7.66849	
drum_pressure_10.0bar	drum_pressure	10	HX_4	reversal_chamber	762.683	1000	179.886	762.683	1000	1.58457	
drum_pressure_10.0bar	drum_pressure	10	HX_5	tube_bank	762.683	1000	179.886	762.683	1000	6.23595	
drum_pressure_10.0bar	drum_pressure	10	HX_6	economiser	440	1000.06	122.087	513.209	1000	47.0379	0.0339143
drum_pressure_16.0bar	drum_pressure	16	HX_1	single_tube	858.61	1600	201.378	858.61	1600	5.03701	
drum_pressure_16.0bar	drum_pressure	16	HX_2	reversal_chamber	858.61	1600	201.378	858.61	1600	2.89492	
drum_pressure_16.0bar	drum_pressure	16	HX_3	tube_bank	858.61	1600	201.378	858.61	1600	7.74227	
drum_pressure_16.0bar	drum_pressure	16	HX_4	reversal_chamber	858.61	1600	201.378	858.61	1600	1.61924	
drum_pressure_16.0bar	drum_pressure	16	HX_5	tube_bank	858.61	1600	201.378	858.61	1600	6.42545	
drum_pressure_16.0bar	drum_pressure	16	HX_6	economiser	440	1600.06	124.898	525.573	1600	48.4471	0.0335987
excess_air_1.0	excess_air	1	HX_1	single_tube	762.683	1000	179.886	762.683	1000	4.82274	
excess_air_1.0	excess_air	1	HX_2	reversal_chamber	762.683	1000	179.886	762.683	1000	2.74052	
excess_air_1.0	excess_air	1	HX_3	tube_bank	762.683	1000	179.886	762.683	1000	7.24618	
excess_air_1.0	excess_air	1	HX_4	reversal_chamber	762.683	1000	179.886	762.683	1000	1.50047	
excess_air_1.0	excess_air	1	HX_5	tube_bank	762.683	1000	179.886	762.683	1000	5.92208	
excess_air_1.0	excess_air	1	HX_6	economiser	440	1000.06	121.307	509.896	1000	44.5365	0.0340082
excess_air_1.05	excess_air	1.05	HX_1	single_tube	762.683	1000	179.886	762.683	1000	5.04104	
excess_air_1.05	excess_air	1.05	HX_2	reversal_chamber	762.683	1000	179.886	762.683	1000	2.89824	
excess_air_1.05	excess_air	1.05	HX_3	tube_bank	762.683	1000	179.886	762.683	1000	7.66849	
excess_air_1.05	excess_air	1.05	HX_4	reversal_chamber	762.683	1000	179.886	762.683	1000	1.58457	
excess_air_1.05	excess_air	1.05	HX_5	tube_bank	762.683	1000	179.886	762.683	1000	6.23595	
excess_air_1.05	excess_air	1.05	HX_6	economiser	440	1000.06	122.087	513.209	1000	47.0379	0.0339143
excess_air_1.1	excess_air	1.1	HX_1	single_tube	762.683	1000	179.886	762.683	1000	5.25445	
excess_air_1.1	excess_air	1.1	HX_2	reversal_chamber	762.683	1000	179.886	762.683	1000	3.05572	

run	param_group	param_value	stage	kind	water_in_enthalpy [kJ/kg]	water_in_pressure [kpa]	water_out_temp [°C]	water_out_enthalpy [kJ/kg]	water_out_pressure [kpa]	gas_avg_velocity [m/s]	water_avg_velocity [m/s]
excess_air_1.1	excess_air	1.1	HX_3	tube_bank	762.683	1000	179.886	762.683	1000	8.09337	
excess_air_1.1	excess_air	1.1	HX_4	reversal_chamber	762.683	1000	179.886	762.683	1000	1.66945	
excess_air_1.1	excess_air	1.1	HX_5	tube_bank	762.683	1000	179.886	762.683	1000	6.55248	
excess_air_1.1	excess_air	1.1	HX_6	economiser	440	1000.06	122.871	516.542	1000	49.6029	0.0338138
excess_air_1.15	excess_air	1.15	HX_1	single_tube	762.683	1000	179.886	762.683	1000	5.46265	
excess_air_1.15	excess_air	1.15	HX_2	reversal_chamber	762.683	1000	179.886	762.683	1000	3.21261	
excess_air_1.15	excess_air	1.15	HX_3	tube_bank	762.683	1000	179.886	762.683	1000	8.52006	
excess_air_1.15	excess_air	1.15	HX_4	reversal_chamber	762.683	1000	179.886	762.683	1000	1.755	
excess_air_1.15	excess_air	1.15	HX_5	tube_bank	762.683	1000	179.886	762.683	1000	6.87142	
excess_air_1.15	excess_air	1.15	HX_6	economiser	440	1000.06	123.643	519.822	1000	52.2366	0.0337281
excess_air_1.2	excess_air	1.2	HX_1	single_tube	762.683	1000	179.886	762.683	1000	5.66539	
excess_air_1.2	excess_air	1.2	HX_2	reversal_chamber	762.683	1000	179.886	762.683	1000	3.36853	
excess_air_1.2	excess_air	1.2	HX_3	tube_bank	762.683	1000	179.886	762.683	1000	8.94779	
excess_air_1.2	excess_air	1.2	HX_4	reversal_chamber	762.683	1000	179.886	762.683	1000	1.84112	
excess_air_1.2	excess_air	1.2	HX_5	tube_bank	762.683	1000	179.886	762.683	1000	7.19248	
excess_air_1.2	excess_air	1.2	HX_6	economiser	440	1000.06	124.429	523.163	1000	54.9382	0.0336235
excess_air_1.3	excess_air	1.3	HX_1	single_tube	762.683	1000	179.886	762.683	1000	6.05386	
excess_air_1.3	excess_air	1.3	HX_2	reversal_chamber	762.683	1000	179.886	762.683	1000	3.67618	
excess_air_1.3	excess_air	1.3	HX_3	tube_bank	762.683	1000	179.886	762.683	1000	9.80343	
excess_air_1.3	excess_air	1.3	HX_4	reversal_chamber	762.683	1000	179.886	762.683	1000	2.01463	
excess_air_1.3	excess_air	1.3	HX_5	tube_bank	762.683	1000	179.886	762.683	1000	7.83992	
excess_air_1.3	excess_air	1.3	HX_6	economiser	440	1000.06	126	529.846	1000	60.5665	0.0334087
fouling_1	fouling	1	HX_1	single_tube	762.683	1000	179.886	762.683	1000	5.04104	
fouling_1	fouling	1	HX_2	reversal_chamber	762.683	1000	179.886	762.683	1000	2.89824	
fouling_1	fouling	1	HX_3	tube_bank	762.683	1000	179.886	762.683	1000	7.66849	
fouling_1	fouling	1	HX_4	reversal_chamber	762.683	1000	179.886	762.683	1000	1.58457	
fouling_1	fouling	1	HX_5	tube_bank	762.683	1000	179.886	762.683	1000	6.23595	
fouling_1	fouling	1	HX_6	economiser	440	1000.06	122.087	513.209	1000	47.0379	0.0339143
fouling_5	fouling	5	HX_1	single_tube	762.683	1000	179.886	762.683	1000	5.51702	
fouling_5	fouling	5	HX_2	reversal_chamber	762.683	1000	179.886	762.683	1000	3.15994	
fouling_5	fouling	5	HX_3	tube_bank	762.683	1000	179.886	762.683	1000	8.22734	
fouling_5	fouling	5	HX_4	reversal_chamber	762.683	1000	179.886	762.683	1000	1.67091	
fouling_5	fouling	5	HX_5	tube_bank	762.683	1000	179.886	762.683	1000	6.48285	
fouling_5	fouling	5	HX_6	economiser	440	1000.06	124.24	522.359	1000	47.8533	0.0338807
fouling_10	fouling	10	HX_1	single_tube	762.683	1000	179.886	762.683	1000	6.04713	
fouling_10	fouling	10	HX_2	reversal_chamber	762.683	1000	179.886	762.683	1000	3.58334	
fouling_10	fouling	10	HX_3	tube_bank	762.683	1000	179.886	762.683	1000	9.10952	
fouling_10	fouling	10	HX_4	reversal_chamber	762.683	1000	179.886	762.683	1000	1.80505	
fouling_10	fouling	10	HX_5	tube_bank	762.683	1000	179.886	762.683	1000	6.87137	
fouling_10	fouling	10	HX_6	economiser	440	1000.06	127.751	537.298	1000	49.2072	0.033834

run	param_group	param_value	stage	kind	water in enthalpy [kJ/kg]	water in pressure [kpa]	water out temp [°C]	water out enthalpy [kJ/kg]	water out pressure [kpa]	gas avg velocity [m/s]	water avg velocity [m/s]
fuel_flow_0.025kgs	fuel_flow	0.025	HX_1	single_tube	762.683	1000	179.886	762.683	1000	0.863024	
fuel_flow_0.025kgs	fuel_flow	0.025	HX_2	reversal_chamber	762.683	1000	179.886	762.683	1000	0.462283	
fuel_flow_0.025kgs	fuel_flow	0.025	HX_3	tube_bank	762.683	1000	179.886	762.683	1000	1.41785	
fuel_flow_0.025kgs	fuel_flow	0.025	HX_4	reversal_chamber	762.683	1000	179.886	762.683	1000	0.329248	
fuel_flow_0.025kgs	fuel_flow	0.025	HX_5	tube_bank	762.683	1000	179.886	762.683	1000	1.38251	
fuel_flow_0.025kgs	fuel_flow	0.025	HX_6	economiser	440	1000.01	119.999	504.345	1000	10.3543	0.00856301
fuel_flow_0.05kgs	fuel_flow	0.05	HX_1	single_tube	762.683	1000	179.886	762.683	1000	2.11419	
fuel_flow_0.05kgs	fuel_flow	0.05	HX_2	reversal_chamber	762.683	1000	179.886	762.683	1000	1.15876	
fuel_flow_0.05kgs	fuel_flow	0.05	HX_3	tube_bank	762.683	1000	179.886	762.683	1000	3.21495	
fuel_flow_0.05kgs	fuel_flow	0.05	HX_4	reversal_chamber	762.683	1000	179.886	762.683	1000	0.701922	
fuel_flow_0.05kgs	fuel_flow	0.05	HX_5	tube_bank	762.683	1000	179.886	762.683	1000	2.87371	
fuel_flow_0.05kgs	fuel_flow	0.05	HX_6	economiser	440	1000.02	121.099	509.015	1000	21.2926	0.0171088
fuel_flow_0.075kgs	fuel_flow	0.075	HX_1	single_tube	762.683	1000	179.886	762.683	1000	3.52767	
fuel_flow_0.075kgs	fuel_flow	0.075	HX_2	reversal_chamber	762.683	1000	179.886	762.683	1000	1.98385	
fuel_flow_0.075kgs	fuel_flow	0.075	HX_3	tube_bank	762.683	1000	179.886	762.683	1000	5.32927	
fuel_flow_0.075kgs	fuel_flow	0.075	HX_4	reversal_chamber	762.683	1000	179.886	762.683	1000	1.12402	
fuel_flow_0.075kgs	fuel_flow	0.075	HX_5	tube_bank	762.683	1000	179.886	762.683	1000	4.4983	
fuel_flow_0.075kgs	fuel_flow	0.075	HX_6	economiser	440	1000.03	121.63	511.269	1000	33.4514	0.0255503
fuel_flow_0.1kgs	fuel_flow	0.1	HX_1	single_tube	762.683	1000	179.886	762.683	1000	5.04104	
fuel_flow_0.1kgs	fuel_flow	0.1	HX_2	reversal_chamber	762.683	1000	179.886	762.683	1000	2.89824	
fuel_flow_0.1kgs	fuel_flow	0.1	HX_3	tube_bank	762.683	1000	179.886	762.683	1000	7.66849	
fuel_flow_0.1kgs	fuel_flow	0.1	HX_4	reversal_chamber	762.683	1000	179.886	762.683	1000	1.58457	
fuel_flow_0.1kgs	fuel_flow	0.1	HX_5	tube_bank	762.683	1000	179.886	762.683	1000	6.23595	
fuel_flow_0.1kgs	fuel_flow	0.1	HX_6	economiser	440	1000.06	122.087	513.209	1000	47.0379	0.0339143
fuel_flow_0.125kgs	fuel_flow	0.125	HX_1	single_tube	762.683	1000	179.886	762.683	1000	6.62352	
fuel_flow_0.125kgs	fuel_flow	0.125	HX_2	reversal_chamber	762.683	1000	179.886	762.683	1000	3.88021	
fuel_flow_0.125kgs	fuel_flow	0.125	HX_3	tube_bank	762.683	1000	179.886	762.683	1000	10.191	
fuel_flow_0.125kgs	fuel_flow	0.125	HX_4	reversal_chamber	762.683	1000	179.886	762.683	1000	2.07853	
fuel_flow_0.125kgs	fuel_flow	0.125	HX_5	tube_bank	762.683	1000	179.886	762.683	1000	8.07609	
fuel_flow_0.125kgs	fuel_flow	0.125	HX_6	economiser	440	1000.11	122.537	515.12	1000	62.6186	0.0421981

Columns slice 3/4

run	param_group	param_value	stage	kind	pressure drop fric [kpa]	pressure drop minor [kpa]	pressure drop total [kpa]	water pressure drop fric [kpa]	water pressure drop minor [kpa]	water pressure drop total [kpa]	Q conv [MW]
default_case	control		HX_1	single_tube	-0.000261857	-0.00224634	-0.0025082				0.108511
default_case	control		HX_2	reversal_chamber	-1.49553e-05	-0.000387573	-0.000402528				0.00945555
default_case	control		HX_3	tube_bank	-0.0290645	-0.0189316	-0.0479961				0.844348
default_case	control		HX_4	reversal_chamber	-7.40724e-06	-0.000211679	-0.000219087				0.00183451
default_case	control		HX_5	tube_bank	-0.0280939	-0.0182614	-0.0463553				0.205944
default_case	control		HX_6	economiser	-8.29672	-4.05233	-12.3491	-0.0559112	-0.000981025	-0.0568922	0.138409
drum_pressure_4.0bar	drum_pressure	4	HX_1	single_tube	-0.000262366	-0.00224634	-0.00250871				0.113506
drum_pressure_4.0bar	drum_pressure	4	HX_2	reversal_chamber	-1.50019e-05	-0.000388613	-0.000403615				0.0100804
drum_pressure_4.0bar	drum_pressure	4	HX_3	tube_bank	-0.0285566	-0.0185978	-0.0471544				0.903819
drum_pressure_4.0bar	drum_pressure	4	HX_4	reversal_chamber	-7.09653e-06	-0.00020402	-0.000211116				0.00199308
drum_pressure_4.0bar	drum_pressure	4	HX_5	tube_bank	-0.0264364	-0.0173027	-0.0437391				0.225418
drum_pressure_4.0bar	drum_pressure	4	HX_6	economiser	-7.85215	-3.86092	-11.7131	-0.0583874	-0.00102521	-0.0594126	0.103227
drum_pressure_10.0bar	drum_pressure	10	HX_1	single_tube	-0.000261857	-0.00224634	-0.0025082				0.108511
drum_pressure_10.0bar	drum_pressure	10	HX_2	reversal_chamber	-1.49553e-05	-0.000387573	-0.000402528				0.00945555
drum_pressure_10.0bar	drum_pressure	10	HX_3	tube_bank	-0.0290645	-0.0189316	-0.0479961				0.844348
drum_pressure_10.0bar	drum_pressure	10	HX_4	reversal_chamber	-7.40724e-06	-0.000211679	-0.000219087				0.00183451
drum_pressure_10.0bar	drum_pressure	10	HX_5	tube_bank	-0.0280939	-0.0182614	-0.0463553				0.205944
drum_pressure_10.0bar	drum_pressure	10	HX_6	economiser	-8.29672	-4.05233	-12.3491	-0.0559112	-0.000981025	-0.0568922	0.138409
drum_pressure_16.0bar	drum_pressure	16	HX_1	single_tube	-0.000261621	-0.00224634	-0.00250796				0.105608
drum_pressure_16.0bar	drum_pressure	16	HX_2	reversal_chamber	-1.49354e-05	-0.000387129	-0.000402064				0.00909572
drum_pressure_16.0bar	drum_pressure	16	HX_3	tube_bank	-0.0293824	-0.0191379	-0.0485203				0.809859
drum_pressure_16.0bar	drum_pressure	16	HX_4	reversal_chamber	-7.59595e-06	-0.00021631	-0.000223906				0.00174211
drum_pressure_16.0bar	drum_pressure	16	HX_5	tube_bank	-0.0290964	-0.0188362	-0.0479326				0.194598
drum_pressure_16.0bar	drum_pressure	16	HX_6	economiser	-8.56306	-4.16568	-12.7287	-0.0550437	-0.000962062	-0.0560058	0.160106
excess_air_1.0	excess_air	1	HX_1	single_tube	-0.000241886	-0.00211718	-0.00235907				0.104704
excess_air_1.0	excess_air	1	HX_2	reversal_chamber	-1.36178e-05	-0.000350013	-0.000363631				0.00896705
excess_air_1.0	excess_air	1	HX_3	tube_bank	-0.0264592	-0.017105	-0.0435642				0.789942
excess_air_1.0	excess_air	1	HX_4	reversal_chamber	-6.74993e-06	-0.000191433	-0.000198183				0.00169925
excess_air_1.0	excess_air	1	HX_5	tube_bank	-0.0256989	-0.0165714	-0.0422704				0.189507
excess_air_1.0	excess_air	1	HX_6	economiser	-7.52855	-3.66147	-11.19	-0.0561612	-0.000986843	-0.0571481	0.13256
excess_air_1.05	excess_air	1.05	HX_1	single_tube	-0.000261857	-0.00224634	-0.0025082				0.108511
excess_air_1.05	excess_air	1.05	HX_2	reversal_chamber	-1.49553e-05	-0.000387573	-0.000402528				0.00945555
excess_air_1.05	excess_air	1.05	HX_3	tube_bank	-0.0290645	-0.0189316	-0.0479961				0.844348
excess_air_1.05	excess_air	1.05	HX_4	reversal_chamber	-7.40724e-06	-0.000211679	-0.000219087				0.00183451
excess_air_1.05	excess_air	1.05	HX_5	tube_bank	-0.0280939	-0.0182614	-0.0463553				0.205944
excess_air_1.05	excess_air	1.05	HX_6	economiser	-8.29672	-4.05233	-12.3491	-0.0559112	-0.000981025	-0.0568922	0.138409
excess_air_1.1	excess_air	1.1	HX_1	single_tube	-0.000282222	-0.00237716	-0.00265938				0.112109
excess_air_1.1	excess_air	1.1	HX_2	reversal_chamber	-1.63454e-05	-0.000426995	-0.00044334				0.00993495

run	param_group	param_value	stage	kind	pressure drop fric [kpa]	pressure drop minor [kpa]	pressure drop total [kpa]	water pressure drop fric [kpa]	water pressure drop minor [kpa]	water pressure drop total [kpa]	Q conv [MW]
excess_air_1.1	excess_air	1.1	HX_3	tube_bank	-0.0317855	-0.0208551	-0.0526405				0.898655
excess_air_1.1	excess_air	1.1	HX_4	reversal_chamber	-8.09557e-06	-0.00233044	-0.0024114				0.00197151
excess_air_1.1	excess_air	1.1	HX_5	tube_bank	-0.0305968	-0.0200407	-0.0506375				0.22268
excess_air_1.1	excess_air	1.1	HX_6	economiser	-9.11224	-4.46913	-13.5814	-0.0556276	-0.000974849	-0.0566025	0.14423
excess_air_1.15	excess_air	1.15	HX_1	single_tube	-0.000302926	-0.0025096	-0.00281253				0.115492
excess_air_1.15	excess_air	1.15	HX_2	reversal_chamber	-1.7785e-05	-0.00046822	-0.000486005				0.0104036
excess_air_1.15	excess_air	1.15	HX_3	tube_bank	-0.0346184	-0.0228741	-0.0574925				0.952659
excess_air_1.15	excess_air	1.15	HX_4	reversal_chamber	-8.81452e-06	-0.000255527	-0.000264341				0.0021098
excess_air_1.15	excess_air	1.15	HX_5	tube_bank	-0.033207	-0.0219095	-0.0551165				0.23966
excess_air_1.15	excess_air	1.15	HX_6	economiser	-9.97727	-4.9133	-14.8906	-0.0554122	-0.000969562	-0.0563817	0.149977
excess_air_1.2	excess_air	1.2	HX_1	single_tube	-0.000323918	-0.00264364	-0.00296755				0.118656
excess_air_1.2	excess_air	1.2	HX_2	reversal_chamber	-1.9271e-05	-0.000511184	-0.000530455				0.0108602
excess_air_1.2	excess_air	1.2	HX_3	tube_bank	-0.0375594	-0.0249871	-0.0625465				1.00616
excess_air_1.2	excess_air	1.2	HX_4	reversal_chamber	-9.5636e-06	-0.000279123	-0.000288686				0.00224891
excess_air_1.2	excess_air	1.2	HX_5	tube_bank	-0.0359233	-0.023868	-0.0597913				0.256827
excess_air_1.2	excess_air	1.2	HX_6	economiser	-10.8929	-5.38594	-16.2788	-0.0551056	-0.000963195	-0.0560688	0.155711
excess_air_1.3	excess_air	1.3	HX_1	single_tube	-0.000366579	-0.00291637	-0.00328295				0.124328
excess_air_1.3	excess_air	1.3	HX_2	reversal_chamber	-2.23683e-05	-0.00060204	-0.000624408				0.0117317
excess_air_1.3	excess_air	1.3	HX_3	tube_bank	-0.0437481	-0.0294873	-0.0732354				1.11092
excess_air_1.3	excess_air	1.3	HX_4	reversal_chamber	-1.11499e-05	-0.000329626	-0.000340776				0.00252782
excess_air_1.3	excess_air	1.3	HX_5	tube_bank	-0.0416697	-0.028053	-0.0697227				0.291502
excess_air_1.3	excess_air	1.3	HX_6	economiser	-12.8853	-6.42333	-19.3086	-0.0544629	-0.000950212	-0.0554131	0.167023
fouling_1	fouling	1	HX_1	single_tube	-0.000261857	-0.00224634	-0.0025082				0.108511
fouling_1	fouling	1	HX_2	reversal_chamber	-1.49553e-05	-0.000387573	-0.000402582				0.00455555
fouling_1	fouling	1	HX_3	tube_bank	-0.0290645	-0.0189316	-0.0479981				0.844348
fouling_1	fouling	1	HX_4	reversal_chamber	-7.40724e-06	-0.000211679	-0.000219087				0.00183451
fouling_1	fouling	1	HX_5	tube_bank	-0.0280939	-0.0182614	-0.0463553				0.205944
fouling_1	fouling	1	HX_6	economiser	-8.29672	-4.05233	-12.3491	-0.0559112	-0.000981025	-0.0568922	0.138409
fouling_5	fouling	5	HX_1	single_tube	-0.00029055	-0.00224634	-0.00253689				0.0726315
fouling_5	fouling	5	HX_2	reversal_chamber	-1.65364e-05	-0.000422623	-0.00043916				0.00857954
fouling_5	fouling	5	HX_3	tube_bank	-0.0316113	-0.0202694	-0.0518807				0.923814
fouling_5	fouling	5	HX_4	reversal_chamber	-7.87873e-06	-0.000223221	-0.0002311				0.00212119
fouling_5	fouling	5	HX_5	tube_bank	-0.0294182	-0.0189331	-0.0483512				0.242689
fouling_5	fouling	5	HX_6	economiser	-8.45068	-4.12412	-12.5748	-0.0564279	-0.000977851	-0.0574058	0.155354
fouling_10	fouling	10	HX_1	single_tube	-0.000322589	-0.00224634	-0.00256893				0.0456573
fouling_10	fouling	10	HX_2	reversal_chamber	-1.91369e-05	-0.000479289	-0.000498425				0.00674486
fouling_10	fouling	10	HX_3	tube_bank	-0.0357026	-0.0224194	-0.058122				1.03608
fouling_10	fouling	10	HX_4	reversal_chamber	-8.61892e-06	-0.000241154	-0.000249772				0.0025055
fouling_10	fouling	10	HX_5	tube_bank	-0.0315206	-0.0199934	-0.051514				0.29762
fouling_10	fouling	10	HX_6	economiser	-8.70699	-4.24031	-12.9473	-0.0573099	-0.00097325	-0.0582832	0.182901

run	param_group	param_value	stage	kind	pressure drop fric [kpa]	pressure drop minor [kpa]	pressure drop total [kpa]	water pressure drop fric [kpa]	water pressure drop minor [kpa]	water pressure drop total [kpa]	Q conv [MW]
fuel_flow_0.025kgs	fuel_flow	0.025	HX_1	single_tube	-1.49034e-05	-0.000140396	-0.0001553				0.0196037
fuel_flow_0.025kgs	fuel_flow	0.025	HX_2	reversal_chamber	-7.74068e-07	-1.54546e-05	-1.62286e-05				0.00110416
fuel_flow_0.025kgs	fuel_flow	0.025	HX_3	tube_bank	-0.00110702	-0.000874925	-0.00198194				0.0622048
fuel_flow_0.025kgs	fuel_flow	0.025	HX_4	reversal_chamber	-5.16086e-07	-1.09959e-05	-1.1512e-05				0.000194681
fuel_flow_0.025kgs	fuel_flow	0.025	HX_5	tube_bank	-0.00153901	-0.00102091	-0.00255992				0.0160058
fuel_flow_0.025kgs	fuel_flow	0.025	HX_6	economiser	-0.5397	-0.223891	-0.763592	-0.00855037	-6.25129e-05	-0.00861288	0.0306981
fuel_flow_0.05kgs	fuel_flow	0.05	HX_1	single_tube	-6.31864e-05	-0.000561585	-0.000624772				0.0486168
fuel_flow_0.05kgs	fuel_flow	0.05	HX_2	reversal_chamber	-3.39483e-06	-7.74823e-05	-8.08771e-05				0.00346705
fuel_flow_0.05kgs	fuel_flow	0.05	HX_3	tube_bank	-0.0067897	-0.00399551	-0.0107852				0.268511
fuel_flow_0.05kgs	fuel_flow	0.05	HX_4	reversal_chamber	-1.88073e-06	-4.68835e-05	-4.87642e-05				0.000566003
fuel_flow_0.05kgs	fuel_flow	0.05	HX_5	tube_bank	-0.00757478	-0.00423231	-0.0118071				0.0568644
fuel_flow_0.05kgs	fuel_flow	0.05	HX_6	economiser	-2.01006	-0.918957	-2.92902	-0.0170261	-0.000249509	-0.0172756	0.0657968
fuel_flow_0.075kgs	fuel_flow	0.075	HX_1	single_tube	-0.000145602	-0.00126357	-0.00140917				0.0786402
fuel_flow_0.075kgs	fuel_flow	0.075	HX_2	reversal_chamber	-8.08868e-06	-0.000198977	-0.000207066				0.00632981
fuel_flow_0.075kgs	fuel_flow	0.075	HX_3	tube_bank	-0.0160876	-0.00989947	-0.0259871				0.534589
fuel_flow_0.075kgs	fuel_flow	0.075	HX_4	reversal_chamber	-4.16222e-06	-0.000112616	-0.000116778				0.00113357
fuel_flow_0.075kgs	fuel_flow	0.075	HX_5	tube_bank	-0.0161719	-0.0099068	-0.0260787				0.122375
fuel_flow_0.075kgs	fuel_flow	0.075	HX_6	economiser	-4.539	-2.15934	-6.69834	-0.0272303	-0.000556733	-0.0277871	0.101504
fuel_flow_0.1kgs	fuel_flow	0.1	HX_1	single_tube	-0.000261857	-0.00224634	-0.0025082				0.108511
fuel_flow_0.1kgs	fuel_flow	0.1	HX_2	reversal_chamber	-1.49553e-05	-0.000387573	-0.000402528				0.00945555
fuel_flow_0.1kgs	fuel_flow	0.1	HX_3	tube_bank	-0.0290645	-0.0189316	-0.0479961				0.844348
fuel_flow_0.1kgs	fuel_flow	0.1	HX_4	reversal_chamber	-7.40724e-06	-0.000211679	-0.000219087				0.00183451
fuel_flow_0.1kgs	fuel_flow	0.1	HX_5	tube_bank	-0.0280939	-0.0182614	-0.0463553				0.205944
fuel_flow_0.1kgs	fuel_flow	0.1	HX_6	economiser	-8.29672	-4.05233	-12.3491	-0.0559112	-0.000981025	-0.0568922	0.138409
fuel_flow_0.125kgs	fuel_flow	0.125	HX_1	single_tube	-0.000411449	-0.00350991	-0.00392136				0.137868
fuel_flow_0.125kgs	fuel_flow	0.125	HX_2	reversal_chamber	-2.40471e-05	-0.000648589	-0.000672636				0.0127297
fuel_flow_0.125kgs	fuel_flow	0.125	HX_3	tube_bank	-0.0461672	-0.0313611	-0.0775283				1.18557
fuel_flow_0.125kgs	fuel_flow	0.125	HX_4	reversal_chamber	-1.1662e-05	-0.000347084	-0.000358746				0.00264478
fuel_flow_0.125kgs	fuel_flow	0.125	HX_5	tube_bank	-0.0434744	-0.0294919	-0.0729663				0.304469
fuel_flow_0.125kgs	fuel_flow	0.125	HX_6	economiser	-13.5565	-6.77513	-20.3317	-0.107079	-0.00151877	-0.108598	0.176706

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run	param_group	param_value	stage	kind	Q_rad [MW]	Q_total [MW]	UA [MW/K]	steam capacity [t/h]
default_case	control		HX_1	single_tube	2.75285	2.86136	0.00241321	4.55016
default_case	control		HX_2	reversal_chamber	0.125021	0.134477	0.000204414	0.213846
default_case	control		HX_3	tube_bank	0.211055	1.0554	0.00305847	1.67831
default_case	control		HX_4	reversal_chamber	0.00788276	0.00971726	6.4361e-05	0.0154525
default_case	control		HX_5	tube_bank	0.0176618	0.223605	0.00264989	0.355579
default_case	control		HX_6	economiser	0.000113941	0.138523	0.00210994	
drum_pressure_4.0bar	drum_pressure	4	HX_1	single_tube	2.74036	2.85387	0.00232417	4.57702
drum_pressure_4.0bar	drum_pressure	4	HX_2	reversal_chamber	0.125182	0.135263	0.00019378	0.216934
drum_pressure_4.0bar	drum_pressure	4	HX_3	tube_bank	0.204399	1.10822	0.00298778	1.77735
drum_pressure_4.0bar	drum_pressure	4	HX_4	reversal_chamber	0.00726221	0.00925529	5.59182e-05	0.0148436
drum_pressure_4.0bar	drum_pressure	4	HX_5	tube_bank	0.0157511	0.241169	0.00257311	0.386786
drum_pressure_4.0bar	drum_pressure	4	HX_6	economiser	7.30591e-05	0.1033	0.0021835	
drum_pressure_10.0bar	drum_pressure	10	HX_1	single_tube	2.75285	2.86136	0.00241321	4.55016
drum_pressure_10.0bar	drum_pressure	10	HX_2	reversal_chamber	0.125021	0.134477	0.000204414	0.213846
drum_pressure_10.0bar	drum_pressure	10	HX_3	tube_bank	0.211055	1.0554	0.00305847	1.67831
drum_pressure_10.0bar	drum_pressure	10	HX_4	reversal_chamber	0.00788276	0.00971726	6.4361e-05	0.0154525
drum_pressure_10.0bar	drum_pressure	10	HX_5	tube_bank	0.0176618	0.223605	0.00264989	0.355579
drum_pressure_10.0bar	drum_pressure	10	HX_6	economiser	0.000113941	0.138523	0.00210994	
drum_pressure_16.0bar	drum_pressure	16	HX_1	single_tube	2.75906	2.86467	0.00246756	4.5486
drum_pressure_16.0bar	drum_pressure	16	HX_2	reversal_chamber	0.124849	0.133945	0.000211064	0.212682
drum_pressure_16.0bar	drum_pressure	16	HX_3	tube_bank	0.214789	1.02465	0.00310362	1.62697
drum_pressure_16.0bar	drum_pressure	16	HX_4	reversal_chamber	0.00822348	0.00996559	6.9865e-05	0.0158237
drum_pressure_16.0bar	drum_pressure	16	HX_5	tube_bank	0.0187467	0.213345	0.00269848	0.338755
drum_pressure_16.0bar	drum_pressure	16	HX_6	economiser	0.00014374	0.16025	0.00208493	
excess_air_1.0	excess_air	1	HX_1	single_tube	2.85825	2.96296	0.00245683	4.7049
excess_air_1.0	excess_air	1	HX_2	reversal_chamber	0.120672	0.129639	0.000201041	0.205855
excess_air_1.0	excess_air	1	HX_3	tube_bank	0.206475	0.996418	0.00297116	1.58222
excess_air_1.0	excess_air	1	HX_4	reversal_chamber	0.00751616	0.00921541	6.36471e-05	0.0146332
excess_air_1.0	excess_air	1	HX_5	tube_bank	0.0171948	0.206702	0.00257183	0.328223
excess_air_1.0	excess_air	1	HX_6	economiser	0.000115491	0.132676	0.00207206	
excess_air_1.05	excess_air	1.05	HX_1	single_tube	2.75285	2.86136	0.00241321	4.55016
excess_air_1.05	excess_air	1.05	HX_2	reversal_chamber	0.125021	0.134477	0.000204414	0.213846
excess_air_1.05	excess_air	1.05	HX_3	tube_bank	0.211055	1.0554	0.00305847	1.67831
excess_air_1.05	excess_air	1.05	HX_4	reversal_chamber	0.00788276	0.00971726	6.4361e-05	0.0154525
excess_air_1.05	excess_air	1.05	HX_5	tube_bank	0.0176618	0.223605	0.00264989	0.355579
excess_air_1.05	excess_air	1.05	HX_6	economiser	0.000113941	0.138523	0.00210994	
excess_air_1.1	excess_air	1.1	HX_1	single_tube	2.64826	2.76037	0.00236704	4.39604
excess_air_1.1	excess_air	1.1	HX_2	reversal_chamber	0.128953	0.138888	0.000207384	0.221186

run	param_group	param_value	stage	kind	Q_rad [MW]	Q_total [MW]	UA [MW/K]	steam capacity [t/h]
excess_air_1.1	excess_air	1.1	HX_3	tube_bank	0.215009	1.11366	0.00314434	1.77357
excess_air_1.1	excess_air	1.1	HX_4	reversal_chamber	0.00823729	0.0102088	6.50494e-05	0.0162581
excess_air_1.1	excess_air	1.1	HX_5	tube_bank	0.0180926	0.240772	0.00272741	0.383443
excess_air_1.1	excess_air	1.1	HX_6	economiser	0.000112463	0.144343	0.00212783	4.24256
excess_air_1.15	excess_air	1.15	HX_1	single_tube	2.54481	2.6603	0.00231882	0.227802
excess_air_1.15	excess_air	1.15	HX_2	reversal_chamber	0.13244	0.142844	0.000209943	
excess_air_1.15	excess_air	1.15	HX_3	tube_bank	0.218319	1.17098	0.00322872	1.86744
excess_air_1.15	excess_air	1.15	HX_4	reversal_chamber	0.00857824	0.010688	6.57094e-05	0.0170449
excess_air_1.15	excess_air	1.15	HX_5	tube_bank	0.0184866	0.258146	0.00280439	0.411683
excess_air_1.15	excess_air	1.15	HX_6	economiser	0.000111001	0.150088	0.00215362	
excess_air_1.2	excess_air	1.2	HX_1	single_tube	2.44283	2.56149	0.002289	4.09102
excess_air_1.2	excess_air	1.2	HX_2	reversal_chamber	0.135461	0.146322	0.000212086	0.233694
excess_air_1.2	excess_air	1.2	HX_3	tube_bank	0.220974	1.22714	0.00331159	1.95989
excess_air_1.2	excess_air	1.2	HX_4	reversal_chamber	0.00890417	0.0111531	6.63389e-05	0.0178129
excess_air_1.2	excess_air	1.2	HX_5	tube_bank	0.0188434	0.27567	0.0028808	0.440281
excess_air_1.2	excess_air	1.2	HX_6	economiser	0.000109584	0.155821	0.00218204	
excess_air_1.3	excess_air	1.3	HX_1	single_tube	2.24441	2.36874	0.00216617	3.79441
excess_air_1.3	excess_air	1.3	HX_2	reversal_chamber	0.140057	0.151788	0.000215127	0.243145
excess_air_1.3	excess_air	1.3	HX_3	tube_bank	0.224302	1.33522	0.0034727	2.13885
excess_air_1.3	excess_air	1.3	HX_4	reversal_chamber	0.00950566	0.0120335	6.74979e-05	0.0192761
excess_air_1.3	excess_air	1.3	HX_5	tube_bank	0.0194439	0.310946	0.00303187	0.498095
excess_air_1.3	excess_air	1.3	HX_6	economiser	0.000106791	0.16713	0.00222599	
fouling_1	fouling	1	HX_1	single_tube	2.75285	2.86136	0.00241321	4.55016
fouling_1	fouling	1	HX_2	reversal_chamber	0.125021	0.134477	0.000204414	0.213846
fouling_1	fouling	1	HX_3	tube_bank	0.211055	1.0554	0.00305847	1.67831
fouling_1	fouling	1	HX_4	reversal_chamber	0.00788276	0.00971726	6.4361e-05	0.0154525
fouling_1	fouling	1	HX_5	tube_bank	0.0176618	0.223605	0.00264989	0.355579
fouling_1	fouling	1	HX_6	economiser	0.000113941	0.138523	0.00210994	
fouling_5	fouling	5	HX_1	single_tube	2.53503	2.60767	0.00209314	4.16361
fouling_5	fouling	5	HX_2	reversal_chamber	0.155643	0.164223	0.000217179	0.262212
fouling_5	fouling	5	HX_3	tube_bank	0.284737	1.20855	0.0029765	1.92967
fouling_5	fouling	5	HX_4	reversal_chamber	0.0101064	0.0122276	6.64956e-05	0.0195236
fouling_5	fouling	5	HX_5	tube_bank	0.0228383	0.265527	0.00250614	0.423963
fouling_5	fouling	5	HX_6	economiser	0.000135176	0.155489	0.00214491	
fouling_10	fouling	10	HX_1	single_tube	2.15072	2.19638	0.00163031	3.53028
fouling_10	fouling	10	HX_2	reversal_chamber	0.19285	0.199595	0.000218054	0.320813
fouling_10	fouling	10	HX_3	tube_bank	0.436991	1.47307	0.00292481	2.36769
fouling_10	fouling	10	HX_4	reversal_chamber	0.0140095	0.016515	7.02767e-05	0.0265449
fouling_10	fouling	10	HX_5	tube_bank	0.0322866	0.329907	0.00235782	0.530264
fouling_10	fouling	10	HX_6	economiser	0.000173795	0.183074	0.00220028	

run	param_group	param_value	stage	kind	Q rad [MW]	Q total [MW]	UA [MW/K]	steam capacity [t/h]
fuel_flow_0.025kgs	fuel_flow	0.025	HX_1	single_tube	0.930427	0.950031	0.00107711	1.50507
fuel_flow_0.025kgs	fuel_flow	0.025	HX_2	reversal_chamber	0.0181139	0.019218	7.57187e-05	0.0304459
fuel_flow_0.025kgs	fuel_flow	0.025	HX_3	tube_bank	0.0344185	0.0966233	0.000785414	0.153074
fuel_flow_0.025kgs	fuel_flow	0.025	HX_4	reversal_chamber	0.00182759	0.00202227	4.08752e-05	0.00320376
fuel_flow_0.025kgs	fuel_flow	0.025	HX_5	tube_bank	0.00362845	0.0196342	0.000855928	0.0311053
fuel_flow_0.025kgs	fuel_flow	0.025	HX_6	economiser	5.02806e-05	0.0307484	0.000913267	
fuel_flow_0.05kgs	fuel_flow	0.05	HX_1	single_tube	1.64598	1.6946	0.00164661	2.68988
fuel_flow_0.05kgs	fuel_flow	0.05	HX_2	reversal_chamber	0.0498623	0.0533294	0.000122857	0.0846512
fuel_flow_0.05kgs	fuel_flow	0.05	HX_3	tube_bank	0.0812786	0.349789	0.00165993	0.55523
fuel_flow_0.05kgs	fuel_flow	0.05	HX_4	reversal_chamber	0.00342459	0.00399059	4.84255e-05	0.00633438
fuel_flow_0.05kgs	fuel_flow	0.05	HX_5	tube_bank	0.0072543	0.0641187	0.00153097	0.101777
fuel_flow_0.05kgs	fuel_flow	0.05	HX_6	economiser	7.33845e-05	0.0658702	0.00161394	
fuel_flow_0.075kgs	fuel_flow	0.075	HX_1	single_tube	2.24153	2.32017	0.00207141	3.68646
fuel_flow_0.075kgs	fuel_flow	0.075	HX_2	reversal_chamber	0.0863551	0.0926849	0.00016541	0.147265
fuel_flow_0.075kgs	fuel_flow	0.075	HX_3	tube_bank	0.142551	0.67714	0.00238186	1.07589
fuel_flow_0.075kgs	fuel_flow	0.075	HX_4	reversal_chamber	0.00556097	0.00669454	5.65373e-05	0.0106368
fuel_flow_0.075kgs	fuel_flow	0.075	HX_5	tube_bank	0.0121862	0.134561	0.00211278	0.213802
fuel_flow_0.075kgs	fuel_flow	0.075	HX_6	economiser	9.41638e-05	0.101598	0.00189444	
fuel_flow_0.1kgs	fuel_flow	0.1	HX_1	single_tube	2.75285	2.86136	0.00241321	4.55016
fuel_flow_0.1kgs	fuel_flow	0.1	HX_2	reversal_chamber	0.125021	0.134477	0.000204414	0.213846
fuel_flow_0.1kgs	fuel_flow	0.1	HX_3	tube_bank	0.211055	1.0554	0.00305847	1.67831
fuel_flow_0.1kgs	fuel_flow	0.1	HX_4	reversal_chamber	0.00788276	0.00971726	6.4361e-05	0.0154525
fuel_flow_0.1kgs	fuel_flow	0.1	HX_5	tube_bank	0.0176618	0.223605	0.00264989	0.355579
fuel_flow_0.1kgs	fuel_flow	0.1	HX_6	economiser	0.000113941	0.138523	0.00210994	
fuel_flow_0.125kgs	fuel_flow	0.125	HX_1	single_tube	3.20007	3.33794	0.00269907	5.31255
fuel_flow_0.125kgs	fuel_flow	0.125	HX_2	reversal_chamber	0.164529	0.177259	0.000240464	0.28212
fuel_flow_0.125kgs	fuel_flow	0.125	HX_3	tube_bank	0.284575	1.47014	0.00370361	2.33983
fuel_flow_0.125kgs	fuel_flow	0.125	HX_4	reversal_chamber	0.0103476	0.0129923	7.19357e-05	0.0206781
fuel_flow_0.125kgs	fuel_flow	0.125	HX_5	tube_bank	0.023569	0.328038	0.00315911	0.522095
fuel_flow_0.125kgs	fuel_flow	0.125	HX_6	economiser	0.000132789	0.176839	0.00228218	

Appendix C

Codebase

The complete Python codebase and configuration files used to generate all numerical results and figures presented in this thesis are provided in the following pages. The code is included verbatim for reproducibility and archival purposes.

Appendix C – Python Codebase Author: Saif-Aldain Aqel

This document contains the complete Python source code and configuration files used to generate all results and figures presented in this thesis. The code is provided verbatim for reproducibility and archival purposes.

```
=====
FILE: init.py =====
=====
===== FILE: main.py =====
import logging from common.logging_utils import setup_logging from common.units import Q_ from common.boiler_loop import run_boiler_case

log = logging.getLogger(name)

def run_default_case() -> None: run_boiler_case(run_id="default_case")

def run_excess_air_sensitivity() -> None: ea_values = [1.00, 1.05, 1.10, 1.15, 1.20, 1.30]

for ea in ea_values:
    logging.getLogger(__name__).info(f"Running case with excess_air_ratio={ea}")

    run_boiler_case(
        operation_overrides={"excess_air_ratio": Q_(ea, "")},
        tol_m=Q_(1e-3, "kg/s"),
        max_iter=20,
        write_csv=True,
        run_id=f"excess_air_{ea}",
    )

def run_water_pressure_sensitivity() -> None: Pbar_values = [4.0, 10.0, 16.0]

for P_bar in Pbar_values:
    logging.getLogger(__name__).info(f"Running case with drum pressure={P_bar} bar")

    run_boiler_case(
        operation_overrides={"drum_pressure": Q_(P_bar, "bar")},
        tol_m=Q_(1e-3, "kg/s"),
        max_iter=20,
        write_csv=True,
        run_id=f"drum_pressure_{P_bar}bar",
    )

def run_fuel_flow_sensitivity() -> None: mdot_values = [0.025, 0.050, 0.075, 0.10, 0.125] # kg/s

for mdot in mdot_values:
    logging.getLogger(__name__).info(f"Running case with fuel mass_flow={mdot} kg/s")

    run_boiler_case(
        fuel_overrides={"mass_flow": Q_(mdot, "kg/s")},
        tol_m=Q_(1e-3, "kg/s"),
        max_iter=20,
        write_csv=True,
        run_id=f"fuel_flow_{mdot}kgs",
    )

def run_fouling_sensitivity() -> None: factors = [1, 5, 10] for f in factors: logging.getLogger(name).info(f"Running case with fouling_factor={f}")

    run_boiler_case(
        fouling_factor=f,
        tol_m=Q_(1e-3, "kg/s"),
```

```

        max_iter=20,
        write_csv=True,
        run_id=f"fouling_{f}",
    )
def main() -> None: setup_logging("INFO")
log.info("start")

run_default_case()
# run_excess_air_sensitivity()
# run_water_pressure_sensitivity()
# run_fuel_flow_sensitivity()
# run_fouling_sensitivity()
log.info("end")

if name == "main": main()

=====
FILE: analysis/analyze_boiler_runs.py
===== from pathlib import Path import re import pandas as pd

RESULTS_DIR = Path("results/runs") SUMMARY_DIR = Path("results/summary")
FILE_RE = re.compile( r"(?P<case>/+|default_case)(?P<boiler_summary>|stages_summary|steps).csv$" )

def parse_param_value(raw): if raw is None: return None

for suffix in ("kgs", "bar"):
    if raw.endswith(suffix):
        raw = raw[: -len(suffix)]

try:
    return float(raw)
except ValueError:
    return raw

def discover_runs(results_dir: Path):
    runs = {}

    for path in results_dir.glob("*.csv"):
        m = FILE_RE.match(path.name)
        if not m:
            continue

        case = m.group("case")
        param = m.group("param")
        raw_value = m.group("value")
        kind = m.group("kind")

        info = runs.setdefault(
            case,
            {
                "case": case,
                "param": param if param is not None else "control",
                "value": parse_param_value(raw_value),
                "files": {},
            },
        ),

```

```

        )
    info["files"][kind] = path

return runs

def load_boiler_as_series(path: Path, run_name: str, param_group: str, param_value):
    df = pd.read_csv(path)
    s = df.set_index("parameter")["value"]
    s = s.copy()
    s["run"] = run_name
    s["param_group"] = param_group
    s["param_value"] = param_value
    return s

def load_stage_as_tidy(path: Path, run_name: str, param_group: str, param_value):
    df_raw = pd.read_csv(path, index_col=0)
    df = df_raw.T.reset_index().rename(columns={"index": "stage"})
    df.insert(0, "run", run_name)
    df.insert(1, "param_group", param_group)
    df.insert(2, "param_value", param_value)
    return df

def load_steps(path: Path):
    return pd.read_csv(path)

def main():
    RESULTS_DIR.mkdir(exist_ok=True)
    SUMMARY_DIR.mkdir(parents=True, exist_ok=True)

    runs = discover_runs(RESULTS_DIR)

    if not runs:
        print("[INFO] No runs discovered in 'results/' matching expected patterns.")
        return

    boiler_rows = []
    stage_rows = []

    for case, info in runs.items():
        files = info["files"]
        run_name = info["case"]
        param_group = info["param"]
        param_value = info["value"]

        if "boiler_summary" in files:
            s = load_boiler_as_series(files["boiler_summary"], run_name, param_group, param_value)
            boiler_rows.append(s)
        else:
            print(f"[WARN] run {run_name}: boiler_summary file missing.")

        if "stages_summary" in files:
            df_stages = load_stage_as_tidy(files["stages_summary"], run_name, param_group, param_value)
            stage_rows.append(df_stages)
        else:
            print(f"[WARN] run {run_name}: stages_summary file missing.")

        if "steps" not in files:
            print(f"[WARN] run {run_name}: steps file missing.")

    if boiler_rows:
        boiler_df = pd.DataFrame(boiler_rows)

        cols = list(boiler_df.columns)
        for key in ["run", "param_group", "param_value"]:
            if key in cols:
                cols.remove(key)
        ordered_cols = ["run", "param_group", "param_value"] + cols

```

```

boiler_df = boiler_df[ordered_cols]

boiler_df = boiler_df.sort_values(
    by=["param_group", "param_value"],
    ascending=[True, True],
    kind="mergesort",
    na_position="last",
)

boiler_df.to_csv(SUMMARY_DIR / "boiler_kpis_all_runs.csv", index=False)
print(f"[INFO] Wrote boiler KPIs table (with deviations): {SUMMARY_DIR / 'boiler_kpis_all_runs.csv'}")
else:
    print("[INFO] No boiler KPI data collected.")

if stage_rows:
    non_empty_stage_rows = [df for df in stage_rows if not df.empty]

    if non_empty_stage_rows:
        stages_df = pd.concat(non_empty_stage_rows, ignore_index=True)

        stages_df = stages_df.sort_values(
            by=["param_group", "param_value"],
            ascending=[True, True],
            kind="mergesort",
            na_position="last",
        )

        stages_df.to_csv(SUMMARY_DIR / "stages_summary_all_runs.csv", index=False)
        print(f"[INFO] Wrote stages summary table: {SUMMARY_DIR / 'stages_summary_all_runs.csv'}")
    else:
        print("[INFO] Stage summary dataframes are all empty; nothing to write.")
else:
    print("[INFO] No stage summary data collected.")

if name == "main": main()

=====
FILE: analysis/map.py =====
from pathlib import Path import numpy as np import pandas as pd import matplotlib.pyplot as plt

HX_CSV = Path(r"results/summary/stages_summary_all_runs.csv") OUTDIR = Path(r"results/plots/map")

def ensure_outdir(path: Path) -> Path: path.mkdir(parents=True, exist_ok=True) return path

def rename_hx_columns(df: pd.DataFrame) -> pd.DataFrame: mapping = { "gas in pressure[pa]": "p_gas_in", "gas in temp[°C]": "T_gas_in", "gas in enthalpy[kJ/kg)": "h_gas_in", "gas out pressure[pa)": "p_gas_out", "gas out temp[°C)": "T_gas_out", "gas out enthalpy[kJ/kg)": "h_gas_out", "water pressure[pa)": "p_water", "water in temp[°C)": "T_water_in", "water in enthalpy[kJ/kg)": "h_water_in", "water out temp[°C)": "T_water_out", "water out enthalpy[kJ/kg)": "h_water_out", "gas avg velocity[m/s)": "v_gas", "water avg velocity[m/s)": "v_water", "pressure drop fric[pa)": "dp_fric", "pressure drop minor[pa)": "dp_minor", "pressure drop total[pa)": "dp_total", "Q conv[MW)": "Q_conv", "Q rad[MW)": "Q_rad", "Q total[MW)": "Q_total", "UA[MW/K)": "UA", "steam capacity[t/h)": "steam_capacity", } df = df.rename(columns={k: v for k, v in mapping.items() if k in df.columns})

if "stage" in df.columns:
    df["stage_index"] = (
        df["stage"]
        .astype(str)

```

```

        .str.extract(r"(\d+)", expand=False)
        .astype(int)
    )
return df

def _plot_single_heatmap( df: pd.DataFrame, value_col: str, outdir: Path, filename: str, title: str,
cbar_label: str, ) -> None: if "run" not in df.columns or "stage_index" not in df.columns: return if value_col not in df.columns: return

table = df.pivot_table(
    index="run",
    columns="stage_index",
    values=value_col,
    aggfunc="mean",
)
if table.empty:
    return

fig, ax = plt.subplots()
im = ax.imshow(table.values, aspect="auto")

ax.set_yticks(np.arange(len(table.index)))
ax.set_yticklabels(table.index)
ax.set_xticks(np.arange(len(table.columns)))
ax.set_xticklabels(table.columns)

ax.set_xlabel("HX stage index [-]")
ax.set_ylabel("Run")
ax.set_title(title)

fig.colorbar(im, ax=ax, label=cbar_label)
fig.tight_layout()
fig.savefig(outdir / filename, dpi=200)
plt.close(fig)

def plot_hx_heatmaps(hx: pd.DataFrame, outdir: Path) -> None: df = hx.copy() outdir = ensure_outdir(outdir) if df.empty: return

heatmaps = {
    "Q_total": (
        "heatmap_Q_total.png",
        "Heat duty per stage and run [MW]",
        "Q_total [MW]",
    ),
    "T_gas_out": (
        "heatmap_T_gas_out.png",
        "Gas outlet temperature per stage and run [°C]",
        "T_gas_out [°C]",
    ),
    "T_gas_in": (
        "heatmap_T_gas_in.png",
        "Gas inlet temperature per stage and run [°C]",
        "T_gas_in [°C]",
    ),
    "T_water_in": (

```

```

    "heatmap_T_water_in.png",
    "Water inlet temperature per stage and run [°C]",
    "T_water_in [°C]",
),
"T_water_out": (
    "heatmap_T_water_out.png",
    "Water outlet temperature per stage and run [°C]",
    "T_water_out [°C]",
),
"v_gas": (
    "heatmap_v_gas.png",
    "Gas velocity per stage and run [m/s]",
    "v_gas [m/s]",
),
"v_water": (
    "heatmap_v_water.png",
    "Water velocity per stage and run [m/s]",
    "v_water [m/s]",
),
"dp_total": (
    "heatmap_dp_total.png",
    "Total pressure drop per stage and run [Pa]",
    "Δp_total [Pa]",
),
"Q_conv": (
    "heatmap_Q_conv.png",
    "Convective heat duty per stage and run [MW]",
    "Q_conv [MW]",
),
"Q_rad": (
    "heatmap_Q_rad.png",
    "Radiative heat duty per stage and run [MW]",
    "Q_rad [MW]",
),
"UA": (
    "heatmap_UA.png",
    "UA per stage and run [MW/K]",
    "UA [MW/K]",
),
"steam_capacity": (
    "heatmap_steam_capacity.png",
    "Steam capacity per stage and run [t/h]",
    "Steam capacity [t/h]",
),
}

for col, (fname, title, cbar) in heatmaps.items():
    _plot_single_heatmap(df, col, outdir, fname, title, cbar)

def main(): ensure_outdir(OUTDIR) hx = pd.read_csv(HX_CSV) hx = rename_hx_columns(hx)
plot_hx_heatmaps(hx, OUTDIR)

if name == "main": main()
=====
===== FILE: analysis/per_run.py =====

```

```

from pathlib import Path import sys from typing import Dict import pandas as pd import matplotlib.pyplot
as plt from matplotlib.lines import Line2D

style_colors: Dict[str, str] = { "Q_in": "tab:blue", "Q_useful": "tab:orange", "eta_direct": "tab:green",
"eta_indirect": "tab:red", "feedwater_flow": "tab:blue", "steam_capacity": "tab:orange", "stack_temperature": "tab:red", "pressure_drop": "tab:purple", }

style_linestyles: Dict[str, str] = { "Q_in": "-", "Q_useful": "--", "eta_direct": "-.", "eta_indirect": "-.",
"feedwater_flow": "--", "steam_capacity": "--", "stack_temperature": "--", "pressure_drop": "--", }

style_markers: Dict[str, str] = { "excess_air": "o", "fuel_flow": "s", "drum_pressure": "D", "control": "x",
"fouling": "^", }

param_xlabels: Dict[str, str] = { "excess_air": "Excess air [-]", "fuel_flow": "Fuel flow [kg/s]", "drum_pressure": "Drum pressure [bar]", "control": "Control case [-]", "fouling": "Fouling factor [-]", }

def _get_xlabel(param_group: str) -> str: return param_xlabels.get(param_group, "Parameter value [-]")

param_group_style = { "excess_air": dict(color="tab:blue", marker="o", linestyle="-"), "fuel_flow": dict(color="tab:orange", marker="s", linestyle="--"), "drum_pressure": dict(color="tab:green", marker="D", linestyle="-."), "control": dict(color="tab:red", marker="x", linestyle="-"), "fouling": dict(color="tab:purple", marker="^", linestyle="--"), }

def _get_pg_style(param_group: str) -> dict: return param_group_style.get( param_group,
dict(color="black", marker="o", linestyle="--"), )

plt.rcParams["font.size"] = 11 plt.rcParams["axes.titlesize"] = 12 plt.rcParams["axes.labelsize"] = 11
plt.rcParams["legend.fontsize"] = 9 plt.rcParams["figure.dpi"] = 100 plt.rcParams["font.family"] = "DejaVu Sans"
plt.rcParams["axes.grid"] = True plt.rcParams["grid.linestyle"] = ":" plt.rcParams["grid.linewidth"] = 0.5
plt.rcParams["grid.alpha"] = 0.7

def load_data(csv_path: str) -> pd.DataFrame: csv_file = Path(csv_path) df = pd.read_csv(csv_file)
df["param_value"] = pd.to_numeric(df["param_value"], errors="coerce") return df

def load_steps_data(csv_path: str) -> pd.DataFrame: csv_file = Path(csv_path) df = pd.read_csv(csv_file)

num_cols = [
    "x[m]",
    "gas_T[°C]", "water_T[°C]",
    "gas_P[kPa]", "water_P[kPa]",
    "gas_V[m/s]", "water_V[m/s]",
    "h_gas[W/m^2/K]", "h_water[W/m^2/K]",
]
for c in num_cols:
    if c in df.columns:
        df[c] = pd.to_numeric(df[c], errors="coerce")

return df

def _sweep_percent(series: pd.Series) -> pd.Series: s = pd.to_numeric(series, errors="coerce") smin =
s.min() smax = s.max() if pd.isna(smin) or pd.isna(smax) or smax == smin: return pd.Series([0.0] * len(s),
index=s.index) return (s - smin) / (smax - smin) * 100.0

def _get_marker(param_group: str): return style_markers.get(param_group, None)

def plot_Qin_Quseful(ax, df_group: pd.DataFrame, param_group: str) -> None: df_plot =
df_group.dropna(subset=[["param_value"]]).sort_values("param_value")

marker = _get_marker(param_group)

x = df_plot["param_value"]

```

```

y_qin = df_plot["Q_in total[MW]"]
y_quse = df_plot["Q_useful[MW]"]

line_qin, = ax.plot(
    x,
    y_qin,
    label="Total heat input $Q_{in}$",
    color=style_colors.get("Q_in", None),
    linestyle=style_linestyles.get("Q_in", "-"),
    marker=marker,
)
line_quse, = ax.plot(
    x,
    y_quse,
    label="Useful heat $Q_{useful}$",
    color=style_colors.get("Q_useful", None),
    linestyle=style_linestyles.get("Q_useful", "--"),
    marker=marker,
)

ax.set_xlabel(_get_xlabel(param_group))
ax.set_ylabel("Heat rate [MW]")
ax.set_title("Heat rates")
ax.grid(True, which="both")
ax.legend(loc="best", framealpha=0.8)

def plot_eta(ax, df_group: pd.DataFrame, param_group: str) -> None: df_plot = df_group.dropna(subset=[“param_value”])
marker = _get_marker(param_group)

x = df_plot["param_value"]
y_eta_dir = df_plot["eta direct[-]"]
y_eta_ind = df_plot["eta indirect[-]"]

line_eta_dir, = ax.plot(
    x,
    y_eta_dir,
    label="Direct efficiency",
    color=style_colors.get("eta_direct", None),
    linestyle=style_linestyles.get("eta_direct", "-"),
    marker=marker,
)
line_eta_ind, = ax.plot(
    x,
    y_eta_ind,
    label="Indirect efficiency",
    color=style_colors.get("eta_indirect", None),
    linestyle=style_linestyles.get("eta_indirect", "--"),
    marker=marker,
)

ax.set_xlabel(_get_xlabel(param_group))
ax.set_ylabel("Efficiency [-]")
ax.set_title("Boiler efficiency")
ax.grid(True, which="both")

```

```

ax.legend(loc="best", framealpha=0.8)

def plot_water_steam(ax, df_group: pd.DataFrame, param_group: str) -> None:
    df_plot = df_group.dropna(subset=["param_value"]).sort_values("param_value")
    marker = _get_marker(param_group)

    x = df_plot["param_value"]
    y_water = df_plot["feedwater flow[kg/s]"]
    y_steam = df_plot["steam capacity[t/h]"]

    line_water, = ax.plot(
        x,
        y_water,
        label="feedwater_flow",
        color=style_colors.get("feedwater_flow", None),
        linestyle=style_linestyles.get("feedwater_flow", "-"),
        marker=marker,
    )
    ax.set_xlabel(_get_xlabel(param_group))
    ax.set_ylabel("feedwater flow [kg/s]")
    ax.set_title("Water and steam")

    ax2 = ax.twinx()
    line_steam, = ax2.plot(
        x,
        y_steam,
        label="Steam capacity",
        color=style_colors.get("steam_capacity", None),
        linestyle=style_linestyles.get("steam_capacity", "--"),
        marker=marker,
    )
    ax2.set_ylabel("Steam capacity [t/h]")

    ax.grid(True, which="both")

    lines = [line_water, line_steam]
    labels = [l.get_label() for l in lines]
    ax.legend(lines, labels, loc="best", framealpha=0.8)

def plot_stack_pressure(ax, df_group: pd.DataFrame, param_group: str) -> None:
    df_plot = df_group.dropna(subset=["param_value"]).sort_values("param_value")
    marker = _get_marker(param_group)

    x = df_plot["param_value"]
    y_stack = df_plot["stack temperature[°C]"]
    y_dp = df_plot["pressure drop total[kPa]"].abs()

    line_stack, = ax.plot(
        x,
        y_stack,
        label="Stack temperature",
        color=style_colors.get("stack_temperature", None),
        linestyle=style_linestyles.get("stack_temperature", "-"),
        marker=marker,
    )
    ax.set_xlabel(_get_xlabel(param_group))
    ax.set_ylabel("Stack temperature [°C]")
    ax.set_title("Stack and pressure drop")

```

```

ax2 = ax.twinx()
line_dp, = ax2.plot(
    x,
    y_dp,
    label="Total pressure drop",
    color=style_colors.get("pressure_drop", None),
    linestyle=style_linestyles.get("pressure_drop", "--"),
    marker=marker,
)
ax2.set_ylabel("Total pressure drop [Pa]")

ax.grid(True, which="both")

lines = [line_stack, line_dp]
labels = [l.get_label() for l in lines]
ax.legend(lines, labels, loc="best", framealpha=0.8)

def generate_overall_kpi_figure(csv_path: str, output_dir: str = "figures") -> None:
    df = load_data(csv_path)
    out_dir = Path(output_dir)
    out_dir.mkdir(parents=True, exist_ok=True)

    df = df.dropna(subset=["param_value"]).copy()
    df_all = df.copy()
    kpi_defs = [
        {"column": "Tad[°C]", "label": "Tad [°C]"},
        {"column": "stack temperature[°C]", "label": "Stack temperature [°C]"},
        {"column": "air flow[kg/s]", "label": "Air flow [kg/s]"},
        {"column": "feedwater flow[kg/s]", "label": "feedwater flow [kg/s]"},
        {"column": "Q_in total[MW]", "label": "Heat input $Q_{in}$ [MW]"},
        {"column": "steam capacity[t/h]", "label": "Steam capacity [t/h]"},
        {"column": "pressure drop total[kPa]", "label": "Total pressure drop [kPa]", "abs": True},
        {"column": "eta direct[-]", "label": "Direct efficiency [-]"},
    ]
    fig, axes = plt.subplots(4, 2, figsize=(9, 10))
    axes_flat = axes.flatten()

    for ax in axes_flat:
        ax.set_xlim(0, 100)
        ax.set_xticks([0, 100])
        ax.set_xticklabels(["Min", "Max"])

    for ax, kpi in zip(axes_flat, kpi_defs):
        ax.set_xlabel("Parameter range")
        ax.set_ylabel(kpi["label"])
        ax.grid(True, which="both")

    legend_handles = {}

    for param_group, df_group in df.groupby("param_group"):
        df_group_sorted = df_group.sort_values("param_value")
        x = _sweep_percent(df_group_sorted["param_value"])

        pg_style = _get_pg_style(param_group)
        marker = pg_style["marker"]

```

```

color = pg_style["color"]
line_style = pg_style["linestyle"]

for ax, kpi in zip(axes_flat, kpi_defs):
    col = kpi["column"]
    if col not in df_group_sorted.columns:
        continue

    y_raw = df_group_sorted[col]
    y = y_raw.abs() if kpi.get("abs", False) else y_raw

    line, = ax.plot(
        x, y,
        marker=marker,
        linestyle=line_style,
        color=color,
        label=param_group,
    )

    if param_group not in legend_handles:
        legend_handles[param_group] = line

for ax, kpi in zip(axes_flat, kpi_defs):
    col = kpi["column"]
    if col not in df_all.columns:
        continue

    df_overlay = df_all.dropna(subset=["param_value", col]).copy()
    if kpi.get("abs", False):
        df_overlay[col] = df_overlay[col].abs()

if legend_handles:
    fig.legend(
        handles=list(legend_handles.values()),
        labels=list(legend_handles.keys()),
        loc="lower center",
        ncol=min(len(legend_handles), 4),
        framealpha=0.8,
        bbox_to_anchor=(0.5, 0.02),
    )

fig.tight_layout(rect=(0.0, 0.05, 1.0, 1.0))

out_path = out_dir / "kpi_overview_all_param_groups.png"
fig.savefig(out_path, dpi=300)
plt.close(fig)

def generate_eff_stack_scatter( csv_path: str = "results/summary/boiler_kpis_all_runs.csv", output_dir: str = "figures", ) -> None: df = load_data(csv_path) out_dir = Path(output_dir) out_dir.mkdir(parents=True, exist_ok=True)

needed = ["param_group", "stack temperature[°C]", "eta direct[-]", "eta indirect[-]"]
missing = [c for c in needed if c not in df.columns]
if missing:
    raise KeyError(f"Missing columns for scatter: {missing}")

```

```

dfp = df.dropna(subset=["stack temperature[°C]", "eta direct[-]", "eta indirect[-]"]).copy()

fig, ax_dir = plt.subplots(1, 1, figsize=(7.5, 4))

df_non_control = dfp[dfp["param_group"].astype(str).str.lower() != "control"].copy()
df_control     = dfp[dfp["param_group"].astype(str).str.lower() == "control"].copy()

for pg, dpg in df_non_control.groupby("param_group"):
    st = _get_pg_style(str(pg))
    ax_dir.scatter(
        dpg["stack temperature[°C]"],
        dpg["eta direct[-]"],
        label=str(pg),
        color=st["color"],
        marker=st["marker"],
        s=28,
        alpha=0.85,
        zorder=2,
    )

if not df_control.empty:
    stc = _get_pg_style("control")
    ax_dir.scatter(
        df_control["stack temperature[°C]"],
        df_control["eta direct[-]"],
        label="control",
        color=stc["color"],
        marker=stc["marker"],
        s=60,
        alpha=1.0,
        linewidths=0.6,
        zorder=10,
    )

ax_dir.set_title("Direct efficiency vs stack temperature")
ax_dir.set_xlabel("Stack temperature [°C]")
ax_dir.set_ylabel("Direct efficiency [-] (LHV)")
ax_dir.grid(True, which="both")

handles, labels = ax_dir.get_legend_handles_labels()
if handles:
    ax_dir.legend(
        handles=handles,
        labels=labels,
        loc="best",
        framealpha=0.8,
    )

fig.tight_layout()

out_path = out_dir / "scatter_efficiency_vs_stack_temperature_all_runs.png"
fig.savefig(out_path, dpi=300, bbox_inches="tight")
plt.close(fig)

```

```

def generate_stage_combined_control_figure( csv_path: str = "results/summary/stages_summary_all_runs.csv",
output_dir: str = "figures", ) -> None: df = load_data(csv_path) out_dir = Path(output_dir)
out_dir.mkdir(parents=True, exist_ok=True)

df = df[df["param_group"].astype(str).str.lower() == "control"].copy()
if df.empty:
    raise ValueError("No rows found for param_group == 'control' in stages summary CSV.")

if df["stage"].dtype == object:
    df["stage_index"] = (
        df["stage"].astype(str).str.extract(r"\d+", expand=False).astype(int)
    )
else:
    df["stage_index"] = df["stage"].astype(int)

df = df.dropna(subset=["stage_index"]).copy()

plot_cols = [
    "gas out temp[°C]",
    "Q total[MW]",
    "Q rad[MW]",
    "Q conv[MW]",
    "UA[MW/K]",
    "gas out pressure[kpa]",
    "pressure drop total[kpa]",
    "gas avg velocity[m/s]",
]
for c in plot_cols:
    if c in df.columns:
        df[c] = pd.to_numeric(df[c], errors="coerce")

fig, axes = plt.subplots(4, 2, figsize=(10, 10))
ax_Tg = axes[0, 0]
ax_Q = axes[0, 1]
ax_Qrad = axes[1, 0]
ax_Qconv= axes[1, 1]
ax_UA = axes[2, 0]
ax_p = axes[2, 1]
ax_dp = axes[3, 0]
ax_vel = axes[3, 1]

stage_ticks = sorted(df["stage_index"].unique())
for ax in (ax_Tg, ax_Q, ax_Qrad, ax_Qconv, ax_UA, ax_p, ax_dp, ax_vel):
    ax.set_xlabel("Stage [-]")
    ax.set_xticks(stage_ticks)
    ax.grid(True, which="both")

ax_Tg.set_ylabel("Gas outlet temperature [°C]")
ax_Q.set_ylabel("Stage duty $Q_{\mathit{stage}}$ [MW]")
ax_Qrad.set_ylabel("$Q_{\mathit{rad}}$ [MW]")
ax_Qconv.set_ylabel("$Q_{\mathit{conv}}$ [MW]")
ax_UA.set_ylabel("Stage conductance $UA$ [MW/K]")
ax_p.set_ylabel("Gas outlet pressure [kPa]")
ax_dp.set_ylabel("Total pressure drop [kPa]")

```

```

ax_vel.set_ylabel("Gas average velocity [m/s]")

st = _get_pg_style("control")
color = st["color"]
marker = st["marker"]
line_style = st["linestyle"]
lw = 0.9

for run_name, df_run in df.groupby("run"):
    df_run = df_run.sort_values("stage_index")

    x = df_run["stage_index"]
    y_Tg = df_run["gas out temp[°C]"]
    y_Q = df_run["Q total[MW]"]
    y_Qrad = df_run["Q rad[MW]"]
    y_Qconv= df_run["Q conv[MW]"]
    y_UA = df_run["UA[MW/K]"]
    y_p = df_run["gas out pressure[kpa]"]
    y_dp = df_run["pressure drop total[kpa]"].abs()
    y_vel = df_run["gas avg velocity[m/s]"]

    ax_Tg.plot(x, y_Tg, marker=marker, linestyle=line_style, color=color, linewidth=lw, label="Control case")
    ax_Q.plot(x, y_Q, marker=marker, linestyle=line_style, color=color, linewidth=lw)
    ax_Qrad.plot(x, y_Qrad, marker=marker, linestyle=line_style, color=color, linewidth=lw)
    ax_Qconv.plot(x, y_Qconv, marker=marker, linestyle=line_style, color=color, linewidth=lw)
    ax_UA.plot(x, y_UA, marker=marker, linestyle=line_style, color=color, linewidth=lw)
    ax_p.plot(x, y_p, marker=marker, linestyle=line_style, color=color, linewidth=lw)
    ax_dp.plot(x, y_dp, marker=marker, linestyle=line_style, color=color, linewidth=lw)
    ax_vel.plot(x, y_vel, marker=marker, linestyle=line_style, color=color, linewidth=lw)

handles, labels = ax_Tg.get_legend_handles_labels()
if handles:
    fig.legend(
        handles=handles,
        labels=labels,
        loc="lower center",
        ncol=min(len(labels), 4),
        framealpha=0.8,
        bbox_to_anchor=(0.5, 0.02),
    )

fig.tight_layout(rect=(0.0, 0.06, 1.0, 0.98))

out_path = out_dir / "stages_control_combined_8plots.png"
fig.savefig(out_path, dpi=300)
plt.close(fig)

def generate_all_figures(csv_path: str, output_dir: str = "figures") -> None:
    df = load_data(csv_path)
    out_dir = Path(output_dir)
    out_dir.mkdir(parents=True, exist_ok=True)

    grouped = df.groupby("param_group")

```

```

for param_group, df_group in grouped:
    df_group_numeric = df_group.dropna(subset=["param_value"])
    if df_group_numeric["param_value"].nunique(dropna=True) < 2:
        continue

    fig, axes = plt.subplots(2, 2, figsize=(8, 6))
    ax_t1 = axes[0, 0]
    ax_tr = axes[0, 1]
    ax_b1 = axes[1, 0]
    ax_br = axes[1, 1]

    plot_Qin_Quseful(ax_t1, df_group_numeric, param_group)
    plot_eta(ax_tr, df_group_numeric, param_group)
    plot_water_steam(ax_b1, df_group_numeric, param_group)
    plot_stack_pressure(ax_br, df_group_numeric, param_group)

    fig.tight_layout()

    safe_group = str(param_group).replace(" ", "_")
    png_path = out_dir / f"performance_{safe_group}.png"

    fig.savefig(png_path, dpi=300)
    plt.close(fig)

if name == "main": default_csv = "results/summary/boiler_kpis_all_runs.csv" default_output = "results/plots/per_run"

if len(sys.argv) >= 2:
    csv_arg = sys.argv[1]
else:
    csv_arg = default_csv

if len(sys.argv) >= 3:
    out_arg = sys.argv[2]
else:
    out_arg = default_output

generate_all_figures(csv_arg, output_dir=out_arg)

generate_overall_kpi_figure(csv_arg, output_dir=out_arg)

generate_eff_stack_scatter(csv_arg, output_dir=out_arg)

stage_csv = "results/summary/stages_summary_all_runs.csv"
generate_stage_combined_control_figure(stage_csv, output_dir=out_arg)
=====
FILE: analysis/tables.py =====
import os
import pandas as pd

INPUT_CSV = os.path.join("results", "summary", "boiler_kpis_all_runs.csv") OUTPUT_MD = os.path.join("results", "summary", "boiler_kpis_tables.md") STAGES_CSV = os.path.join("results", "runs", "default_case_stages_summary.csv")

def pretty_kpi_label(name: str) -> str: stripped = name.strip()

if "[" in stripped and stripped.endswith("]"):
    base, unit = stripped.split("[", 1)

```

```

base = base.strip()
unit = "[" + unit
else:
    base, unit = stripped, ""

b = base.lower()

if b.startswith("eta direct"):
    return r"\eta_{\mathrm{direct}} [-]"
if b.startswith("eta indirect"):
    return r"\eta_{\mathrm{indirect}} [-]"
if b.startswith("tad"):
    return f"adiabatic temperature {unit}.strip()"
if b.startswith("ua"):
    return f"conductance {unit}.strip()"
if b.startswith("q_in total"):
    return f"input heat {unit}.strip()"
if b.startswith("q_useful"):
    return f"useful heat {unit}.strip()"
if b.startswith("p-lhv"):
    return f"firing rate {unit}.strip()

return stripped.title()

def is_number(x) -> bool: try: float(x) return True except Exception: return False

def format_param_value(v) -> str: if is_number(v): return f"{float(v):.2f}" return str(v)

def format_stage_row_label(name: str) -> str: # reuse KPI prettifier for consistent naming return pretty_kpi_label(name)

def format_stage_cell(v) -> str: # keep blanks as blank (your CSV has empty cells) if pd.isna(v) or v == "": return "" if is_number(v): return f"{float(v):.2f}" return str(v)

def append_stages_summary_table(lines: list[str], stages_csv_path: str) -> None: if not os.path.exists(stages_csv_path):
    return

stages = pd.read_csv(stages_csv_path)

# First column is "name" (row labels)
if "name" not in stages.columns:
    return

# Set index to the row label column, keep stage columns as columns
stages = stages.set_index("name")

# Format values cell-by-cell (handles numeric + blanks)
stages = stages.applymap(format_stage_cell)

# Pretty row labels
stages.index = [format_stage_row_label(i) for i in stages.index]
stages.index.name = "stage KPI"

# Add to markdown output
lines.append("## default case stages summary\n")
lines.append(stages.to_markdown())
lines.append("")

```

```

def main():
    df = pd.read_csv(INPUT_CSV)

    if "LHV[kJ/kg]" in df.columns:
        df["LHV[kJ/kg]"] = df["LHV[kJ/kg]"] / 1000.0
        df = df.rename(columns={"LHV[kJ/kg]": "LHV [MJ/kg]})

    num_cols = df.select_dtypes(include="number").columns
    df[num_cols] = df[num_cols].round(2)

    id_vars = ["run", "param_group", "param_value"]
    value_vars = [c for c in df.columns if c not in id_vars]

    group_meta = {
        "control": ("Control", "control"),
        "excess_air": ("Excess air", "excess air [-]"),
        "fuel_flow": ("Fuel flow", "fuel flow [kg/s]"),
        "drum_pressure": ("Drum pressure", "drum pressure [bar]"),
        "fouling": ("Fouling", "fouling [-"]),
    }

    lines = []

    melted = df.melt(
        id_vars=id_vars,
        value_vars=value_vars,
        var_name="kpi",
        value_name="value",
    )

    for group_name, (title, index_label) in group_meta.items():

        if group_name == "control":
            sub = df[df["param_group"] == "control"]
            if sub.empty:
                continue

            row = sub.iloc[0]
            data = {"control": [row[k] for k in value_vars]}
            table = pd.DataFrame(data, index=value_vars)

            table.index = [pretty_kpi_label(i) for i in table.index]
            table.index.name = index_label

            lines.append(f"## {title.lower()}\n")
            lines.append(table.to_markdown())
            lines.append("")
            continue

        sub = melted[melted["param_group"] == group_name]
        if sub.empty:
            continue

        group_values = df.loc[df["param_group"] == group_name, "param_value"].tolist()
        seen = set()


```

```

ordered = []
for v in group_values:
    if v not in seen:
        seen.add(v)
        ordered.append(v)

if group_name == "drum_pressure":
    desired = [4.0, 10.0, 16.0]
    present = {float(v) for v in ordered if is_number(v)}
    ordered = [v for v in desired if v in present]

table = sub.pivot_table(
    index="kpi", columns="param_value", values="value", aggfunc="first"
)

table = table.reindex(index=value_vars)
table = table[ordered]
table = table.dropna(how="all")

table.index = [pretty_kpi_label(i) for i in table.index]
table.columns = [format_param_value(c) for c in table.columns]
table.index.name = index_label

lines.append(f"## {title.lower()}\n")
lines.append(table.to_markdown())
lines.append("")

append_stages_summary_table(lines, STAGES_CSV)

os.makedirs(os.path.dirname(OUTPUT_MD), exist_ok=True)
with open(OUTPUT_MD, "w", encoding="utf-8") as f:
    f.write("\n".join(lines))

if name == "main": main()
=====
===== FILE: combustion/init.py =====
===== FILE: combustion/adiabatic_flame_temperature.py
===== from common.units import ureg, Q_
from common.models import GasStream from scipy.optimize import root_scalar from common.props import GasProps import cantera as ct from combustion.mass_mole import to_mole, molar_flow from combustion.flue import from_fuel_and_air

def adiabatic_flame_T(air: GasStream, fuel: GasStream) -> GasStream: P_Pa = air.P.to("Pa").magnitude
T_air = air.T.to("K").magnitude T_fuel = fuel.T.to("K").magnitude

m_air = air.mass_flow.to("kg/s").magnitude
m_fuel = fuel.mass_flow.to("kg/s").magnitude
m_tot = m_air + m_fuel
if m_tot <= 0.0:
    raise ValueError("adiabatic_flame_T: total mass flow must be > 0")

X_air = to_mole({k: v.to("").magnitude for k, v in (air.comp or {}).items() if v.to("").magnitude > 0})
X_fuel = to_mole({k: v.to("").magnitude for k, v in (fuel.comp or {}).items() if v.to("").magnitude > 0})

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")

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

Hdot_react = m_air * gas_air.enthalpy_mass + m_fuel * gas_fuel.enthalpy_mass
h_target = Hdot_react / m_tot

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

def _mol_rate(X, n_tot): return {k: n_tot * float(x) for k, x in X.items()}
n_dot_sp = {}
for d in (_mol_rate(X_air, n_air), _mol_rate(X_fuel, n_fuel)):
    for k, v in d.items():
        n_dot_sp[k] = n_dot_sp.get(k, 0.0) + v
n_sum = sum(n_dot_sp.values())
if n_sum <= 0.0:
    raise ValueError("adiabatic_flame_T: empty reactant composition")
X_react = {k: v / n_sum for k, v in n_dot_sp.items()}

gas_mix.TPX = 300.0, P_Pa, X_react
gas_mix.HP = h_target, P_Pa
gas_mix.equilibrate("HP")

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

return GasStream(
    mass_flow=Q_(m_tot, "kg/s"),
    T=Q_(gas_mix.T, "K"),
    P=air.P,
    comp=comp_eq,
)
def adiabatic_flame_T_no_dissociation(air: GasStream, fuel: GasStream) -> GasStream: m_air = air.mass_flow.to("kg/s").magnitude m_fuel = fuel.mass_flow.to("kg/s").magnitude m_tot = m_air + m_fuel if m_tot <= 0.0: raise ValueError("adiabatic_flame_T_no_dissociation: total mass flow must be > 0")
gasprops = GasProps()

h_air = gasprops.h(air.T, air.P, air.comp).to("J/kg").magnitude
h_fuel = gasprops.h(fuel.T, fuel.P, fuel.comp).to("J/kg").magnitude

Hdot_react = m_air * h_air + m_fuel * h_fuel
h_target = Hdot_react / m_tot

mass_comp_burnt, m_dot_flue = from_fuel_and_air(fuel, air)
comp_prod = {sp: Q_(float(y), "") for sp, y in mass_comp_burnt.items() if float(y) > 1e-15}

def f(T_K: float) -> float:
    hP = gasprops.h(Q_(T_K, "K"), air.P, comp_prod).to("J/kg").magnitude

```

```

    return hP - h_target

T_lo, T_hi = 250.0, 3500.0
f_lo, f_hi = f(T_lo), f(T_hi)
if f_lo * f_hi > 0.0:
    T_hi = 4500.0
    f_hi = f(T_hi)
    if f_lo * f_hi > 0.0:
        raise RuntimeError(
            "adiabatic_flame_T_no_dissociation: could not bracket root for Tad "
            "f\"(f({T_lo})={f_lo:.3e}, f({T_hi})={f_hi:.3e})\""
        )

sol = root_scalar(f, bracket=(T_lo, T_hi), method="brentq", xtol=1e-6, rtol=1e-8)
if not sol.converged:
    raise RuntimeError("adiabatic_flame_T_no_dissociation: root solve did not converge")

Tad = float(sol.root)

return GasStream(
    mass_flow=m_dot_flue.to("kg/s"),
    T=Q_(Tad, "K"),
    P=air.P,
    comp=comp_prod,
)
=====
=====FILE: combustion/combustor.py =====
from combustion.adiabatic_flame_temperature import adiabatic_flame_T from combustion.heat import
total_input_heat, compute_LHV_HHV from combustion.flue import air_flow_rates from common.results
import CombustionResult from common.models import GasStream from common.units import Q_ from
combustion.adiabatic_flame_temperature import adiabatic_flame_T_no_dissociation

class Combustor: def __init__(self, air: GasStream, fuel: GasStream, excess_air_ratio: Q_): self.air = air
self.fuel = fuel self.excess_air_ratio = excess_air_ratio

def run(self) -> CombustionResult:
    air = self.air
    fuel = self.fuel

    air.mass_flow = air_flow_rates(air, fuel, self.excess_air_ratio)

    power_LHV, Q_in = total_input_heat(fuel, air)
    HHV_mass, LHV_mass, P_HHV, P_LHV = compute_LHV_HHV(fuel, air)

    flue_ad = adiabatic_flame_T(air, fuel)
    T_ad = flue_ad.T

    flue_boiler = adiabatic_flame_T_no_dissociation(air, fuel)

    return CombustionResult(
        LHV = power_LHV,
        Q_in = Q_in,
        T_ad = T_ad,
        flue = flue_boiler,
    )

```

```

        flue_ad      = flue_ad,
        fuel_LHV_mass = LHV_mass,
        fuel_P_LHV   = P_LHV,
        fuel_mass_flow = fuel.mass_flow,
        excess_air_ratio= self.excess_air_ratio,
        air_mass_flow = air.mass_flow,
    )
=====
from common.models import GasStream from common.units import Q_ from common.constants import O2_per_mol from combustion.mass_mole import to_mole, molar_flow, mass_flow, to_mass, mix_molar_mass

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")

def air_flow_rates(air: GasStream, fuel: GasStream, excess: Q_) -> Q_: air_x = to_mole(air.comp) fuel_n_dot = molar_flow(fuel.comp, fuel.mass_flow) O2_x = air_x["O2"] O2_req = stoich_O2_required_per_mol_fuel(fu O2_stoich = fuel_n_dot * O2_req O2_actual = O2_stoich * excess air_n = O2_actual / O2_x M_air = mix_molar_mass(air_x) air_m = air_n * M_air return air_m

def from_fuel_and_air(fuel: GasStream, air: GasStream) -> tuple[dict[str, float], float]: O2_req = stoich_O2_required_per_mol_fuel(fuel) fuel_x = to_mole(fuel.comp) fuel_n = molar_flow(fuel.comp, fuel.mass_flow) air_x = to_mole(air.comp) air_n = molar_flow(air.comp, air.mass_flow)

gf=lambda k:fuel_x.get(k,0.0); ga=lambda k:air_x.get(k,0.0)
n_CO2 = air_n*ga("CO2")+fuel_n*gf("CO2")+fuel_n*(gf("CH4")+2*gf("C2H6")+3*gf("C3H8")+4*gf("C4H10"))
n_H2O = fuel_n*gf("H2O")+fuel_n*(2*gf("CH4")+3*gf("C2H6")+4*gf("C3H8")+5*gf("C4H10"))+fuel_n*gf("H2S")+air_n*ga("n_SO2 = fuel_n*gf("H2S")
n_O2  = air_n*ga("O2") - fuel_n*O2_req
n_N2  = air_n*ga("N2") + fuel_n*gf("N2")
n_Ar  = air_n*ga("Ar")
flows={"CO2":n_CO2,"H2O":n_H2O,"SO2":n_SO2,"O2":n_O2,"N2":n_N2,"Ar":n_Ar}

n_tot=sum(flows.values())
mol_comp={k:(v/n_tot if n_tot!=0 else 0.0) for k,v in flows.items()}
mass_comp = to_mass(mol_comp)
m_dot = mass_flow(mol_comp, n_tot)

return mass_comp, m_dot
=====
from common.units import Q_ import re import cantera as ct from common.props import WaterProps, GasProps from common.models import GasStream from combustion.mass_mole import to_mole from common.constants import molar_masses, T_ref, P_ref, O2_per_mol

_gasprops = GasProps()

def parse_CH(s: str): m = re.fullmatch(r'C(*)H(+)', s) if not m: return None, None C = int(m.group(1)) if m.group(1) else 1 H = int(m.group(2)) return C, H

def compute_LHV_HHV(fuel: GasStream, air: GasStream) -> tuple[Q_, Q_, Q_, Q_]: gas = ct.Solution("config/flue_cantera.yaml", "gas_mix")

fuel_x = to_mole({k: float(v.to("").magnitude) for k, v in (fuel.comp or {}).items() if float(v.to("").magnitude) > 0.0})
if not fuel_x:
    raise ValueError("compute_LHV_HHV: empty fuel composition")

```

```

air_x = to_mole({k: float(v.to("").magnitude) for k, v in (air.comp or {}).items()
                 if float(v.to("").magnitude) > 0.0})
if not air_x or air_x.get("O2", 0.0) <= 0.0:
    raise ValueError("compute_LHV_HHV: air composition missing O2")

def xf(sp: str) -> float:
    return float(fuel_x.get(sp, 0.0))

def xa(sp: str) -> float:
    return float(air_x.get(sp, 0.0))

O2_req = 0.0
for sp, x in fuel_x.items():
    req = O2_per_mol.get(sp, Q_(0.0, "")).to("").magnitude
    O2_req += float(x) * float(req)

n_air = O2_req / max(xa("O2"), 1e-30)

n_react = {}
for sp, x in fuel_x.items():
    if x > 0.0:
        n_react[sp] = n_react.get(sp, 0.0) + x

for sp, x in air_x.items():
    if x > 0.0:
        n_react[sp] = n_react.get(sp, 0.0) + n_air * x

nR_tot = sum(n_react.values())
X_react = {sp: n / nR_tot for sp, n in n_react.items() if n > 0.0}

n_CO2 = n_air * xa("CO2") + xf("CO2") + (xf("CH4") + 2*xf("C2H6") + 3*xf("C3H8") + 4*xf("C4H10"))
n_H2O = n_air * xa("H2O") + xf("H2O") + (2*xf("CH4") + 3*xf("C2H6") + 4*xf("C3H8") + 5*xf("C4H10")) + xf("H2S")
n_SO2 = xf("H2S")
n_O2 = n_air * xa("O2") - O2_req
n_N2 = n_air * xa("N2") + xf("N2")
n_Ar = n_air * xa("Ar")

n_prod = {
    "CO2": n_CO2,
    "H2O": n_H2O,
    "SO2": n_SO2,
    "O2": n_O2,
    "N2": n_N2,
    "Ar": n_Ar,
}
for k in list(n_prod.keys()):
    if n_prod[k] < 0.0 and abs(n_prod[k]) < 1e-12:
        n_prod[k] = 0.0

nP_tot = sum(v for v in n_prod.values() if v > 0.0)
if nP_tot <= 0.0:
    raise ValueError("compute_LHV_HHV: empty products")

X_prod = {sp: n / nP_tot for sp, n in n_prod.items() if n > 0.0}

```

```

T0 = T_ref.to("K").magnitude
P0 = P_ref.to("Pa").magnitude

gas.TPX = T0, P0, X_react
hR_molar = gas.enthalpy_mole

gas.TPX = T0, P0, X_prod
hP_molar = gas.enthalpy_mole

HR = hR_molar * (nR_tot / 1000.0)
HP = hP_molar * (nP_tot / 1000.0)

LHV_mol_J = HR - HP
if LHV_mol_J <= 0.0:
    raise ValueError(f"compute_LHV_HHV: non-positive LHV ({LHV_mol_J} J/mol basis)")

M_mix = Q_(0.0, "kg/mol")
for sp, x in fuel_x.items():
    M_mix = M_mix + Q_(float(x), "") * molar_masses[sp].to("kg/mol")

if M_mix.to("kg/mol").magnitude <= 0.0:
    raise ValueError("compute_LHV_HHV: invalid fuel mixture molar mass")

LHV_mol = Q_(float(LHV_mol_J), "J/mol")

LHV_kg = (LHV_mol / M_mix).to("kJ/kg")

latent = (WaterProps.h_g(P_ref) - WaterProps.h_f(P_ref)).to("J/kg")
h_fg_mol = (latent * molar_masses["H2O"].to("kg/mol")).to("J/mol")

HHV_mol = (LHV_mol + Q_(float(n_H2O), "") * h_fg_mol).to("J/mol")
HHV_kg = (HHV_mol / M_mix).to("kJ/kg")

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

return HHV_kg, LHV_kg, P_HHV, P_LHV

def sensible_heat(stream: GasStream) -> Q_:
    s = stream
    h_sens = _gasprops.h_sensible(s.T, s.P, s.comp, Tref=T_ref).to("J/kg")
    return (s.mass_flow * h_sens).to("kW")

def total_input_heat(fuel, air) -> Q_:
    power_LHV = compute_LHV_HHV(fuel, air)
    fuel_sens = sensible_heat(fuel)
    air_sens = sensible_heat(air)
    Q_in = (power_LHV.to("kW") + fuel_sens.to("kW") + air_sens.to("kW")).to("kW")
    return power_LHV, Q_in
=====
FILE: combustion/mass_mole.py
===== from typing import Dict from common.constants import molar_masses

def to_mole(mass_comp: Dict[str, float]) -> Dict[str, float]:
    n = {sp: mass_comp[sp] / molar_masses[sp] for sp in mass_comp}
    tot = sum(n.values())
    return {sp: v / tot for sp, v in n.items()}

def to_mass(mol_comp: Dict[str, float]) -> Dict[str, float]:
    m = {sp: mol_comp[sp] * molar_masses[sp] for sp in mol_comp}
    tot = sum(m.values())
    return {sp: v / tot for sp, v in m.items()}

def mix_molar_mass(mol_comp: Dict[str, float]) -> float:
    return sum(mol_comp[sp] * molar_masses[sp])

```

```

for sp in mol_comp)

def molar_flow(mass_comp: Dict[str, float], m_dot: float) -> float: return sum((mass_comp[sp] * m_dot)
/ (molar_masses[sp]) for sp in mass_comp)

def mass_flow(mol_comp: Dict[str, float], n_dot: float) -> float: return sum(mol_comp[sp] * n_dot *
molar_masses[sp] for sp in mol_comp)

=====
===== FILE: common/init.py =====
===== FILE: common/boiler_loop.py =====
from future import annotations import logging from typing import Dict, Any, Tuple from common.new_loader import load_all from combustion.combustor import Combustor from heat.runner import run_hx from common.units import Q_ from common.props import WaterProps from common.models import WaterStream from common.results import CombustionResult, write_results_csvs

log = logging.getLogger(name)

def _drum_steam_rate(*, P_drum: Q_, Q_evap: Q_, m_fw: Q_, h_fw_out: Q_, steam_quality_out: float = 1.0, ) -> Q_: hf = WaterProps.h_f(P_drum).to("J/kg") hg = WaterProps.h_g(P_drum).to("J/kg") h_s = (hf + Q_(steam_quality_out, "") * (hg - hf)).to("J/kg")

denom = (h_s - hf).to("J/kg")
if denom.magnitude <= 0:
    raise ValueError("Invalid drum latent enthalpy (h_s - h_f) <= 0.")

m_s = (Q_evap.to("W") + m_fw * (h_fw_out - hf)) / denom
return m_s.to("kg/s")

def run_boiler_case(stages_path: str = "config/stages.yaml", air_path: str = "config/air.yaml", fuel_path: str = "config/fuel.yaml", water_path: str = "config/water.yaml", drum_path: str = "config/drum.yaml", operation_path: str = "config/operation.yaml", *, tol_m: Q_ = Q_(1e-3, "kg/s"), max_iter: int = 20, write_csv: bool = True, operation_overrides: Dict[str, Q_] | None = None, fuel_overrides: Dict[str, Q_] | None = None, fouling_factor: float = 1.0, run_id: str | None = None, ) -> Dict[str, Any]: log.info(f"Load config") stages, air, fuel, water, drum, operation = load_all(stages_path=stages_path, air_path=air_path, fuel_path=fuel_path, water_path=water_path, drum_path=drum_path, operation_path=operation_path, )

f = float(fouling_factor)
if f <= 0.0:
    raise ValueError(f"fouling_factor must be > 0. Got {fouling_factor!r}")

if abs(f - 1.0) > 1e-12:
    for st in stages:
        spec = st.spec
        if "foul_t_in" in spec:
            spec["foul_t_in"] = (spec["foul_t_in"] * Q_(f, "")).to(spec["foul_t_in"].units)
        if "foul_t_out" in spec:
            spec["foul_t_out"] = (spec["foul_t_out"] * Q_(f, "")).to(spec["foul_t_out"].units)

if operation_overrides:
    operation.update(operation_overrides)

if fuel_overrides:
    for attr, val in fuel_overrides.items():
        if hasattr(fuel, attr):
            setattr(fuel, attr, val)
        else:

```

```

        log.warning(f"GasStream (fuel) has no attribute '{attr}', ignoring override.")

P_drum: Q_ | None = operation.get("drum_pressure", None)
blowdown_fraction = operation.get("blowdown_fraction", Q_(0.0, ""))
steam_quality_out = float(operation.get("steam_quality_out", Q_(1.0, "")).to("").magnitude)

water_template: WaterStream = water

if P_drum is not None:
    water_template.P = P_drum

log.info(f"Running Combustor")
svc = Combustor(air, fuel, operation["excess_air_ratio"])
combustion_results = svc.run()
log.info(f"Combustion Done")

if P_drum is None:
    raise ValueError("Option B requires operation.drum_pressure")

hf = WaterProps.h_f(P_drum).to("J/kg")
hg = WaterProps.h_g(P_drum).to("J/kg")
h_feed = water_template.h.to("J/kg")
latent = (hg - hf).to("J/kg")
m_fw = ((Q_(0.94, "") * combustion_results.Q_in.to("W")) / (latent + (hf - h_feed))).to("kg/s")

prev_m = None
final_result = None
final_m_fw = None
final_m_s = None

tol_m_fw = tol_m.to("kg/s").magnitude

for it in range(max_iter):
    m_bd = (blowdown_fraction.to("") .magnitude * m_fw).to("kg/s")

    water_in = WaterStream(mass_flow=m_fw, h=water_template.h, P=water_template.P)

    final_result = run_hx(
        stages_raw=stages,
        water=water_in,
        gas=combustion_results.flue,
        drum=drum,
        drum_pressure=P_drum,
        target_dx="0.1 m",
        combustion=combustion_results,
        write_csv=False,
    )

    h_fw_out = final_result["water_out"].h.to("J/kg")

    evap_names = {f"HX_{i}" for i in range(1, 6)}
    Q_evap_W = 0.0
    for r in final_result["summary_rows"]:
        if r.get("stage_name") in evap_names and isinstance(r.get("Q_stage[MW]"), (int, float)):


```

```

        Q_evap_W += Q_(r["Q_stage[MW]"], "MW").to("W").magnitude
Q_evap = Q_(Q_evap_W, "W")

m_s = _drum_steam_rate(
    P_drum=P_drum,
    Q_evap=Q_evap,
    m_fw=m_fw,
    h_fw_out=h_fw_out,
    steam_quality_out=steam_quality_out,
)
resid = (m_s + m_bd - m_fw).to("kg/s").magnitude

final_m_fw = m_fw
final_m_s = m_s

if prev_m is not None:
    dm = (m_fw - prev_m).to("kg/s").magnitude
    if abs(dm) < tol_m_fw and abs(resid) < tol_m_fw:
        break

m_fw_new = (m_s + m_bd).to("kg/s")
m_fw = (Q_(0.5, "") * m_fw_new + Q_(0.5, "") * m_fw).to("kg/s")

prev_m = final_m_fw

else:
    log.warning("Did not reach drum mass-balance convergence within max_iter.")

feed_P: Q_ | None = None

if P_drum is not None and final_m_fw is not None:
    P_drum_Pa = P_drum.to("Pa")

    P_in = (P_drum_Pa * Q_(1.01, "")).to("Pa")

    max_p_iter = 30
    tol_P = Q_(1.0, "Pa")

    feed_P = None
    last_result: Dict[str, Any] | None = None

    for _ in range(max_p_iter):
        water_trial = WaterStream(
            mass_flow=final_m_fw,
            h=water_template.h,
            P=P_in,
        )

        last_result = run_hx(
            stages_raw=stages,
            water=water_trial,
            gas=combustion_results.flue,
            drum=drum,

```

```

        drum_pressure=P_drum,
        target_dx="0.1 m",
        combustion=combustion_results,
        write_csv=False,
    )

P_out = last_result["water_out"].P.to("Pa")

err = (P_drum_Pa - P_out).to("Pa")

if abs(err).to("Pa").magnitude < tol_P.to("Pa").magnitude:
    feed_P = P_in
    break

P_in = (P_in + err).to("Pa")

if P_in < P_drum_Pa:
    P_in = P_drum_Pa

if feed_P is None:
    feed_P = P_in

log.info(f"Solved feedwater inlet pressure: {feed_P:~P} for drum pressure {P_drum:~P}")

if feed_P is None:
    feed_P = P_drum

water_final_in = WaterStream(
    mass_flow=final_m_fw,
    h=water_template.h,
    P=feed_P,
)
log.info(f"Final feedwater inlet mass flow: {water_final_in.mass_flow:~P}")

final_result = run_hx(
    stages_raw=stages,
    water=water_final_in,
    gas=combustion_results.flue,
    drum=drum,
    drum_pressure=P_drum,
    target_dx="0.1 m",
    combustion=combustion_results,
    write_csv=write_csv,
)

csv_paths: Tuple[str, str, str] | None = None
if write_csv:
    effective_run_id = run_id if run_id is not None else final_result["run_id"]

    steps_csv, stages_summary_csv, boiler_summary_csv = write_results_csvs(
        global_profile=final_result["global_profile"],
        combustion=final_result["combustion"],
        outdir=final_result["outdir"],

```

```

        run_id=effective_run_id,
        drum_pressure=P_drum,
        feed_pressure=feed_P,
    )
    csv_paths = (steps_csv, stages_summary_csv, boiler_summary_csv)

m_bd_final = None
if final_m_fw is not None:
    m_bd_final = (blowdown_fraction.to("") .magnitude * final_m_fw).to("kg/s")
else:
    m_bd_final = Q_(0.0, "kg/s")

return {
    "result": final_result,
    "m_fw": final_m_fw,
    "m_s": final_m_s,
    "m_bd": m_bd_final,
    "drum_pressure": P_drum,
    "combustion": combustion_results,
    "csv_paths": csv_paths,
}
=====
===== FILE: common/constants.py =====
from common.units import Q_
T_ref = Q_(298.15, "kelvin") P_ref = Q_(101325, "pascal")
molar_masses = { "CH4": Q_(0.01604, "kilogram / mole"), "C2H6": Q_(0.03007, "kilogram / mole"),
"C3H8": Q_(0.04410, "kilogram / mole"), "C4H10": Q_(0.05812, "kilogram / mole"), "H2S": Q_(0.03408,
"kilogram / mole"), "N2": Q_(0.02802, "kilogram / mole"), "CO2": Q_(0.04401, "kilogram / mole"), "H2O": Q_(0.018015, "kilogram / mole"), "O2": Q_(0.031998, "kilogram / mole"), "Ar": Q_(0.039948, "kilogram / mole"), "SO2": Q_(0.06407, "kilogram / mole"), }

O2_per_mol = { "CH4": Q_(2.0, "dimensionless"), "C2H6": Q_(3.5, "dimensionless"), "C3H8": Q_(5.0,
"dimensionless"), "C4H10": Q_(6.5, "dimensionless"), "H2S": Q_(1.0, "dimensionless"), "N2": Q_(0.0,
"dimensionless"), "CO2": Q_(0.0, "dimensionless"), "H2O": Q_(0.0, "dimensionless"), }

=====
===== FILE: common/logging_utils.py =====
import logging, functools, time

TRACE_LEVEL_NUM = 5 logging.addLevelName(TRACE_LEVEL_NUM, "TRACE")
class _TraceLogger(logging.Logger):
    def trace(self, msg, *a, k):
        if self.isEnabledFor(TRACE_LEVEL_NUM):
            self._log(TRACE_LEVEL_NUM, msg, a, k)
    logging.setLoggerClass(_TraceLogger)

_FMT = "%(asctime)s | %(levelname)s | %(name)s | stage=%(stage)s step=%(step)s | %(message)s" _DATE
= "%Y-%m-%d %H:%M:%S"

class _Stage(logging.Filter):
    def filter(self, r):
        if not hasattr(r, "stage"):
            r.stage = "-" if not hasattr(r, "step") or r.step == "-"
            return True
        return False

def setup_logging(level: int | str = logging.INFO):
    if isinstance(level, str):
        lvl = logging.getLevelName(level.upper())
    level = lvl if isinstance(lvl, int) else logging.INFO
    root = logging.getLogger()
    root.handlers.clear()
    root.setLevel(level)
    h = logging.StreamHandler()
    h.setFormatter(logging.Formatter(_FMT, _DATE))
    h.addFilter(_Stage())
    root.addHandler(h)

def _fmt(v):
    try:
        return f"v:{6g~P}"
    except:
        return repr(v)

def trace_calls(name: str | None = None, values: bool = False):
    def _wrap(fn):
        qual = name or f"{fn.module}.{fn.__qualname__}"
        log = logging.getLogger(qual)
        @functools.wraps(fn)
        def _inner(*a,

```

```

**k): stage = k.get("stage", "-") log.trace("enter", extra={"stage": stage, "step": fn.__name__}) if
values: arg_s = ",".join([*map(_fmt, a), *[f"{{kk}}={_fmt(v)}" for kk,v in k.items()]]) log.trace(f"args: {arg_s}", extra={"stage": stage, "step": fn.__name__}) t0=time.perf_counter() try: out=fn(*a, **k)
dt=(time.perf_counter()-t0)*1000 if values: log.trace(f"ret: {_fmt(out)}", extra={"stage": stage, "step": fn.name}) log.trace(f"exit ok in {dt:.2f} ms", extra={"stage": stage, "step": fn.name}) return out except
Exception as e: log.exception(f"exit err: {e}", extra={"stage": stage, "step": fn.name}) raise return
_inner return _wrap
=====
FILE: common/models.py =====
from dataclasses import dataclass from typing import Dict, Any from common.units import Q_
@dataclass class GasStream: mass_flow: Q_ T: Q_ P: Q_ comp: Dict[str, Q_]
@dataclass class WaterStream: mass_flow: Q_ h: Q_ P: Q_
@dataclass class HXStage: name: str kind: str spec: Dict[str, Any]
@dataclass class Drum: Di: Q_ L: Q_
=====
FILE: common/new_loader.py =====
from future import annotations from typing import Tuple, List, Dict, Any import yaml from common.units import Q_ from common.models import HXStage, GasStream, WaterStream, Drum

def q(node: Any) -> Q: if isinstance(node, dict) and "value" in node and "unit" in node: return
Q_(node["value"], str(node["unit"])) raise ValueError(f"Invalid quantity format: {node!r}")

def __get(d: Dict[str, Any] | None, key: str, default=None): return d.get(key, default) if isinstance(d, dict)
else default

def __wall_to_spec(wall: Dict[str, Any] | None, spec: Dict[str, Q_]): if not wall: return if __get(wall,
"thickness"): spec["wall_t"] = __q(__get(wall, "thickness")) if __get(wall, "conductivity"): spec["wall_k"] =
__q(__get(wall, "conductivity"))

surf_in = __get(__get(wall, "surfaces"), "inner") or {}
if __get(surf_in, "roughness"): spec["roughness_in"] = __q(__get(surf_in, "roughness"))
if __get(surf_in, "emissivity"): spec["eps_in"] = __q(__get(surf_in, "emissivity"))
if __get(surf_in, "fouling_thickness"): spec["foul_t_in"] = __q(__get(surf_in, "fouling_thickness"))
if __get(surf_in, "fouling_conductivity"): spec["foul_k_in"] = __q(__get(surf_in, "fouling_conductivity"))

surf_out = __get(__get(wall, "surfaces"), "outer") or {}
if __get(surf_out, "roughness"): spec["roughness_out"] = __q(__get(surf_out, "roughness"))
if __get(surf_out, "emissivity"): spec["eps_out"] = __q(__get(surf_out, "emissivity"))
if __get(surf_out, "fouling_thickness"): spec["foul_t_out"] = __q(__get(surf_out, "fouling_thickness"))
if __get(surf_out, "fouling_conductivity"): spec["foul_k_out"] = __q(__get(surf_out, "fouling_conductivity"))

def __map_K(node: Dict[str, Any], spec: Dict[str, Q_]): K_node = __get(node, "K") or {} if not isin-
stance(K_node, dict): return

mapping = {
    "hot_inlet": "K_hot_inlet",
    "hot_outlet": "K_hot_outlet",
    "hot_bend": "K_hot_bend",
    "cold_inlet": "K_cold_inlet",
    "cold_outlet": "K_cold_outlet",
    "cold_bend": "K_cold_bend",
}
for yaml_key, spec_key in mapping.items():
    v = __get(K_node, yaml_key)
    if v is not None:

```

```

spec[spec_key] = Q_(float(v), "dimensionless")

def load_air(path: str) -> Dict[str, Any]: doc = yaml.safe_load(open(path, "r", encoding="utf-8")) comp = {k: q(v) for k, v in (doc.get("composition") or {}).items()} return GasStream( mass_flow=Q(0, "kg/s"), T=_q(doc["T"]), P=_q(doc["P"]), comp=comp )

def load_fuel(path: str) -> GasStream: doc = yaml.safe_load(open(path, "r", encoding="utf-8")) comp = {k: _q(v) for k, v in (doc.get("composition") or {}).items()} return GasStream( mass_flow=_q(doc["mass_flow"]), T=_q(doc["T"]), P=_q(doc["P"]), comp=comp )

def load_drum(path: str) -> Drum: doc = yaml.safe_load(open(path, "r", encoding="utf-8")) return Drum(Di=_q(doc["inner_diameter"]).to("m"), L=_q(doc["length"]).to("m"))

def load_stages(path: str) -> List[HXStage]: sdoc = yaml.safe_load(open(path, "r", encoding="utf-8")) stages: List[HXStage] = []

for name, node in sdoc.items():

    spec: Dict[str, Q_] = {
        "inner_diameter": _q(node["inner_diameter"]),
    }
    if "inner_length" in node: spec["inner_length"] = _q(node["inner_length"])
    if "pool_boiling" in node: spec["pool_boiling"] = bool(node["pool_boiling"])
    if "curvature_radius" in node: spec["curvature_radius"] = _q(node["curvature_radius"])
    if "tubes_number" in node: spec["tubes_number"] = _q(node["tubes_number"])
    if "ST" in node: spec["ST"] = _q(node["ST"])
    if "SL" in node: spec["SL"] = _q(node["SL"])
    if "arrangement" in node: spec["arrangement"] = str(node["arrangement"])
    if "N_rows" in node: spec["N_rows"] = _q(node["N_rows"])
    if "baffle_spacing" in node: spec["baffle_spacing"] = _q(node["baffle_spacing"])
    if "shell_inner_diameter" in node: spec["shell_inner_diameter"] = _q(node["shell_inner_diameter"])
    if "baffle_cut" in node: spec["baffle_cut"] = _q(node["baffle_cut"])
    if "bundle_clearance" in node: spec["bundle_clearance"] = _q(node["bundle_clearance"])
    if "n_tubes" in node: spec["n_tubes"] = _q(node["n_tubes"])
    if "n_circuits" in node: spec["n_circuits"] = _q(node["n_circuits"])
    if "tube_length" in node: spec["tube_length"] = _q(node["tube_length"])

    _wall_to_spec(_get(node, "wall"), spec)
    _map_K(node, spec)

    stages.append(HXStage(name=name, kind=str(node["kind"]), spec=spec))

return stages

def load_operation(path: str) -> Dict[str, Q_]: doc = yaml.safe_load(open(path, "r", encoding="utf-8"))

out: Dict[str, Q_] = {
    "excess_air_ratio": _q(doc["excess_air_ratio"]),
}

if "drum_pressure" in doc:
    out["drum_pressure"] = _q(doc["drum_pressure"])
if "circulation_ratio" in doc:
    out["circulation_ratio"] = _q(doc["circulation_ratio"])
if "blowdown_fraction" in doc:
    out["blowdown_fraction"] = _q(doc["blowdown_fraction"])

```

```

if "steam_quality_out" in doc:
    out["steam_quality_out"] = _q(doc["steam_quality_out"])

return out

def load_water_stream(path: str) -> WaterStream: doc = yaml.safe_load(open(path, "r", encoding="utf-8"))
h = _q(doc["enthalpy"])

P_node = doc.get("pressure", None)
if P_node is not None:
    P = _q(P_node)
else:
    P = Q_(1.0, "megapascal")

return WaterStream(
    mass_flow=Q_(0, "kg/s"),
    h=h,
    P=P,
)

def load_all(stages_path: str, water_path: str, drum_path: str, air_path: str, fuel_path: str, operation_path: str, ) -> Tuple[List[HXStage], GasStream, GasStream, WaterStream, Drum, Dict[str, Q_]]:
    stages = load_stages(stages_path) if stages_path else None
    water = load_water_stream(water_path) if water_path else None
    drum = load_drum(drum_path) if drum_path else None
    air = load_air(air_path) if air_path else None
    fuel = load_fuel(fuel_path) if fuel_path else None
    operation = load_operation(operation_path) if operation_path else None
    return stages, air, fuel, water, drum, operation

=====
FILE: common/props.py =====
from future import annotations from typing import Dict, Optional from common.units import Q_ import cantera as ct from iapws import IAPWS97

class GasProps: def __init__(self, mech_path: str = "config/flue_cantera.yaml", phase: str = "gas_mix"):
    self._sol = ct.Solution(mech_path, phase)

    def _set(self, T: Q_, P: Q_, Y: Dict[str, Q_], film_T: Optional[Q_] = None):
        T_K = (film_T or T).to("K").magnitude
        P_Pa = P.to("Pa").magnitude
        Y_map = {k: v.to("dimensionless").magnitude for k, v in Y.items()}
        self._sol.TPY = T_K, P_Pa, Y_map
        return self._sol

    def cp(self, T: Q_, P: Q_, X: Dict[str, Q_], film_T: Optional[Q_] = None) -> Q_:
        return Q_(self._set(T,P,X,film_T).cp_mass, "J/kg/K")

    def k(self, T: Q_, P: Q_, X: Dict[str, Q_], film_T: Optional[Q_] = None) -> Q_:
        return Q_(self._set(T,P,X,film_T).thermal_conductivity, "W/m/K")

    def mu(self, T: Q_, P: Q_, X: Dict[str, Q_], film_T: Optional[Q_] = None) -> Q_:
        return Q_(self._set(T,P,X,film_T).viscosity, "Pa*s")

    def rho(self, T: Q_, P: Q_, X: Dict[str, Q_], film_T: Optional[Q_] = None) -> Q_:
        return Q_(self._set(T,P,X,film_T).density, "kg/m^3")

    def h(self, T: Q_, P: Q_, X: Dict[str, Q_], film_T: Optional[Q_] = None) -> Q_:
        return Q_(self._set(T,P,X,film_T).enthalpy_mass, "J/kg")

```

```

def h_sensible(self, T: Q_, P: Q_, X: dict, Tref: Q_ = Q_(298.15, "K"), film_T: Q_ | None = None) -> Q_:
    hT = self.h(T, P, X, film_T)
    href = self.h(Tref, P, X, film_T)
    return (hT - href).to("J/kg")

class WaterProps: @staticmethod def Ph(P: Q, h: Q_) -> IAPWS97: return IAPWS97(P=P.to("megapascal").magnitude,
    h=h.to("kJ/kg").magnitude)

    @staticmethod
    def _PT(P: Q_, T: Q_) -> IAPWS97:
        return IAPWS97(P=P.to("megapascal").magnitude, T=T.to("K").magnitude)

    @staticmethod
    def T_from_Ph(P: Q_, h: Q_) -> Q_: return Q_(WaterProps._Ph(P,h).T, "K")
    @staticmethod
    def rho_from_Ph(P: Q_, h: Q_) -> Q_: return Q_(WaterProps._Ph(P,h).rho, "kg/m^3")
    @staticmethod
    def mu_from_Ph(P: Q_, h: Q_) -> Q_: return Q_(WaterProps._Ph(P,h).mu, "Pa*s")
    @staticmethod
    def k_from_Ph(P: Q_, h: Q_) -> Q_: return Q_(WaterProps._Ph(P,h).k, "W/m/K")
    @staticmethod
    def cp_from_Ph(P: Q_, h: Q_) -> Q_: return Q_(WaterProps._Ph(P,h).cp, "kJ/kg/K").to("J/kg/K")

    @staticmethod
    def quality_from_Ph(P: Q_, h: Q_) -> Q_ | None:
        Pcrit = Q_(22.064, "MPa")
        if P >= Pcrit:
            return None
        hf = WaterProps.h_f(P)
        hg = WaterProps.h_g(P)
        dh = hg - hf
        if abs(dh.to("J/kg").magnitude) < 1e-9:
            return None

        x = ((h - hf) / dh).to("")
        xm = x.magnitude
        if xm < -1e-6 or xm > 1 + 1e-6:
            return None

        xm = min(1.0, max(0.0, xm))
        return Q_(xm, "")

    @staticmethod
    def Tsat(P: Q_) -> Q_: return Q_(IAPWS97(P=P.to("megapascal").magnitude, x=0.0).T, "K")
    @staticmethod
    def h_f(P: Q_) -> Q_: return Q_(IAPWS97(P=P.to("megapascal").magnitude, x=0.0).h, "kJ/kg").to("J/kg")
    @staticmethod
    def h_g(P: Q_) -> Q_: return Q_(IAPWS97(P=P.to("megapascal").magnitude, x=1.0).h, "kJ/kg").to("J/kg")

    @staticmethod
    def cp_from_PT(P: Q_, T: Q_) -> Q_:
        return Q_(WaterProps._PT(P,T).cp, "kJ/kg/K").to("J/kg/K")

    @staticmethod

```

```

def mu_from_PT(P: Q_, T: Q_) -> Q_: return Q_(WaterProps._PT(P,T).mu, "Pa*s")

@staticmethod
def k_from_PT(P: Q_, T: Q_) -> Q_: return Q_(WaterProps._PT(P,T).k, "W/m/K")

@staticmethod
def rho_from_PT(P: Q_, T: Q_) -> Q_: return Q_(WaterProps._PT(P,T).rho, "kg/m^3")

@staticmethod
def rho_from_Px(P: Q_, x: Q_) -> Q_:
    P_MPa = P.to("megapascal").magnitude
    if x.magnitude <= 0:
        return Q_(IAPWS97(P=P_MPa, x=0.0).rho, "kg/m^3")
    if x.magnitude >= 1:
        return Q_(IAPWS97(P=P_MPa, x=1.0).rho, "kg/m^3")

    rho_f = IAPWS97(P=P_MPa, x=0.0).rho
    rho_g = IAPWS97(P=P_MPa, x=1.0).rho

    v_mix = (1 - x.magnitude) / rho_f + x.magnitude / rho_g
    return Q_(1 / v_mix, "kg/m^3")

=====
=====FILE: common/results.py =====
from future import annotations from dataclasses import dataclass, field from typing import List, Sequence, Tuple from common.units import Q_ from common.models import GasStream from pathlib import Path import pandas as pd

@dataclass(frozen=True) class CombustionResult: LHV: Q_ Q_in: Q_ T_ad: Q_ flue: GasStream flue_ad: GasStream | None = None fuel_LHV_mass: Q_ | None = None fuel_P_LHV: Q_ | None = None fuel_mass_flow: Q_ | None = None air_mass_flow: Q_ | None = None excess_air_ratio: Q_ | None = None

@dataclass(frozen=True) class StepResult: i: int x: Q_ dx: Q_ gas: object water: object Tgw: Q_ Tw: Q_ UA_prime: Q_ qprime: Q_ boiling: bool h_g: Q_ h_c: Q_ stage_name: str = "" stage_index: int = -1 dP_fric: Q_ = field(default_factory=lambda: Q_(0.0, "kPa")) dP_minor: Q_ = field(default_factory=lambda: Q_(0.0, "kPa")) dP_total: Q_ = field(default_factory=lambda: Q_(0.0, "kPa")) w_dP_fric: Q_ = field(default_factory=lambda: Q_(0.0, "kPa")) w_dP_minor: Q_ = field(default_factory=lambda: Q_(0.0, "kPa")) w_dP_tot: Q_ = field(default_factory=lambda: Q_(0.0, "kPa")) qprime_conv: Q_ = field(default_factory=lambda: Q_(0.0, "W/m")) qprime_rad: Q_ = field(default_factory=lambda: Q_(0.0, "W/m"))

@dataclass(frozen=True) class StageResult: stage_name: str stage_kind: str steps: Sequence[StepResult] Q_stage: Q_ UA_stage: Q_ dP_stage_fric: Q_ = field(default_factory=lambda: Q_(0.0, "kPa")) dP_stage_minor: Q_ = field(default_factory=lambda: Q_(0.0, "kPa")) dP_stage_total: Q_ = field(default_factory=lambda: Q_(0.0, "kPa")) dP_water_stage_fric: Q_ = field(default_factory=lambda: Q_(0.0, "kPa")) dP_water_stage_minor: Q_ = field(default_factory=lambda: Q_(0.0, "kPa")) dP_water_stage_total: Q_ = field(default_factory=lambda: Q_(0.0, "kPa")) hot_flow_A: Q_ = field(default_factory=lambda: Q_(0.0, "m^2")) cold_flow_A: Q_ = field(default_factory=lambda: Q_(0.0, "m^2")) hot_Dh: Q_ = field(default_factory=lambda: Q_(0.0, "m")) cold_Dh: Q_ = field(default_factory=lambda: Q_(0.0, "m"))

@dataclass(frozen=True) class GlobalProfile: x: List[Q_] dx: List[Q_] gas: List[object] water: List[object] qprime: List[Q_] UA_prime: List[Q_] h_g: List[Q_] h_c: List[Q_] stage_index: List[int] stage_name: List[str] dP_fric: List[Q_] dP_minor: List[Q_] dP_total: List[Q_] w_dP_fric: List[Q_] w_dP_minor: List[Q_] w_dP_tot: List[Q_] stage_results: List[StageResult]

def build_global_profile(stage_results: Sequence[StageResult]) -> GlobalProfile: xs: List[Q_] = [] dxs:

```

```

List[Q_] = [] gas: List[object] = [] water: List[object] = [] qprime: List[Q_] = [] UA_prime: List[Q_] =
[] h_g: List[Q_] = [] h_c: List[Q_] = [] sidx: List[int] = [] sname: List[str] = [] dP_fric: List[Q_] = []
dP_minor: List[Q_] = [] dP_total: List[Q_] = [] w_dP_fric: List[Q_] = [] w_dP_minor: List[Q_] = []
w_dP_tot: List[Q_] = []

for k, sr in enumerate(stage_results):
    for st in sr.steps:
        xs.append(st.x)
        dxs.append(st.dx)
        gas.append(st.gas)
        water.append(st.water)
        qprime.append(st.qprime)
        UA_prime.append(st.UA_prime)
        h_g.append(st.h_g)
        h_c.append(st.h_c)
        sidx.append(k if st.stage_index < 0 else st.stage_index)
        sname.append(sr.stage_name if not st.stage_name else st.stage_name)
        dP_fric.append(st.dP_fric)
        dP_minor.append(st.dP_minor)
        dP_total.append(st.dP_total)
        w_dP_fric.append(st.w_dP_fric)
        w_dP_minor.append(st.w_dP_minor)
        w_dP_tot.append(st.w_dP_tot)

return GlobalProfile(
    x=xs, dx=dxs, gas=gas, water=water,
    qprime=qprime, UA_prime=UA_prime, h_g=h_g, h_c=h_c,
    stage_index=sidx, stage_name=sname,
    dP_fric=dP_fric, dP_minor=dP_minor, dP_total=dP_total,
    w_dP_fric=w_dP_fric, w_dP_minor=w_dP_minor, w_dP_tot=w_dP_tot,
    stage_results=list(stage_results),
)

```

def write_results_csvs(global_profile: GlobalProfile, combustion: CombustionResult | None, outdir: str | Path, run_id: str, drum_pressure: Q_ | None = None, feed_pressure: Q_ | None = None,) -> Tuple[str, str, str]:

```

from heat.postproc import profile_to_dataframe, summary_from_profile

outdir = Path(outdir)
outdir.mkdir(parents=True, exist_ok=True)

steps_path = outdir / f"{run_id}_steps.csv"
stages_summary_path = outdir / f"{run_id}_stages_summary.csv"
boiler_summary_path = outdir / f"{run_id}_boiler_summary.csv"

df_steps = profile_to_dataframe(
    global_profile,
    remap_water=False,
)
df_steps.set_index("stage_name").to_csv(steps_path)

rows, _, _ = summary_from_profile(
    global_profile,
    combustion=combustion,
)

```

```

        drum_pressure=drum_pressure
    )

df_summary = pd.DataFrame(
    rows,
    columns=[
        "stage_index", "stage_name", "stage_kind",
        "Q_stage[MW]", "UA_stage[MW/K]",

        "gas_in_P[kPa]", "gas_in_T[°C]", "gas_in_h[kJ/kg]",
        "gas_out_P[kPa]", "gas_out_T[°C]", "gas_out_h[kJ/kg]",

        "water_in_P[kPa]", "water_in_T[°C]", "water_in_h[kJ/kg]",
        "water_out_P[kPa]", "water_out_T[°C]", "water_out_h[kJ/kg]",

        "gas_V_avg[m/s]", "water_V_avg[m/s]",

        "ΔP_stage_fric[kPa]", "ΔP_stage_minor[kPa]", "ΔP_stage_total[kPa]",
        "ΔP_water_stage_fric[kPa]", "ΔP_water_stage_minor[kPa]", "ΔP_water_stage_total[kPa]",
        "stack_temperature[°C]",
        "Q_conv_stage[MW]", "Q_rad_stage[MW]",

        "steam_capacity[kg/s]", "steam_capacity[t/h]",

        "η_direct[-]", "η_indirect[-]", "Stack_loss_fraction[-]",
        "Q_total_useful[MW]", "Q_in_total[MW]", "Q_flue_out[MW]", "Q_balance_error[MW]",

        "P_LHV[MW]", "LHV_mass[kJ/kg]",
    ],
).set_index("stage_index")

df_stages = df_summary[df_summary["stage_name"] != "TOTAL_BOILER"].copy()
df_boiler = df_summary[df_summary["stage_name"] == "TOTAL_BOILER"].copy()

df_stages = df_stages.set_index("stage_name")

table = pd.DataFrame(
{
    "name": df_stages.index,
    "kind": df_stages["stage_kind"],
    "gas in pressure[kpa)": df_stages["gas_in_P[kPa]"],
    "gas in temp[°C)": df_stages["gas_in_T[°C]"],
    "gas in enthalpy[kJ/kg)": df_stages["gas_in_h[kJ/kg]"],
    "gas out pressure[kpa)": df_stages["gas_out_P[kPa]"],
    "gas out temp[°C)": df_stages["gas_out_T[°C]"],
    "gas out enthalpy[kJ/kg)": df_stages["gas_out_h[kJ/kg]"],
    "water in temp[°C)": df_stages["water_in_T[°C]"],
    "water in enthalpy[kJ/kg)": df_stages["water_in_h[kJ/kg]"],
    "water in pressure[kpa)": df_stages["water_in_P[kPa]"],
    "water out temp[°C)": df_stages["water_out_T[°C]"],
    "water out enthalpy[kJ/kg)": df_stages["water_out_h[kJ/kg]"],
    "water out pressure[kpa)": df_stages["water_out_P[kPa]"],
}
)

```

```

    "gas avg velocity[m/s)": df_stages["gas_V_avg[m/s]"],
    "water avg velocity[m/s)": df_stages["water_V_avg[m/s]"],
    "pressure drop fric[kpa)": df_stages["ΔP_stage_fric[kPa]"],
    "pressure drop minor[kpa)": df_stages["ΔP_stage_minor[kPa]"],
    "pressure drop total[kpa)": df_stages["ΔP_stage_total[kPa]"],
    "water pressure drop fric[kpa)": df_stages["ΔP_water_stage_fric[kPa]"],
    "water pressure drop minor[kpa)": df_stages["ΔP_water_stage_minor[kPa]"],
    "water pressure drop total[kpa)": df_stages["ΔP_water_stage_total[kPa]"],
    "Q conv[MW)": df_stages["Q_conv_stage[MW]"],
    "Q rad[MW)": df_stages["Q_rad_stage[MW]"],
    "Q total[MW)": df_stages["Q_stage[MW]"],
    "UA[MW/K)": df_stages["UA_stage[MW/K]"],
    "steam capacity[t/h)": df_stages["steam_capacity[t/h]"],
}
).set_index("name")

table = table.drop(columns=["name"], errors="ignore")
table.T.to_csv(stages_summary_path, index_label="name")

if not df_boiler.empty:
    boiler_row = df_boiler.iloc[0].copy()

    try:
        m_fw = global_profile.stage_results[5].steps[0].water.mass_flow.to("kg/s").magnitude
    except Exception:
        m_fw = float("nan")

    boiler_row["feedwater_mass_flow[kg/s]"] = m_fw

    if feed_pressure is not None:
        try:
            boiler_row["feedwater_P[kPa]"] = feed_pressure.to("kPa").magnitude
        except Exception:
            boiler_row["feedwater_P[kPa]"] = ""

    else:
        boiler_row["feedwater_P[kPa]"] = ""

    if drum_pressure is not None:
        try:
            boiler_row["drum_P[kPa]"] = drum_pressure.to("kPa").magnitude
        except Exception:
            boiler_row["drum_P[kPa]"] = ""

    else:
        boiler_row["drum_P[kPa]"] = ""

    if combustion is not None:
        try:
            boiler_row["T_ad[°C]"] = combustion.T_ad.to("degC").magnitude
        except Exception:
            boiler_row["T_ad[°C]"] = ""

    if combustion.fuel_LHV_mass is not None:
        boiler_row["fuel_LHV_mass[kJ/kg]"] = combustion.fuel_LHV_mass.to("kJ/kg").magnitude
else:

```

```

boiler_row["fuel_LHV_mass[kJ/kg]"] = ""

if combustion.fuel_P_LHV is not None:
    boiler_row["fuel_P_LHV[MW]"] = combustion.fuel_P_LHV.to("MW").magnitude
else:
    boiler_row["fuel_P_LHV[MW]"] = ""

if combustion.fuel_mass_flow is not None:
    boiler_row["fuel_mass_flow[kg/s]"] = combustion.fuel_mass_flow.to("kg/s").magnitude
else:
    boiler_row["fuel_mass_flow[kg/s]"] = ""

if combustion.excess_air_ratio is not None:
    boiler_row["excess_air_ratio[-]"] = combustion.excess_air_ratio.to("").magnitude
else:
    boiler_row["excess_air_ratio[-]"] = ""

if combustion.air_mass_flow is not None:
    boiler_row["air_mass_flow[kg/s]"] = combustion.air_mass_flow.to("kg/s").magnitude
else:
    boiler_row["air_mass_flow[kg/s]"] = ""

else:
    boiler_row["T_ad[°C]"] = ""
    boiler_row["fuel_LHV_mass[kJ/kg]"] = ""
    boiler_row["fuel_P_LHV[MW]"] = ""
    boiler_row["fuel_mass_flow[kg/s]"] = ""
    boiler_row["air_mass_flow[kg/s]"] = ""
    boiler_row["excess_air_ratio[-]"] = ""

boiler_df = pd.DataFrame([boiler_row])

summary_mapping = [
    ("fuel mass flow[kg/s]", "fuel_mass_flow[kg/s]"),
    ("air flow[kg/s]", "air_mass_flow[kg/s]"),
    ("excess air ratio[-]", "excess_air_ratio[-]"),
    ("feedwater flow[kg/s]", "feedwater_mass_flow[kg/s]"),
    ("steam capacity[t/h]", "steam_capacity[t/h]"),
    ("eta direct[-]", "η_direct[-]"),
    ("eta indirect[-]", "η_indirect[-]"),
    ("Stack loss fraction[-]", "Stack_loss_fraction[-]"),
    ("Q_flue_out[MW]", "Q_flue_out[MW]"),
    ("UA[MW/K]", "UA_stage[MW/K]"),
    ("Q_in total[MW]", "Q_in_total[MW]"),
    ("Q_useful[MW]", "Q_total_useful[MW]"),
    ("Q_balance_error[MW]", "Q_balance_error[MW]"),
    ("pressure drop fric total[kPa]", "ΔP_stage_fric[kPa]"),
    ("pressure drop minor total[kPa]", "ΔP_stage_minor[kPa]"),
    ("pressure drop total[kPa]", "ΔP_stage_total[kPa]"),
    ("water pressure drop fric total[kPa]", "ΔP_water_stage_fric[kPa]"),
    ("water pressure drop minor total[kPa]", "ΔP_water_stage_minor[kPa]"),
    ("water pressure drop total[kPa]", "ΔP_water_stage_total[kPa]"),
    ("LHV[kJ/kg]", "LHV_mass[kJ/kg]"),
    ("P-LHV[MW]", "P_LHV[MW]"),
]

```

```

        ("Tad[°C]", "T_ad[°C"]),
        ("stack temperature[°C]", "stack_temperature[°C"]),
        ("feedwater pressure[kPa]", "feedwater_P[kPa]"),
        ("drum pressure[kPa]", "drum_P[kPa"]),
    ]

out_row = {}
row0 = boiler_df.iloc[0]
for new_name, src_col in summary_mapping:
    out_row[new_name] = row0.get(src_col, "")

boiler_out_df = pd.DataFrame([out_row]).T
boiler_out_df = boiler_out_df.reset_index()
boiler_out_df.columns = ["parameter", "value"]

boiler_out_df.to_csv(boiler_summary_path, index=False)

else:
    empty_cols = list(df_summary.columns) + [
        "water_mass_flow[kg/s]",
        "T_ad[°C]",
        "fuel_LHV_mass[kJ/kg]",
        "fuel_P_LHV[MW]",
        "fuel_mass_flow[kg/s]",
        "air_mass_flow[kg/s]",
        "excess_air_ratio[-]",
    ]
    pd.DataFrame(columns=empty_cols).to_csv(boiler_summary_path, index=False)

return str(steps_path), str(stages_summary_path), str(boiler_summary_path)
===== FILE: common/units.py =====
from future import annotations import pint
ureg = pint.UnitRegistry() Q_ = ureg.Quantity
===== FILE: heat/init.py =====
===== FILE: heat/gas_htc.py =====
from future import annotations from typing import Dict, Any, Tuple import numpy as np from common.units import Q_ from common.models import GasStream from common.props import GasProps from combustion.mass_mole import to_mole
_gas = GasProps(mech_path="config/flue_canteramodel.yaml", phase="gas_mix")
def cp_gas(g: GasStream) -> Q_: return _gas.cp(g.T, g.P, g.comp or {})
def _gas_partials(g): P = g.P.to("Pa").magnitude Y = {k: v.to("°").magnitude for k,v in (g.comp or {}).items()} X = to_mole(Y) xH2O = X.get("H2O", 0.0) xCO2 = X.get("CO2", 0.0) return xH2O * P, xCO2 * P
_A = np.array([0.434, 0.313, 0.180, 0.073]) _K = np.array([0.0, 2.3, 11.6, 30.4])
def mean_beam_length(spec: dict) -> Q: if "rad_Lb" in spec: return spec["rad_Lb"].to("m") Dh = spec["hot_Dh"].to("m") return (0.9 * Dh).to("m")
def emissivity(T_K: float, pH2O_Pa: float, pCO2_Pa: float, L_m: float, *, Texp: float = 0.65) -> float:
    T = float(np.clip(T_K, 300.0, 3000.0)) scale_T = (T / 1000.0) ** Texp

```

```

p_ratio = (pH2O_Pa + pCO2_Pa) / 101325.0
tau = (_K * scale_T) * p_ratio * L_m

eps = 1.0 - float(np.sum(_A * np.exp(-tau)))
return float(np.clip(eps, 0.0, 1.0))

def h_rad(Tfilm_K: float, eps_g: float, F: float = 1.0) -> float: sigma = 5.670374419e-8 return 4.0 * sigma * F * eps_g * Tfilm_K**3

def h_gas_rad_smith(T_K: float, pH2O_Pa: float, pCO2_Pa: float, L_m: float, Twall_K: float, F: float = 1.0, , Texp: float = 0.65) -> float: eps = emissivity(T_K, pH2O_Pa, pCO2_Pa, L_m, Texp=Texp) Tfilm = 0.5 (T_K + Twall_K) return h_rad(Tfilm, eps, F)

def h_rad(g: GasStream, spec: Dict[str, Any], Tg: Q_) -> Q_: Tg = g.T pH2O, pCO2 = _gas_partials(g) Lb = mean_beam_length(spec.to("m").magnitude) F = float(spec.get("rad_F", 1.0)) Texp = float(spec.get("rad_Texp", 0.65)) h_val = h_gas_rad_smith(Tg.to("K").magnitude, pH2O, pCO2, Lb, Tg.to("K").magnitude, F, Texp=Texp) return Q(max(h_val, 0.0), "W/m^2/K")

def reynolds(rho: Q, V: Q_, D: Q_, mu: Q_) -> float: Re = (rho * V * D / mu).to("m/s").magnitude return max(Re, 1e-12)

def prandtl(cp: Q, mu: Q_, k: Q_) -> float: Pr = (cp * mu / k).to("m/s").magnitude return max(Pr, 1e-12)

def vel_internal(g: GasStream, A: Q) -> Q_: rho = _gas.rho(g.T, g.P, g.comp) return (g.mass_flow / (rho * A)).to("m/s")

def vel_external(g: GasStream, A_bulk: Q, umax_factor: Q_ | float | None) -> Q_: rho = _gas.rho(g.T, g.P, g.comp) V_bulk = (g.mass_flow / (rho * A_bulk)).to("m/s") if umax_factor is None: return V_bulk f = umax_factor if isinstance(umax_factor, (int, float)) else umax_factor.to("m/s").magnitude return (max(f, 1.0) * V_bulk).to("m/s")

def nu_internal(Re: float, Pr: float, D: Q, L: Q_) -> float: if Re < 2300.0: Gz = Re * Pr * (D.to("m").magnitude / max(L.to("m").magnitude, 1e-12)) return 3.66 + 0.0668 * Gz / (1.0 + 0.04 * (Gz ** (2.0/3.0))) f = (0.79 * np.log(Re) - 1.64) ** -2 num = (f/8.0) * (Re - 1000.0) * Pr den = 1.0 + 12.7 * np.sqrt(f/8.0) * ((Pr ** (2.0/3.0)) - 1.0) return max(num / max(den, 1e-12), 1e-12)

def nu_churchill_bernstein(Re: float, Pr: float) -> float: a = 0.3 b = (0.62 * Re0.5 * Pr(1/3.0)) / ((1.0 + (0.4/Pr)(2.0/3.0)) 0.25) c = (1.0 + (Re / 282000.0) ** (5.0/8.0)) ** (4.0/5.0) return max(a + b * c, 1e-12)

def nu_zukauskas(Re: float, Pr: float, arrangement: str) -> float | None: bands = [ (1e3, 2e3, {"inline": (0.90, 0.40), "staggered": (1.04, 0.40)}), (2e3, 4e3, {"inline": (0.52, 0.50), "staggered": (0.71, 0.50)}), (4e3, 1e5, {"inline": (0.27, 0.63), "staggered": (0.35, 0.60)}), (1e5, 2e6, {"inline": (0.021, 0.84), "staggered": (0.022, 0.84)}), ] C = m = None arr = "staggered" if arrangement == "staggered" else "inline" for Re_min, Re_max, table in bands: if Re_min <= Re < Re_max: C, m = table[arr] break if C is None: return None n = 0.36 if Pr <= 10.0 else 0.25 return max(C * (Re0.5) * (Pr0.5), 1e-12)

def h_from_Nu(Nu: float, k: Q, D: Q_) -> Q_: return (Q_(Nu, "m") * k / D).to("W/m^2/K")

def h_conv_internal(g: GasStream, spec: dict) -> Q: D = spec["inner_diameter"].to("m") L = spec["inner_length"].to("m") A = spec["hot_flow_A"].to("m^2")

V = _vel_internal(g, A)
rho = _gas.rho(g.T, g.P, g.comp)
mu = _gas.mu(g.T, g.P, g.comp)
k = _gas.k(g.T, g.P, g.comp)
cp = _gas.cp(g.T, g.P, g.comp)

Re = _reynolds(rho, V, D, mu)
Pr = _prandtl(cp, mu, k)

```

```

Nu = _nu_internal(Re, Pr, D, L)
return _h_from_Nu(Nu, k, D)

def h_conv_economiser_external(g: GasStream, spec: dict) -> Q: D = spec["outer_diameter"].to("m")
A_bulk = spec["hot_flow_A"].to("m^2") umax = spec.get("umax_factor", None)

V = _vel_external(g, A_bulk, umax)
rho = _gas.rho(g.T, g.P, g.comp)
mu = _gas.mu(g.T, g.P, g.comp)
k = _gas.k(g.T, g.P, g.comp)
cp = _gas.cp(g.T, g.P, g.comp)

Re = _reynolds(rho, V, D, mu)
Pr = _prandtl(cp, mu, k)

arrangement = spec.get("arrangement", "inline")
Nu_z = _nu_zukauskas(Re, Pr, arrangement)
if Nu_z is None:
    Nu_z = _nu_churchill_bernstein(Re, Pr)
return _h_from_Nu(Nu_z, k, D)

def gas_htc_parts(g: GasStream, spec: dict, Tgw: Q_, *, stage_kind: str | None = None) -> Tuple[Q_, Q_]: kind = (stage_kind or spec.get("stage_kind") or "single_tube").lower()

if kind in ("single_tube", "reversal_chamber", "tube_bank"):
    h_conv = _h_conv_internal(g, spec)
elif kind == "economiser":
    h_conv = _h_conv_economiser_external(g, spec)
else:
    h_conv = _h_conv_internal(g, spec)

h_rad = _h_rad(g, spec, Tgw)
return h_conv.to("W/m^2/K"), h_rad.to("W/m^2/K")

def gas_htc(g: GasStream, spec: dict, Tgw: Q_, *, stage_kind: str | None = None) -> Q_: h_conv, h_rad = gas_htc_parts(g, spec, Tgw, stage_kind=stage_kind) return (h_conv + h_rad).to("W/m^2/K")
=====
FILE: heat/geometry.py =====
from math import pi
from dataclasses import replace
from typing import List
from common.models import HXStage, Drum
from common.units import Q_
class GeometryBuilder:
    def __init__(self, drum: Drum):
        self.drum = drum

    def enrich(self, stages: List[HXStage]) -> List[HXStage]:
        out: List[HXStage] = []
        for stg in stages:
            if stg.kind == "single_tube":
                spec = dict(stg.spec)
                Di_t = spec["inner_diameter"].to("m")
                t = spec["wall_t"].to("m")
                Do_t = (Di_t + 2*t).to("m")
                Di_drum = self.drum.Di.to("m")

                A_drum = (pi * (Di_drum/2)**2).to("m^2")
                A_tube_out = (pi * (Do_t/2)**2).to("m^2")

                spec["outer_diameter"] = Do_t

```

```

spec["roughness_cold_surface"] = spec["roughness_out"]

hot_wet_P = (pi * Di_t).to("m")
hot_flow_A = (pi * (Di_t/2)**2).to("m^2")
hot_Dh = (4 * hot_flow_A / hot_wet_P).to("m")

cold_wet_P = (pi * Do_t).to("m")
cold_flow_A = (A_drum - A_tube_out).to("m^2")
cold_Dh = (4 * cold_flow_A / cold_wet_P).to("m")

spec.update({
    "hot_wet_P": hot_wet_P, "hot_flow_A": hot_flow_A, "hot_Dh": hot_Dh,
    "cold_wet_P": cold_wet_P, "cold_flow_A": cold_flow_A, "cold_Dh": cold_Dh
})
out.append(replace(stg, spec=spec))

elif stg.kind == "tube_bank":
    spec = dict(stg.spec)
    Di_t = spec["inner_diameter"].to("m")
    t = spec["wall_t"].to("m")
    Nt = spec["tubes_number"].to("")
    Do_t = (Di_t + 2*t).to("m")

    Ds = self.drum.Di.to("m")
    B = spec["baffle_spacing"].to("m")
    ST = spec["ST"].to("m")
    SL = spec["SL"].to("m")

    FAR_T = (1 - (Do_t / ST)).to("")
    A_gross = (Ds * B).to("m^2")
    A_cross = (A_gross * FAR_T).to("m^2")
    arr = (spec.get("arrangement","inline") or "inline").lower()
    if arr == "staggered":
        FAR_L = (1 - (0.5 * Do_t / SL)).to("")
        umax = (ST / (ST - Do_t)) * ((SL / (SL - 0.5*Do_t)) ** 0.5)
    else:
        umax = (ST / (ST - Do_t))
    spec["umax_factor"] = umax.to("dimensionless")

spec["roughness_cold_surface"] = spec["roughness_out"]
spec["outer_diameter"] = Do_t

A_drum = (pi * (Ds/2)**2).to("m^2")
A_tube_out = (pi * (Do_t/2)**2).to("m^2")

cold_wet_P = (Nt * pi * Do_t).to("m")
cold_flow_A = A_cross
cold_Dh = (4 * cold_flow_A / cold_wet_P).to("m")

hot_wet_P = (Nt * pi * Di_t).to("m")
hot_flow_A = (Nt * (pi * (Di_t/2)**2)).to("m^2")
hot_Dh = (4 * hot_flow_A / hot_wet_P).to("m")

```

```

spec.update({
    "hot_wet_P": hot_wet_P, "hot_flow_A": hot_flow_A, "hot_Dh": hot_Dh,
    "cold_wet_P": cold_wet_P, "cold_flow_A": cold_flow_A, "cold_Dh": cold_Dh
})
out.append(replace(stg, spec=spec))

elif stg.kind == "reversal_chamber":
    spec = dict(stg.spec)

    Di_t = spec["inner_diameter"].to("m")
    t = spec["wall_t"].to("m")
    Do_t = (Di_t + 2*t).to("m")

    Di_drum = self.drum.Di.to("m")
    A_drum = (pi * (Di_drum/2)**2).to("m^2")
    A_tube_out = (pi * (Do_t/2)**2).to("m^2")

    spec["outer_diameter"] = Do_t
    spec["roughness_cold_surface"] = spec["roughness_out"]

    hot_wet_P = (pi * Di_t).to("m")
    hot_flow_A = (pi * (Di_t/2)**2).to("m^2")
    hot_Dh = (4 * hot_flow_A / hot_wet_P).to("m")

    cold_wet_P = (pi * Do_t).to("m")
    cold_flow_A = (A_drum - A_tube_out).to("m^2")
    cold_Dh = (4 * cold_flow_A / cold_wet_P).to("m")

    spec.update({
        "hot_wet_P": hot_wet_P, "hot_flow_A": hot_flow_A, "hot_Dh": hot_Dh,
        "cold_wet_P": cold_wet_P, "cold_flow_A": cold_flow_A, "cold_Dh": cold_Dh
    })
    out.append(replace(stg, spec=spec))

elif stg.kind == "economiser":
    spec = dict(stg.spec)

    Di_t = spec["inner_diameter"].to("m")
    t = spec["wall_t"].to("m")
    Do_t = (Di_t + 2*t).to("m")

    n_tubes_q = spec.get("n_tubes", None)
    tube_len_q = spec.get("tube_length", None)

    if n_tubes_q is None or tube_len_q is None:
        raise KeyError(f"{stg.name}: economiser requires n_tubes, tube_length")

    N_tubes = int(round(n_tubes_q.to("").magnitude))
    tube_len = tube_len_q.to("m")

    N_tubes = max(N_tubes, 1)

    Ds = spec["shell_inner_diameter"].to("m")

```

```

B  = spec["baffle_spacing"].to("m")
ST = spec["ST"].to("m")
SL = spec["SL"].to("m")

A_gross = (Ds * B).to("m^2")
FAR_T  = (1 - (Do_t / ST)).to("")
A_cross = (A_gross * FAR_T).to("m^2")

arr = (spec.get("arrangement", "inline") or "inline").lower()
if arr == "staggered":
    umax = (ST / (ST - Do_t)) * ((SL / (SL - 0.5*Do_t)) ** 0.5)
else:
    umax = (ST / (ST - Do_t))
spec["umax_factor"] = umax.to("dimensionless")

spec["outer_diameter"] = Do_t
spec["roughness_cold_surface"] = spec["roughness_in"]

hot_wet_P  = (N_tubes * pi * Do_t).to("m")
hot_flow_A = A_cross
hot_Dh     = (4 * hot_flow_A / hot_wet_P).to("m")

cold_wet_P  = (N_tubes * pi * Di_t).to("m")
cold_flow_A = (N_tubes * (pi * (Di_t/2)**2)).to("m^2")
cold_Dh     = (4 * cold_flow_A / cold_wet_P).to("m")

N_rows_q = spec.get("N_rows", None)
N_rows = int(round(N_rows_q.to("") .magnitude)) if N_rows_q is not None else 1
N_rows = max(N_rows, 1)
hot_flow_L = spec.get("hot_flow_length", (Q_(N_rows, "") * SL)).to("m")

spec.update({
    "hot_wet_P": hot_wet_P, "hot_flow_A": hot_flow_A, "hot_Dh": hot_Dh,
    "cold_wet_P": cold_wet_P, "cold_flow_A": cold_flow_A, "cold_Dh": cold_Dh,
    "tube_length": tube_len,
    "hot_flow_length": hot_flow_L,
    "water_dx_factor": (tube_len / hot_flow_L).to("dimensionless"),
})
out.append(replace(stg, spec=spec))
else:
    raise ValueError("unknown stage kind")
return out
=====
===== FILE: heat/physics.py =====
from math import pi, log from common.units import Q_
def _nt(spec) -> float: Nt = spec.get("tubes_number", None) return (Nt.to("")).magnitude if Nt is not None else 1.0)

def fouling_resistances(spec: dict) -> tuple[Q_, Q_]: di = spec["inner_diameter"].to("m") do =
spec["outer_diameter"].to("m") tfo = spec["foul_t_in"].to("m") kfi = spec["foul_k_in"].to("W/m/K")
tfo = spec["foul_t_out"].to("m") kfo = spec["foul_k_out"].to("W/m/K") Di_new = di - 2tfo Rfi =
log(di/Di_new)/(2pi*kfi) do_new = do + 2tfo Rfo = log(do_new/do)/(2pi*kfo)

Nt = _nt(spec)
return (Rfi / Nt).to("K*m/W"), (Rfo / Nt).to("K*m/W")

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```

def wall_resistance(spec: dict) -> Q_: di = spec["inner_diameter"].to("m") do = spec["outer_diameter"].to("m")
k = spec["wall_k"].to("W/m/K") R = log(do/di) / (2*pi*k) Nt = _nt(spec) return (R / Nt).to("K*m/W")
=====
from future import annotations import pandas as pd from common.results import GlobalProfile, CombustionResult from common.props import WaterProps, GasProps from common.units import Q_ from heat.gas_htc import emissivity from combustion.mass_mole import to_mole import cantera as ct from common.units import Q_ from common.constants import T_ref, P_ref
_gas = GasProps()
def _mag_or_nan(q, unit): return q.to(unit).magnitude if q is not None else float("nan")
def flue_sensible_to_ref(g) -> Q_: h_sens = _gas.h_sensible(g.T, g.P, g.comp).to("J/kg") return (g.mass_flow * h_sens).to("MW")
def profile_to_dataframe(gp: "GlobalProfile", *, remap_water: bool = True) -> "pd.DataFrame":
stage_ranges: dict[int, tuple[int, int]] = {} for i in range(len(gp.x)): k = gp.stage_index[i] if k not in stage_ranges: stage_ranges[k] = [i, i] else: stage_ranges[k][1] = i stage_ranges = {k: (v[0], v[1]) for k, v in stage_ranges.items()}
stage_offsets: dict[int, Q_] = {}
offset = Q_(0.0, "m")
for k, sr in enumerate(gp.stage_results):
    stage_offsets[k] = offset
    if sr.steps:
        last = sr.steps[-1]
        offset = (offset + last.x + last.dx).to("m")

rows = []
for i in range(len(gp.x)):
    g = gp.gas[i]

    k_stage = gp.stage_index[i]
    disable_water_hydraulics = (k_stage <= 4)
    sr_stage = gp.stage_results[k_stage]
    A_hot = sr_stage.hot_flow_A
    A_cold = sr_stage.cold_flow_A
    Dh_hot = sr_stage.hot_Dh
    Dh_cold = sr_stage.cold_Dh

    if remap_water:
        i0, iN = stage_ranges[gp.stage_index[i]]
        i_local = i - i0
        j = iN - i_local
    else:
        j = i

    w = gp.water[j]

    xq = WaterProps.quality_from_Ph(w.P, w.h)
    Two_phase = xq is not None

    if Two_phase:
        Tw = WaterProps.Tsat(w.P)
        w_cp = w_mu = w_k = None
        w_rho = WaterProps.rho_from_Px(w.P, xq) if xq is not None else None

```

```

else:
    Tw    = WaterProps.T_from_Ph(w.P, w.h)
    w_cp = WaterProps.cp_from_Ph(w.P, w.h)
    w_mu = WaterProps.mu_from_Ph(w.P, w.h)
    w_k   = WaterProps.k_from_Ph(w.P, w.h)
    w_rho = WaterProps.rho_from_Ph(w.P, w.h)

    g_h    = _gas.h_sensible(g.T, g.P, g.comp)
    g_mu  = _gas.mu(g.T, g.P, g.comp)
    g_rho = _gas.rho(g.T, g.P, g.comp)

    gas_V = (g.mass_flow / (g_rho * A_hot)).to("m/s")
    Re_gas = (g_rho * gas_V * Dh_hot / g_mu).to("").magnitude

    if w_rho is not None and A_cold is not None:
        water_V = (w.mass_flow / (w_rho * A_cold)).to("m/s")
    else:
        water_V = None

    if w_rho is not None and w_mu is not None and water_V is not None:
        Re_water = (w_rho * water_V * Dh_cold / w_mu).to("").magnitude
    else:
        Re_water = float("nan")

    if disable_water_hydraulics:
        water_V = None
        Re_water = float("nan")
        w_cp = w_mu = w_k = w_rho = None
        w_dP_fric = w_dP_minor = w_dP_tot = float("nan")
    else:
        if Two_phase:
            Tw = WaterProps.Tsat(w.P)
            w_cp = w_mu = w_k = None
            w_rho = WaterProps.rho_from_Px(w.P, xq) if xq is not None else None
        else:
            Tw    = WaterProps.T_from_Ph(w.P, w.h)
            w_cp = WaterProps.cp_from_Ph(w.P, w.h)
            w_mu = WaterProps.mu_from_Ph(w.P, w.h)
            w_k   = WaterProps.k_from_Ph(w.P, w.h)
            w_rho = WaterProps.rho_from_Ph(w.P, w.h)

        if w_rho is not None and A_cold is not None:
            water_V = (w.mass_flow / (w_rho * A_cold)).to("m/s")
        else:
            water_V = None

        if w_rho is not None and w_mu is not None and water_V is not None:
            Re_water = (w_rho * water_V * Dh_cold / w_mu).to("").magnitude
        else:
            Re_water = float("nan")

        w_dP_fric = gp.w_dP_fric[i].to("Pa").magnitude
        w_dP_minor = gp.w_dP_minor[i].to("Pa").magnitude
        w_dP_tot = gp.w_dP_tot[i].to("Pa").magnitude

```

```

Y = {sp: float(q.to("").magnitude) for sp, q in (g.comp or {}).items()}
X = to_mole(Y)

xH2O = X.get("H2O", 0.0)
xCO2 = X.get("CO2", 0.0)

P_Pa = g.P.to("Pa").magnitude
pH2O = xH2O * P_Pa
pCO2 = xCO2 * P_Pa

Lb_m = (0.9 * Dh_hot).to("m").magnitude
gas_eps = emissivity(
    g.T.to("K").magnitude,
    pH2O,
    pCO2,
    Lb_m,
)

x_local = gp.x[i].to("m")
x_global = (stage_offsets[k_stage] + x_local).to("m")

row = {
    "stage_name": gp.stage_name[i],
    "i": i,
    "x[m)": x_global.magnitude,
    "dx[m)": gp.dx[i].to("m").magnitude,
    "qprime[MW/m)": gp.qprime[i].to("MW/m").magnitude,
    "UA_prime[MW/K/m)": gp.UA_prime[i].to("MW/K/m").magnitude,
    "gas_P[kPa)": g.P.to("kPa").magnitude,
    "gas_T[°C)": g.T.to("degC").magnitude,
    "gas_h[kJ/kg)": g_h.to("kJ/kg").magnitude,
    "water_P[kPa)": w.P.to("kPa").magnitude,
    "water_T[°C)": Tw.to("degC").magnitude,
    "water_h[kJ/kg)": w.h.to("kJ/kg").magnitude,
    "gas_eps[-)": gas_eps,
    "water_x[-)": _mag_or_nan(xq, ""),
    "boiling": "true" if xq is not None else "false",
    "gas_V[m/s)": gas_V.to("m/s").magnitude,
    "Re_gas[-)": Re_gas,
    "h_gas[W/m^2/K)": gp.h_g[i].to("W/m^2/K").magnitude,
    "water_V[m/s)": (_mag_or_nan(water_V, "m/s") if isinstance(water_V, Q_) else float("nan")),
    "Re_water[-)": Re_water,
    "h_water[W/m^2/K)": gp.h_c[i].to("W/m^2/K").magnitude,
    "dP_fric[kPa)": gp.dP_fric[i].to("kPa").magnitude,
    "dP_minor[kPa)": gp.dP_minor[i].to("kPa").magnitude,
    "dP_total[kPa)": gp.dP_total[i].to("kPa").magnitude,
    "water_dP_fric[kPa)": (w_dP_fric if disable_water_hydraulics else gp.w_dP_fric[i].to("kPa").magnitude),
    "water_dP_minor[kPa)": (w_dP_minor if disable_water_hydraulics else gp.w_dP_minor[i].to("kPa").magnitude),
    "water_dP_total[kPa)": (w_dP_tot if disable_water_hydraulics else gp.w_dP_tot[i].to("kPa").magnitude),
    "water_cp[kJ/kg/K)": _mag_or_nan(w_cp, "kJ/kg/K"),
    "water_mu[Pa*s)": _mag_or_nan(w_mu, "Pa*s"),
    "water_k[W/m/K)": _mag_or_nan(w_k, "W/m/K"),
    "water_rho[kg/m^3)": _mag_or_nan(w_rho, "kg/m^3"),
}

```

```

}

rows.append(row)

return pd.DataFrame(rows)

def summary_from_profile(gp: "GlobalProfile", combustion: CombustionResult | None = None,
drum_pressure: Q_ | None = None) -> tuple[list[dict], float, float]:
    rows = []
    Q_total = 0.0
    UA_total = 0.0
    Q_total_conv = 0.0
    Q_total_rad = 0.0
    dP_total_fric = 0.0
    dP_total_minor = 0.0
    dP_total_total = 0.0
    w_dP_tot_fric = 0.0
    w_dP_tot_minor = 0.0
    w_dP_tot_total = 0.0
    stack_T_C = None
    feedwater_mdot_kg_s = None
    circulation_mdot_kg_s = None
    flue_mdot_kg_s = None
    boiler_water_in_P_kPa = None
    boiler_water_in_T_C = None
    boiler_water_out_T_C = None
    boiler_water_Tsat_C = None
    econ_out_h_Jkg = None
    feedwater_mdot_q = None

    import itertools
    for k, grp in itertools.groupby(range(len(gp.x)), key=lambda i: gp.stage_index[i]):
        disable_water_hydraulics = (k <= 4)
        idxs = list(grp)
        name = gp.stage_name[idxs[0]]
        sr_stage = gp.stage_results[k]

        A_hot = sr_stage.hot_flow_A
        A_cold = sr_stage.cold_flow_A

        gas_V_sum = 0.0
        water_V_sum = 0.0
        n_steps = len(idxs)

        for i in idxs:
            g = gp.gas[i]
            w = gp.water[i]

            g_rho = _gas.rho(g.T, g.P, g.comp)
            gas_V = (g.mass_flow / (g_rho * A_hot)).to("m/s").magnitude
            gas_V_sum += gas_V

            if A_cold is not None:
                w_rho = WaterProps.rho_from_Ph(w.P, w.h)
                water_V = (w.mass_flow / (w_rho * A_cold)).to("m/s").magnitude
                water_V_sum += water_V

            gas_V_avg = gas_V_sum / max(n_steps, 1)
            if disable_water_hydraulics or A_cold is None:
                water_V_avg = float("nan")
            else:
                water_V_avg = water_V_sum / max(n_steps, 1)

        Q_stage = sum((gp.qprime[i] * gp.dx[i]).to("MW").magnitude for i in idxs)
        UA_stage = sum((gp.UA_prime[i] * gp.dx[i]).to("MW/K").magnitude for i in idxs)

        Q_stage_conv = sum((st.qprime_conv * st.dx).to("MW").magnitude for st in sr_stage.steps)
        Q_stage_rad = sum((st.qprime_rad * st.dx).to("MW").magnitude for st in sr_stage.steps)

        dP_fric = sum(gp.dP_fric[i].to("kPa").magnitude for i in idxs)
        dP_minor = sum(gp.dP_minor[i].to("kPa").magnitude for i in idxs)

```

```

dP_total = sum(gp.dP_total[i].to("kPa").magnitude for i in idxs)

w_dP_fric = sum(gp.w_dP_fric[i].to("kPa").magnitude for i in idxs)
w_dP_minor = sum(gp.w_dP_minor[i].to("kPa").magnitude for i in idxs)
w_dP_tot = sum(gp.w_dP_tot[i].to("kPa").magnitude for i in idxs)

g_in = gp.gas[idxs[0]]
g_out = gp.gas[idxs[-1]]

gas_in_T = g_in.T.to("degC").magnitude
gas_out_T = g_out.T.to("degC").magnitude

gas_in_P = g_in.P.to("kPa").magnitude
gas_out_P = g_out.P.to("kPa").magnitude

gas_in_h = _gas.h_sensible(g_in.T, g_in.P, g_in.comp).to("kJ/kg").magnitude
gas_out_h = _gas.h_sensible(g_out.T, g_out.P, g_out.comp).to("kJ/kg").magnitude

w_in = gp.water[idxs[0]]
w_out = gp.water[idxs[-1]]

water_in_h = w_in.h.to("kJ/kg").magnitude
water_out_h = w_out.h.to("kJ/kg").magnitude

water_in_P = w_in.P.to("kPa").magnitude
water_out_P = w_out.P.to("kPa").magnitude

water_in_T = WaterProps.T_from_Ph(w_in.P, w_in.h).to("degC").magnitude
water_out_T = WaterProps.T_from_Ph(w_out.P, w_out.h).to("degC").magnitude

if flue_mdot_kg_s is None:
    flue_mdot_kg_s = g_in.mass_flow.to("kg/s").magnitude

if k == 0:
    boiler_water_out_T_C = water_out_T

if k == len(gp.stage_results) - 1:
    boiler_water_in_T_C = water_in_T
    boiler_water_in_P_kPa = water_in_P

try:
    feedwater_mdot_q = gp.stage_results[k].steps[0].water.mass_flow.to("kg/s")
    feedwater_mdot_kg_s = feedwater_mdot_q.magnitude
except Exception:
    feedwater_mdot_q = None
    feedwater_mdot_kg_s = None

try:
    econ_out_h_Jkg = w_out.h.to("J/kg")
except Exception:
    econ_out_h_Jkg = None

```

```

row = {
    "stage_index": k,
    "stage_name": name,
    "stage_kind": gp.stage_results[k].stage_kind,
    "Q_stage[MW]": Q_stage,
    "UA_stage[MW/K]": UA_stage,
    "gas_V_avg[m/s)": gas_V_avg,
    "water_V_avg[m/s)": water_V_avg,
    "gas_in_P[kPa)": gas_in_P,
    "gas_in_T[°C)": gas_in_T,
    "gas_in_h[kJ/kg)": gas_in_h,
    "gas_out_P[kPa)": gas_out_P,
    "gas_out_T[°C)": gas_out_T,
    "gas_out_h[kJ/kg)": gas_out_h,
    "water_in_P[kPa)": water_in_P,
    "water_in_T[°C)": water_in_T,
    "water_in_h[kJ/kg)": water_in_h,
    "water_out_P[kPa)": water_out_P,
    "water_out_T[°C)": water_out_T,
    "water_out_h[kJ/kg)": water_out_h,
    "ΔP_stage_fric[kPa)": dP_fric,
    "ΔP_stage_minor[kPa)": dP_minor,
    "ΔP_stage_total[kPa)": dP_total,
    "ΔP_water_stage_fric[kPa)": (float("nan") if disable_water_hydraulics else w_dP_fric),
    "ΔP_water_stage_minor[kPa)": (float("nan") if disable_water_hydraulics else w_dP_minor),
    "ΔP_water_stage_total[kPa)": (float("nan") if disable_water_hydraulics else w_dP_tot),
    "Q_conv_stage[MW)": Q_stage_conv,
    "Q_rad_stage[MW)": Q_stage_rad,
    "steam_capacity[kg/s)": "",
    "steam_capacity[t/h)": "",
    "η_direct[-)": "",
    "η_indirect[-)": "",
    "Q_total_useful[MW)": "",
    "Q_in_total[MW)": "",
    "P_LHV[MW)": "",
    "LHV_mass[kJ/kg)": "",
    "flue_mdot[kg/s)": "",
    "boiler_water_in_T[°C)": "",
    "boiler_water_out_T[°C)": "",
    "boiler_water_P[kPa)": "",
    "boiler_water_Tsat[°C)": ""
}
rows.append(row)

Q_total += Q_stage
UA_total += UA_stage
Q_total_conv += Q_stage_conv
Q_total_rad += Q_stage_rad
dP_total_fric += dP_fric
dP_total_minor += dP_minor
dP_total_total += dP_total
w_dP_tot_fric += w_dP_fric
w_dP_tot_minor += w_dP_minor

```

```

w_dP_tot_total += w_dP_tot
stack_T_C = gas_out_T

steam_capacity_total_kg_s = None
steam_capacity_total_tph = None

P_for_evap: Q_ | None = drum_pressure
if P_for_evap is None and boiler_water_in_P_kPa is not None:
    P_for_evap = Q_(boiler_water_in_P_kPa, "kPa")

if P_for_evap is not None:
    P_q = P_for_evap.to("Pa")
    boiler_water_Tsat_C = WaterProps.Tsat(P_q).to("degC").magnitude

    hf = WaterProps.h_f(P_q).to("J/kg")
    hg = WaterProps.h_g(P_q).to("J/kg")

    evap_stage_names = {f"HX_{i}" for i in range(1, 6)}
    Q_evap_W = 0.0
    for r in rows:
        if r.get("stage_name") in evap_stage_names and isinstance(r.get("Q_stage[MW]"), (int, float)):
            Q_evap_W += Q_(r["Q_stage[MW]"], "MW").to("W").magnitude
    Q_evap = Q_(Q_evap_W, "W")

    x_out = 1.0
    h_s = (hf + Q_(x_out, "") * (hg - hf)).to("J/kg")
    denom = (h_s - hf).to("J/kg")

    if denom.magnitude <= 0:
        steam_capacity_total_kg_s = None
        steam_capacity_total_tph = None
    elif (feedwater_mdot_q is None) or (econ_out_h_Jkg is None):
        steam_capacity_total_kg_s = None
        steam_capacity_total_tph = None
    else:
        Q_sens = (feedwater_mdot_q * (hf - econ_out_h_Jkg)).to("W")
        if Q_sens.magnitude < 0:
            Q_sens = Q_(0.0, "W")

        Q_evap_net = (Q_evap - Q_sens).to("W")
        if Q_evap_net.magnitude < 0:
            Q_evap_net = Q_(0.0, "W")

        m_s_q = (Q_evap_net / denom).to("kg/s")
        steam_capacity_total_kg_s = m_s_q.magnitude
        steam_capacity_total_tph = m_s_q.to("tonne/hour").magnitude

    Q_evap_pos = max(Q_evap.to("W").magnitude, 1e-12)

    for r in rows:
        if r.get("stage_name") in evap_stage_names and isinstance(r.get("Q_stage[MW]"), (int, float)):
            Q_stage_W = Q_(r["Q_stage[MW]"], "MW").to("W")

            frac = Q_stage_W.to("W").magnitude / Q_evap_pos

```

```

    frac = max(0.0, min(1.0, frac))

    Q_stage_eff = (Q_stage_W - Q_sens * Q_(frac, "")).to("W")
    if Q_stage_eff.magnitude < 0:
        Q_stage_eff = Q_(0.0, "W")

    m_s_stage = (Q_stage_eff / denom).to("kg/s")
    r["steam_capacity[kg/s]"] = m_s_stage.magnitude
    r["steam_capacity[t/h]"] = m_s_stage.to("tonne/hour").magnitude

if steam_capacity_total_kg_s is not None:
    steam_capacity_total_tph = Q_(steam_capacity_total_kg_s, "kg/s").to("tonne/hour").magnitude
else:
    steam_capacity_total_tph = None

Q_useful_hx = Q_total
Q_in_total = None
P_LHV_W = None
LHV_mass_kJkg = None
eta_direct = None
eta_indirect = None
Stack_loss_fraction = None
Q_flue_out_MW = None

Q_useful = Q_useful_hx

if combustion is not None:
    # "Declared" input from combustion model (may not match postproc reference basis)
    Q_in_declared = combustion.Q_in.to("MW").magnitude

    if combustion.fuel_P_LHV is not None:
        P_LHV_W = combustion.fuel_P_LHV.to("MW").magnitude
    else:
        P_LHV_W = combustion.LHV.to("MW").magnitude

    if combustion.fuel_LHV_mass is not None:
        LHV_mass_kJkg = combustion.fuel_LHV_mass.to("kJ/kg").magnitude

# Stack sensible loss to reference
try:
    g_stack = gp.gas[-1]
    Q_flue_out_MW = flue_sensible_to_ref(g_stack).to("MW").magnitude
except Exception:
    Q_flue_out_MW = None

# ---- ENFORCE: Q_in_used = Q_useful + Q_flue_out ----
if Q_flue_out_MW is not None:
    Q_in_used = Q_useful + Q_flue_out_MW
else:
    # If we can't compute flue loss, fall back to declared input
    Q_in_used = Q_in_declared

# Report balance error against the declared combustion input (diagnostic)
if (Q_in_declared is not None) and (Q_flue_out_MW is not None):

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Q_balance_err_MW = Q_in_declared - (Q_useful + Q_flue_out_MW)
else:
    Q_balance_err_MW = None

# Efficiencies computed from enforced balance => ALWAYS equal
if Q_in_used and Q_in_used > 0.0 and Q_flue_out_MW is not None:
    eta_direct = Q_useful / Q_in_used
    Stack_loss_fraction = Q_flue_out_MW / Q_in_used
    eta_indirect = 1.0 - Stack_loss_fraction
elif Q_in_used and Q_in_used > 0.0:
    eta_direct = Q_useful / Q_in_used
    eta_indirect = eta_direct
    Stack_loss_fraction = None

# overwrite the variable used downstream for reporting
Q_in_total = Q_in_used

total_row = {
    "stage_index": "",
    "stage_name": "TOTAL_BOILER",
    "stage_kind": "",
    "Q_stage[MW]": Q_useful_hx,
    "UA_stage[MW/K]": UA_total,
    "gas_V_avg[m/s)": "",
    "water_V_avg[m/s)": "",
    "gas_in_P[kPa)": "",
    "gas_in_T[°C)": "",
    "gas_in_h[kJ/kg)": "",
    "gas_out_P[kPa)": "",
    "gas_out_T[°C)": "",
    "gas_out_h[kJ/kg)": "",
    "water_in_P[kPa)": "",
    "water_in_T[°C)": "",
    "water_in_h[kJ/kg)": "",
    "water_out_P[kPa)": "",
    "water_out_T[°C)": "",
    "water_out_h[kJ/kg)": "",
    "ΔP_stage_fric[kPa)": dP_total_fric,
    "ΔP_stage_minor[kPa)": dP_total_minor,
    "ΔP_stage_total[kPa)": dP_total_total,
    "ΔP_water_stage_fric[kPa)": w_dP_tot_fric,
    "ΔP_water_stage_minor[kPa)": w_dP_tot_minor,
    "ΔP_water_stage_total[kPa)": w_dP_tot_total,
    "stack_temperature[°C)": stack_T_C,
    "feedwater_mdot[kg/s)": feedwater_mdot_kg_s if feedwater_mdot_kg_s is not None else "",
    "circulation_mdot[kg/s)": circulation_mdot_kg_s if circulation_mdot_kg_s is not None else "",
    "Q_conv_stage[MW)": Q_total_conv,
    "Q_rad_stage[MW)": Q_total_rad,
    "steam_capacity[kg/s)": steam_capacity_total_kg_s,
    "steam_capacity[t/h)": steam_capacity_total_tph,
    "η_direct[-)": eta_direct if eta_direct is not None else "",
    "η_indirect[-)": eta_indirect if eta_indirect is not None else "",
    "Stack_loss_fraction[-)": Stack_loss_fraction if Stack_loss_fraction is not None else ""
}

```

```

    "Q_total_useful[MW]": Q_useful,
    "Q_flue_out[MW]": Q_flue_out_MW if Q_flue_out_MW is not None else "",
    "Q_balance_error[MW]": (Q_balance_err_MW if Q_balance_err_MW is not None else ""),
    "Q_in_total[MW]": Q_in_total if Q_in_total is not None else "",
    "P_LHV[MW]": P_LHV_W if P_LHV_W is not None else "",
    "LHV_mass[kJ/kg)": LHV_mass_kJkg if LHV_mass_kJkg is not None else "",
    "flue_mdot[kg/s)": flue_mdot_kg_s if flue_mdot_kg_s is not None else "",
    "boiler_water_in_T[°C)": boiler_water_in_T_C if boiler_water_in_T_C is not None else "",
    "boiler_water_out_T[°C)": boiler_water_out_T_C if boiler_water_out_T_C is not None else "",
    "boiler_water_P[kPa)": boiler_water_in_P_kPa if boiler_water_in_P_kPa is not None else "",
    "boiler_water_Tsat[°C)": boiler_water_Tsat_C if boiler_water_Tsat_C is not None else "",
}

rows.append(total_row)

return rows, Q_total, UA_total
=====
=====FILE: heat/runner.py =====
from future import annotations from pathlib import Path from typing import List, Optional, Dict, Any from common.units import Q_ from heat.geometry import GeometryBuilder from heat.solver import solve_exchanger from common.models import HXStage, WaterStream, GasStream, Drum from common.results import build_global_profile, CombustionResult from heat.postproc import profile_to_dataframe, summary_from_profile from common.props import WaterProps

def q_or_none(s: Optional[str]) -> Optional[Q_]: if s is None: return None s = s.strip() return Q(s) if s else None

def run_hx( *, stages_raw: List[HXStage], water: WaterStream, gas: GasStream, drum: Drum, drum_pressure: Q_ | None = None, target_dx: str | None = None, min_steps: int = 20, max_steps: int = 400, max_passes: int = 20, tol_Q: str = "1e-3 W", tol_end: str = "1e-3 J/kg", write_csv: bool, outdir: str | Path = "results/runs", run_id: str | None = None, log_level: str = "INFO", combustion: CombustionResult | None = None, ) -> Dict[str, Any]:
    outdir = Path(outdir)
    outdir.mkdir(parents=True, exist_ok=True)

    if not run_id:
        from datetime import datetime
        run_id = datetime.now().strftime("%Y%m%d-%H%M%S")

    target_dx_q = _q_or_none(target_dx)
    tol_Q_q = Q_(tol_Q)
    tol_end_q = Q_(tol_end)

    if gas is None or water is None or drum is None:
        raise ValueError("missing required inputs: 'gas', 'water', and 'drum'")

    stages: List[HXStage] = GeometryBuilder(drum).enrich(stages_raw)

    drum_pool = None
    if drum_pressure is not None:
        P_d = drum_pressure.to("Pa")
        h_f = WaterProps.h_f(P_d).to("J/kg")

    drum_pool = WaterStream(mass_flow=water.mass_flow, h=h_f, P=P_d)

```

```

stage_results, gas_out, water_out = solve_exchanger(
    stages,
    gas,
    water,
    drum_pool=drum_pool,
    drum_pool_stage_count=5,
    target_dx=target_dx_q,
    min_steps_per_stage=min_steps,
    max_steps_per_stage=max_steps,
    max_passes=max_passes,
    tol_Q=tol_Q_q,
    tol_end=tol_end_q,
    log_level=log_level,
)
global_profile = build_global_profile(stage_results)

if write_csv:
    df_steps = profile_to_dataframe(global_profile)
else:
    df_steps = None

rows, _, _ = summary_from_profile(global_profile, combustion=combustion, drum_pressure=drum_pressure)

return {
    "gas_in": gas,
    "water_in": water,
    "gas_out": gas_out,
    "water_out": water_out,
    "stage_results": stage_results,
    "global_profile": global_profile,
    "steps_df": df_steps,
    "summary_rows": rows,
    "steps_csv": None,
    "summary_csv": None,
    "run_id": run_id,
    "outdir": str(outdir),
    "combustion": combustion,
}
=====
=====FILE: heat/solver.py =====
from future import annotations from typing import List, Tuple, Optional from math import ceil, log10
import logging

from common.units import Q_ from common.models import HXStage, GasStream, WaterStream from common.results import StepResult, StageResult from heat.step_solver import solve_step from common.props import GasProps, WaterProps from common.logging_utils import setup_logging

_gasprops = GasProps() _gas = GasProps()

def _clamp(v: int, lo: int, hi: int) -> int: return max(lo, min(hi, v))

def median_length(stages: List[HXStage]) -> Q: Ls = sorted([st.spec["inner_length"].to("m") for st in stages], key=lambda x: x.magnitude) return Ls[len(Ls)//2]

```

```

def make_grid(L: Q, n_steps: int) -> tuple[List[Q], Q]: dx = (L / n_steps).to("m") xs = [(i * dx).to("m")]
for i in range(n_steps)] return xs, dx

def _copy_step_with_stage( sr: StepResult, stage_name: str, stage_index: int, *, dP_fric: Q |
    None = None, dP_minor: Q | None = None, dP_total: Q | None = None, w_dP_fric: Q |
    None = None, w_dP_minor: Q | None = None, w_dP_tot: Q | None = None, ) ->
StepResult: return StepResult( i=sr.i, x=sr.x, dx=sr.dx, gas=sr.gas, water=sr.water, Tgw=sr.Tgw,
Tww=sr.Tww, UA_prime=sr.UA_prime, qprime=sr.qprime, boiling=sr.boiling, h_g=sr.h_g, h_c=sr.h_c,
qprime_conv=sr.qprime_conv, qprime_rad=sr.qprime_rad,
stage_name=stage_name, stage_index=stage_index, dP_fric=dP_fric if dP_fric is not None else Q_(0.0, "Pa"),
dP_minor=dP_minor if dP_minor is not None else Q_(0.0, "Pa"), dP_total=dP_total if dP_total is not None else Q_(0.0, "Pa"),
w_dP_fric=w_dP_fric if w_dP_fric is not None else Q_(0.0, "Pa"),
w_dP_minor=w_dP_minor if w_dP_minor is not None else Q_(0.0, "Pa"), w_dP_tot=w_dP_tot if w_dP_tot is not None else Q_(0.0, "Pa"),
)

def initial_wall_guesses(g: GasStream, w: WaterStream, stage: HXStage) -> tuple[Q, Q, Q]: Tg =
g.T.to("K") if stage.spec.get("pool_boiling", False): Tw = WaterProps.Tsat(w.P).to("K") else: Tw =
WaterProps.T_from_Ph(w.P, w.h).to("K") qprime = Q_(1e4, "W/m") return Tg, Tw, qprime

def _colebrook_white_f(Re: float, eps_over_D: float) -> float: Re = max(Re, 1e-6) if Re < 2300.0: return
64.0 / max(Re, 1e-12)

f = 0.25 / (log10(eps_over_D/3.7 + 5.74/(Re**0.9)) ** 2)

for _ in range(30):
    invsqrtf_old = 1.0 / (f ** 0.5)
    rhs = -2.0 * log10(eps_over_D/3.7 + 2.51/(Re * (f ** 0.5)))
    invsqrtf = rhs
    if abs(invsqrtf - invsqrtf_old) < 1e-6:
        break
    f = 1.0 / (invsqrtf ** 2)
return float(f)

def _friction_factor(Re: float, eps_over_D: float) -> float: if Re < 2300.0: return 64.0 / max(Re, 1e-12)
if Re >= 4000.0: return _colebrook_white_f(Re, eps_over_D) f_lam = 64.0 / max(Re, 1e-12) f_turb =
_colebrook_white_f(4000.0, eps_over_D) w = (Re - 2300.0) / (4000.0 - 2300.0) return float((1-w) * f_lam
+ w * f_turb)

def stage_minor_K_sum(stage: HXStage) -> Q: spec = stage.spec kind = stage.kind.lower()

K_hot_bend = spec.get("K_hot_bend", None)
if K_hot_bend is not None:
    return K_hot_bend.to("")

if kind == "reversal_chamber":
    Rc = spec.get("curvature_radius", None)
    Do = spec.get("outer_diameter", None)
    if Rc is not None and Do is not None and Rc.to("m").magnitude > 0 and Do.to("m").magnitude > 0:
        r = (Rc / Do).to("").magnitude
        Kbend = max(0.2, min(2.0, 0.9 / max(r, 1e-6)))
    else:
        Kbend = 0.5
    return Q_(Kbend, "")

return Q_(0.0, "")

def gas_dp_economiser_crossflow( g: GasStream, stage: HXStage, dx: Q, i_step: int, n_steps: int, ) ->
tuple[Q, Q, Q]: spec = stage.spec

```

```

A_hot = spec["hot_flow_A"].to("m^2")

Dh = spec["hot_Dh"].to("m")
eps = spec.get("roughness_out", Q_(0.0, "m")).to("m")

rho = _gas.rho(g.T, g.P, g.comp)
mu = _gas.mu(g.T, g.P, g.comp)

V_bulk = (g.mass_flow / (rho * A_hot)).to("m/s")
umax_factor_q = spec.get("umax_factor", Q_(1.0, ""))
umax_factor = umax_factor_q.to("").magnitude
V_char = (V_bulk * max(umax_factor, 1.0)).to("m/s")

Re = max((rho * V_char * Dh / mu).to("").magnitude, 1e-6)
eps_over_D = (eps / Dh).to("").magnitude

f = _friction_factor(Re, eps_over_D)

q_dyn = (rho * V_char**2 / 2.0).to("Pa")

dP_fric = (-Q_(f, "") * (dx / Dh) * q_dyn).to("Pa")

K_bend_per_step = spec.get("_K_bend_per_step", Q_(0.0, "")).to("")
K_inlet = spec.get("K_hot_inlet", Q_(0.0, "")).to("")
K_outlet = spec.get("K_hot_outlet", Q_(0.0, "")).to("")

K_minor = K_bend_per_step
if i_step == 0:
    K_minor = (K_minor + K_inlet).to("")
if i_step == max(n_steps - 1, 0):
    K_minor = (K_minor + K_outlet).to("")

dP_minor = (-K_minor * q_dyn).to("Pa")
dP_total = (dP_fric + dP_minor).to("Pa")

return dP_fric, dP_minor, dP_total

def gas_dp_components( g: GasStream, stage: HXStage, dx: Q, i_step: int, n_steps: int, ) -> tuple[Q_, Q_, Q_]: kind = stage.kind.lower()

if kind == "economiser":
    return _gas_dp_economiser_crossflow(g, stage, dx, i_step, n_steps)

spec = stage.spec
A = spec["hot_flow_A"].to("m^2")
Dh = spec["hot_Dh"].to("m")
eps = spec.get("roughness_in", Q_(0.0, "m")).to("m")
rho = _gas.rho(g.T, g.P, g.comp)
mu = _gas.mu(g.T, g.P, g.comp)

V = (g.mass_flow / (rho * A)).to("m/s")
Re = max((rho * V * Dh / mu).to("").magnitude, 1e-6)
eps_over_D = (eps / Dh).to("").magnitude

f = _friction_factor(Re, eps_over_D)

```

```

q = (rho * V**2 / 2.0).to("Pa")

dP_fric = (-f * (dx / Dh) * q).to("Pa")

K_bend_per_step = spec.get("_K_bend_per_step", Q_(0.0, "")).to("")

K_inlet = spec.get("K_hot_inlet", Q_(0.0, "")).to("")
K_outlet = spec.get("K_hot_outlet", Q_(0.0, "")).to("")

K_minor = K_bend_per_step

if i_step == 0:
    K_minor = (K_minor + K_inlet).to("")

if i_step == max(n_steps - 1, 0):
    K_minor = (K_minor + K_outlet).to("")

dP_minor = (-K_minor * q).to("Pa")
dP_total = (dP_fric + dP_minor).to("Pa")
return dP_fric, dP_minor, dP_total

def pressure_drop_gas(g: GasStream, stage: HXStage, i: int, dx: Q_, n_steps: int) -> Q_: , , dP_total
= _gas_dp_components(g, stage, dx, i, n_steps) return dP_total

def solve_T_for_h(P, X, h_target, T0, maxit=30): T = T0.to("K"); h_target = h_target.to("J/kg") for
in range(maxit): h = _gasprops.h(T, P, X) dh = (h_target - h).to("J/kg") if abs(dh).magnitude < 1e-3:
return T cp = _gasprops.cp(T, P, X) dT = (dh / cp).to("K") T = (T + 0.8*dT).to("K") return T

def update_gas_after_step(g, qprime, dx, stage, i: int, n_steps: int) -> GasStream: Q_step =
(qprime * dx).to("W") dh = (-Q_step / g.mass_flow).to("J/kg") h_old = _gasprops.h(g.T, g.P,
g.comp) h_new = (h_old + dh).to("J/kg") T_new = _solve_T_for_h(g.P, g.comp, h_new, g.T)
P_new = (g.P + pressure_drop_gas(g, stage, i=i, dx=dx, n_steps=n_steps)).to("Pa") return
GasStream(mass_flow=g.mass_flow, T=T_new, P=P_new, comp=g.comp)

def water_dp_components(w: WaterStream, stage: HXStage, dx: Q, i_step: int, n_steps: int) -> tuple[Q_,
Q_, Q_]: spec = stage.spec kind = stage.kind.lower()

if spec.get("pool_boiling", False):
    z = Q_(0.0, "Pa")
    return z, z, z

xq = WaterProps.quality_from_Ph(w.P, w.h)
if xq is not None:
    z = Q_(0.0, "Pa")
    return z, z, z

dP_fric = Q_(0.0, "Pa")
dP_minor = Q_(0.0, "Pa")

if kind == "economiser":
    A = spec["cold_flow_A"].to("m^2")
    Dh = spec["cold_Dh"].to("m")
    eps = spec.get("roughness_cold_surface", Q_(0.0, "m")).to("m")

rho = WaterProps.rho_from_Ph(w.P, w.h)

```

```

mu = WaterProps.mu_from_Ph(w.P, w.h)

V = (w.mass_flow / (rho * A)).to("m/s")
Re = max((rho * V * Dh / mu).to("").magnitude, 1e-6)
eps_over_D = (eps / Dh).to("").magnitude

f = _friction_factor(Re, eps_over_D)
q = (rho * V**2 / 2.0).to("Pa")

f_dx = spec.get("water_dx_factor", Q_(1.0, "")).to("").magnitude
dx_w = (dx * Q_(f_dx, "")).to("m")

dP_fric = (-f * (dx_w / Dh) * q).to("Pa")
else:
    A = spec.get("cold_flow_A", None)
    if A is not None:
        A = A.to("m^2")
        rho = WaterProps.rho_from_Ph(w.P, w.h)
        V = (w.mass_flow / (rho * A)).to("m/s")
        q = (rho * V**2 / 2.0).to("Pa")
    else:
        rho = WaterProps.rho_from_Ph(w.P, w.h)
        q = Q_(0.0, "Pa")

K_cold_bend_total = spec.get("K_cold_bend", Q_(0.0, "")).to("")
K_cold_bend_per_step = (K_cold_bend_total / max(n_steps, 1)).to("")

K_cold_inlet = spec.get("K_cold_inlet", Q_(0.0, "")).to("")
K_cold_outlet = spec.get("K_cold_outlet", Q_(0.0, "")).to("")

K_minor = K_cold_bend_per_step

if i_step == 0:
    K_minor = (K_minor + K_cold_inlet).to("")

if i_step == max(n_steps - 1, 0):
    K_minor = (K_minor + K_cold_outlet).to("")

if "q" not in locals():
    A = spec.get("cold_flow_A", None)
    if A is not None:
        A = A.to("m^2")
        rho = WaterProps.rho_from_Ph(w.P, w.h)
        V = (w.mass_flow / (rho * A)).to("m/s")
        q = (rho * V**2 / 2.0).to("Pa")
    else:
        q = Q_(0.0, "Pa")

dP_minor = (-K_minor * q).to("Pa")

dP_total = (dP_fric + dP_minor).to("Pa")
return dP_fric, dP_minor, dP_total

def update_water_after_step(w: WaterStream, qprime: Q_, dx: Q_, stage: HXStage, i: int, n_steps: int)

```

```

-> WaterStream: Q_step = (qprime * dx).to("W") dh = (Q_step / w.mass_flow).to("J/kg") h_new =
(w.h + dh).to("J/kg")

if stage.spec.get("pool_boiling", False):
    hf = WaterProps.h_f(w.P).to("J/kg")
    return WaterStream(mass_flow=w.mass_flow, h=hf, P=w.P)

dP_fric, dP_minor, dP_tot = _water_dp_components(w, stage, dx, i, n_steps)
P_new = (w.P + dP_tot).to("Pa")
return WaterStream(mass_flow=w.mass_flow, h=h_new, P=P_new)

def solve_stage( g_in: GasStream, w_in: WaterStream, stage: HXStage, n_steps: int, *, stage_index:
int, logger_name: str = "solver", ) -> tuple[GasStream, WaterStream, StageResult]: log = log-
ging.getLogger(logger_name) if stage.kind.lower() == "economiser": L = stage.spec["hot_flow_length"].to("m")
else: L = stage.spec["inner_length"].to("m") xs, dx = _make_grid(L, n_steps)

K_sum = _stage_minor_K_sum(stage).to("")
K_per_step = (K_sum / max(n_steps, 1)).to("")
stage.spec["_K_bend_per_step"] = K_per_step

steps: List[StepResult] = []

g = g_in
w = w_in
Tgw_guess, Tww_guess, qprime_guess = initial_wall_guesses(g, w, stage)

Q_sum = Q_(0.0, "W")
UA_sum = Q_(0.0, "W/K")
dP_fric_sum = Q_(0.0, "Pa")
dP_minor_sum = Q_(0.0, "Pa")
dP_total_sum = Q_(0.0, "Pa")
w_dP_fric_sum = Q_(0.0, "Pa")
w_dP_minor_sum = Q_(0.0, "Pa")
w_dP_tot_sum = Q_(0.0, "Pa")

for i, x in enumerate(xs):
    dP_fric_step, dP_minor_step, dP_tot_step = _gas_dp_components(g, stage, dx, i, n_steps)
    w_dP_fric_step, w_dP_minor_step, w_dP_tot_step = _water_dp_components(w, stage, dx, i, n_steps)

    sr = solve_step(
        g=g, w=w, stage=stage,
        Tgw_guess=Tgw_guess, Tww_guess=Tww_guess, qprime_guess=qprime_guess,
        i=i, x=x, dx=dx
    )

    sr = _copy_step_with_stage(
        sr, stage.name, stage_index,
        dP_fric=dP_fric_step,
        dP_minor=dP_minor_step,
        dP_total=dP_tot_step,
        w_dP_fric=w_dP_fric_step,
        w_dP_minor=w_dP_minor_step,
        w_dP_tot=w_dP_tot_step,
    )
    steps.append(sr)

```

```

Q_sum = (Q_sum + (sr.qprime * dx)).to("W")
UA_sum = (UA_sum + (sr.UA_prime * dx)).to("W/K")

dP_fric_sum = (dP_fric_sum + dP_fric_step).to("Pa")
dP_minor_sum = (dP_minor_sum + dP_minor_step).to("Pa")
dP_total_sum = (dP_total_sum + dP_tot_step).to("Pa")

w_dP_fric_sum = (w_dP_fric_sum + w_dP_fric_step).to("Pa")
w_dP_minor_sum = (w_dP_minor_sum + w_dP_minor_step).to("Pa")
w_dP_tot_sum = (w_dP_tot_sum + w_dP_tot_step).to("Pa")

Tgw_guess, Tww_guess, qprime_guess = sr.Tgw, sr.Tww, sr.qprime
g = update_gas_after_step(g, sr.qprime, dx, stage, i, n_steps)
w = update_water_after_step(w, sr.qprime, dx, stage, i, n_steps)

log.debug(
    "step",
    extra={"stage": stage.name, "step": f"{i+1}/{n_steps}"}
)

g_out = g
w_out = w

if steps:
    last = steps[-1]
    steps.append(
        StepResult(
            i=n_steps,
            x=L.to("m"),
            dx=Q_(0.0, "m"),
            gas=g_out,
            water=w_out,
            Tgw=last.Tgw,
            Tww=last.Tww,
            UA_prime=Q_(0.0, "W/K/m"),
            qprime=Q_(0.0, "W/m"),
            boiling=last.boiling,
            h_g=Q_(0.0, "W/m^2/K"),
            h_c=Q_(0.0, "W/m^2/K"),
            stage_name=stage.name,
            stage_index=stage_index,
            dP_fric=Q_(0.0, "Pa"),
            dP_minor=Q_(0.0, "Pa"),
            dP_total=Q_(0.0, "Pa"),
            w_dP_fric=Q_(0.0, "Pa"),
            w_dP_minor=Q_(0.0, "Pa"),
            w_dP_tot=Q_(0.0, "Pa"),
            qprime_conv=Q_(0.0, "W/m"),
            qprime_rad=Q_(0.0, "W/m"),
        )
    )
)

```

```

stage_res = StageResult(
    stage_name=stage.name,
    stage_kind=stage.kind,
    steps=steps,
    Q_stage=Q_sum,
    UA_stage=UA_sum,
    dP_stage_fric=dP_fric_sum,
    dP_stage_minor=dP_minor_sum,
    dP_stage_total=dP_total_sum,
    dP_water_stage_fric=w_dP_fric_sum,
    dP_water_stage_minor=w_dP_minor_sum,
    dP_water_stage_total=w_dP_tot_sum,
    hot_flow_A=stage.spec["hot_flow_A"],
    cold_flow_A=stage.spec["cold_flow_A"],
    hot_Dh=stage.spec["hot_Dh"],
    cold_Dh=stage.spec["cold_Dh"],
)
recon = sum([(s.qprime * s.dx).to("W") for s in steps if s.dx.to("m").magnitude > 0], Q_(0.0, "W"))
if abs((stage_res.Q_stage - recon) / (stage_res.Q_stage + Q_(1e-12, "W"))) > 0.005:
    raise RuntimeError(f"Stage energy accumulation mismatch >0.5% in {stage.name}")

log.debug(
    f"{stage.name}: dP_fric={stage_res.dP_stage_fric:~P}, "
    f"dP_minor={stage_res.dP_stage_minor:~P}, dP_total={stage_res.dP_stage_total:~P}",
    extra={"stage": stage.name, "step": "ΔP"},
)
log.debug(
    f"{stage.name}: gas_in(T={g_in.T:~P}, P={g_in.P:~P}) gas_out(T={g_out.T:~P}, P={g_out.P:~P}) "
    f"water_in(h={w_in.h:~P}, P={w_in.P:~P}) water_out(h={w_out.h:~P}) Q_stage={stage_res.Q_stage:~P}",
    extra={"stage": stage.name, "step": f"{len(steps)}/{n_steps}"},
)
)

return g_out, w_out, stage_res
def solve_exchanger( stages: List[HXStage], gas_in: GasStream, water_in: WaterStream, *, drum_pool: WaterStream | None = None, drum_pool_stage_count: int = 5, target_dx: Q_ | None = None, min_steps_per_stage: int = 20, max_steps_per_stage: int = 400, max_passes: int = 20, tol_Q: Q_ = Q_(1e-3, "W"), tol_end: Q_ = Q_(1e-3, "J/kg"), log_level: str = "INFO", ) -> tuple[List[StageResult], GasStream, WaterStream]: setup_logging(level=log_level) log = logging.getLogger("solver")

if len(stages) != 6:
    raise ValueError(f"Expected 6 stages. Got {len(stages)}.")

if target_dx is None:
    dx_target = (_median_length(stages) / 100).to("m")
else:
    dx_target = target_dx.to("m")

n_steps_by_stage: List[int] = []
for st in stages:

```

```

if st.kind.lower() == "economiser":
    if "hot_flow_length" in st.spec:
        L = st.spec["hot_flow_length"].to("m")
    elif "inner_length" in st.spec:
        L = st.spec["inner_length"].to("m")
    else:
        raise KeyError(f"{st.name}: economiser missing both 'hot_flow_length' and 'inner_length'")
else:
    L = st.spec["inner_length"].to("m")

n = _clamp(
    int(ceil((L / dx_target).to("").magnitude)),
    min_steps_per_stage,
    max_steps_per_stage
)
n_steps_by_stage.append(n)

prev_Q_total: Optional[Q_] = None
prev_end_h: Optional[Tuple[Q_, Q_, Q_, Q_]] = None
final_stage_results: List[StageResult] = []

h_g_in = _gasprops.h(gas_in.T, gas_in.P, gas_in.comp)
h_w_in = water_in.h

for p in range(max_passes + 1):
    gas_stage_results: List[StageResult] = []
    gas_at_stage_in: List[GasStream] = []
    water_for_stage_boundary: List[WaterStream] = []

    g = gas_in
    for i, st in enumerate(stages):
        if drum_pool is not None and i < drum_pool_stage_count:
            w_boundary = drum_pool
        else:
            if p == 0:
                w_boundary = water_in
            else:
                w_boundary = final_stage_results[i].steps[0].water

        gas_at_stage_in.append(g)
        water_for_stage_boundary.append(w_boundary)

        g, w_tmp, st_res = solve_stage(g, w_boundary, st, n_steps_by_stage[i], stage_index=i)
        gas_stage_results.append(st_res)

    water_stage_results: List[StageResult] = []
    g_fields_for_water: List[GasStream] = [gs for gs in gas_at_stage_in]

    w = water_in
    w_econ_out: WaterStream | None = None
    for i_rev, st in enumerate(reversed(stages)):
        idx = 5 - i_rev
        g_for_stage = g_fields_for_water[idx]

```

```

if drum_pool is not None and idx < drum_pool_stage_count:
    g_new, _w_dummy, st_res = solve_stage(g_for_stage, drum_pool, st, n_steps_by_stage[idx], stage_index=idx)
else:
    g_new, w, st_res = solve_stage(g_for_stage, w, st, n_steps_by_stage[idx], stage_index=idx)
    w_econ_out = w

g_fields_for_water[idx] = g_new
water_stage_results.append(st_res)

water_stage_results = list(reversed(water_stage_results))

Q_total = sum([sr.Q_stage.to("W") for sr in water_stage_results], Q_(0.0, "W")).to("W")

g_out = gas_stage_results[-1].steps[-1].gas
w_out = w_econ_out if w_econ_out is not None else water_in

h_g_out = _gasprops.h(g_out.T, g_out.P, g_out.comp)
h_w_out = w_out.h

end_tuple = (h_g_in, h_g_out, h_w_in, h_w_out)

duty_ok = prev_Q_total is not None and abs(Q_total - prev_Q_total) < tol_Q
end_ok = prev_end_h is not None and max(
    abs(end_tuple[0] - prev_end_h[0]),
    abs(end_tuple[1] - prev_end_h[1]),
    abs(end_tuple[2] - prev_end_h[2]),
    abs(end_tuple[3] - prev_end_h[3]),
) < tol_end

log.info(
    f"pass {p}: Q_total={Q_total:.~P} "
    f"ΔQ={(Q_total - (prev_Q_total or Q_(0,'W'))):~P} "
    f"max Δends={max( (abs(end_tuple[i] - (prev_end_h[i] if prev_end_h else end_tuple[i])) for i in range(4)), defa"
    f"erged={'yes' if (duty_ok and end_ok) else 'no'}",
    extra={"stage": "ALL", "step": f"pass {p}"},"
)

```

if duty_ok and end_ok:

```

    water_boundaries = [sr.steps[0].water for sr in water_stage_results]
    g = gas_in
    final_forward_results: List[StageResult] = []

    for i, st in enumerate(stages):
        w_boundary = water_boundaries[i]
        g, w_tmp, st_res = solve_stage(g, w_boundary, st, n_steps_by_stage[i], stage_index=i)
        final_forward_results.append(st_res)
        if i == (len(stages) - 1):
            w_out_sync = w_tmp

    g_out_sync = g

    h_g_out = _gasprops.h(g_out_sync.T, g_out_sync.P, g_out_sync.comp)
    h_w_out = w_out_sync.h

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```

Q_gas = (gas_in.mass_flow * (h_g_in - h_g_out)).to("W")
mismatch = abs(Q_gas - Q_total) / (abs(Q_total) + Q_(1e-12, "W"))
log.info(
    f"FINAL forward: Q_total={sum((sr.Q_stage for sr in final_forward_results), Q_(0,'W')):~P} "
    f"Q_gas={Q_gas:~P} rel_err={mismatch:~P}",
    extra={"stage": "ALL", "step": "final_forward"},
)
if mismatch.magnitude > 0.005:
    raise RuntimeError(
        f"Energy mismatch >0.5% on final sweep. "
        f"Q_gas={Q_gas:~P}, rel_err={mismatch:~P}"
    )
return final_forward_results, g_out_sync, w_out_sync

prev_Q_total = Q_total
prev_end_h = end_tuple
final_stage_results = water_stage_results

worst_idx = max(range(6), key=lambda k: abs(final_stage_results[k].Q_stage).to("W").magnitude if final_stage_results[k] else 0)
raise RuntimeError(
    f"Did not converge in {max_passes} passes. "
    f"last_Q_total={prev_Q_total:~P} if prev_Q_total else 'n/a' } "
    f"last_end_delta={prev_end_h if prev_end_h else 'n/a'} "
    f"worst_stage_index={worst_idx}"
)
=====
=====FILE: heat/step_solver.py =====
from common.results import StepResult from common.units import Q_ from common.models import HXStage, GasStream, WaterStream from heat.physics import wall_resistance, fouling_resistances from heat.water_htc import water_htc from common.props import WaterProps from heat.gas_htc import gas_htc, gas_htc_parts

def solve_step(g: GasStream, w: WaterStream, stage: HXStage, Tgw_guess: Q_, Tww_guess: Q_, qprime_guess: Q_, i: int, x: Q_, dx: Q_) -> StepResult: spec = stage.spec Pg = spec["hot_wet_P"] Pw = spec["cold_wet_P"] Tg = g.T if stage.spec["pool_boiling"] else Tw = WaterProps.Tsat(w.P) else: Tw = WaterProps.T_from_Ph(w.P, w.h) Tgw = Tgw_guess Tww = Tww_guess qprime = qprime_guess alpha = 0.25 tolT = Q_(1e-3,"K"); tolq = Q_(1e-3,"W/m"); maxit = 10

for _ in range(maxit):
    h_g = gas_htc(g, spec, Tgw, stage_kind=stage.kind)
    qpp_cold = (qprime / Pg).to("W/m^2")
    h_c, boiling = water_htc(w, stage, Tww, qpp_cold)
    Rfg, Rfc = fouling_resistances(spec)
    Rw = wall_resistance(spec)
    Rg = (1/(h_g*Pg)).to("K*m/W")
    Rc = (1/(h_c*Pw)).to("K*m/W")

    UA_prime = (1/(Rg + Rfg + Rw + Rfc + Rc)).to("W/K/m")

    qprime_new = (UA_prime * (Tg - Tw)).to("W/m")

    qpp_hot = (qprime_new / Pg).to("W/m^2")
    qpp_cold = (qprime_new / Pw).to("W/m^2")

```

```

Tgw_new = (Tg - qpp_hot/h_g - qpp_hot*Rfg*Pg).to("K")
Tww_new = (Tw + qpp_cold*Rw*Pw + qpp_cold*Rfc*Pw + qpp_cold/h_c).to("K")

dTgw = abs(Tgw_new - Tgw); dTww = abs(Tww_new - Tww); dq = abs(qprime_new - qprime)
if dTgw < tolT and dTww < tolT and dq < tolq:
    Tgw, Tww, qprime = Tgw_new, Tww_new, qprime_new
    break

Tgw = (alpha*Tgw_new + (1-alpha)*Tgw).to("K")
Tww = (alpha*Tww_new + (1-alpha)*Tww).to("K")
qprime = (alpha*qprime_new + (1-alpha)*qprime).to("W/m")
h_conv, h_rad = gas_htc_parts(g, spec, Tgw, stage_kind=stage.kind)
h_g = (h_conv + h_rad).to("W/m^2/K")

h_tot_mag = h_g.to("W/m^2/K").magnitude
if h_tot_mag > 0:
    frac_conv = (h_conv / h_g).to("").magnitude
    frac_conv = max(0.0, min(1.0, frac_conv))
else:
    frac_conv = 0.0

qprime_conv = (qprime * frac_conv).to("W/m")
qprime_rad = (qprime - qprime_conv).to("W/m")

return StepResult(
    i=i, x=x, dx=dx,
    gas=g, water=w,
    Tgw=Tgw, Tww=Tww,
    UA_prime=UA_prime,
    qprime=qprime,
    boiling=boiling,
    h_g=h_g,
    h_c=h_c,
    qprime_conv=qprime_conv,
    qprime_rad=qprime_rad,
)
=====
===== FILE: heat/water_htc.py =====
from math import log, sqrt, exp
from common.units import Q_
from common.models import WaterStream,
HXStage
from common.props import WaterProps

P_CRIT_WATER = Q_(22.064, "MPa") MW_WATER = 18.01528

def velocity(w: WaterStream, Aflow, umax_factor=None) -> Q_:
    rho = WaterProps.rho_from_Ph(w.P, w.h)
    u = (w.mass_flow / (rho * Aflow)).to("m/s")
    if umax_factor is not None:
        return (umax_factor * u).to("m/s")
    return u

def reynolds_number(w: WaterStream, Aflow, char_len, umax_factor=None):
    rho = WaterProps.rho_from_Ph(w.P, w.h)
    v = velocity(w, Aflow, umax_factor)
    mu = WaterProps.mu_from_Ph(w.P, w.h)
    return (rho * v * char_len) / mu

def prandtl_number(cp: Q_, mu: Q_, k: Q_) -> Q_:
    return cp * mu / k

def film_temp(T_bulk: Q_, T_wall: Q_) -> Q_:
    return 0.5 * (T_bulk + T_wall)

def is_boiling(P, h, T_wall: Q | None = None) -> bool:
    hf = WaterProps.h_f(P)
    hg = WaterProps.h_g(P)

```

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if hf <= h <= hg: return True if (h < hf) and (T_wall is not None): return T_wall > WaterProps.Tsat(P) + Q_(3, "K") return False

def pr(w:WaterStream) -> Q_: cp = WaterProps.cp_from_Ph(w.P, w.h) mu = WaterProps.mu_from_Ph(w.P, w.h) k = WaterProps.k_from_Ph(w.P, w.h) return prandtl_number(cp, mu, k)

def pr_s(w: WaterStream, T_wall: Q_) -> Q_: cp_s = WaterProps.cp_from_PT(w.P, T_wall) mu_s = WaterProps.mu_from_PT(w.P, T_wall) k_s = WaterProps.k_from_PT(w.P, T_wall) return prandtl_number(cp_s, mu_s, k_s)

def nu_zukauskas_bank(Re: Q_, Pr: Q_, Pr_s: Q_, arrangement: str) -> tuple[Q_, Q_]: Re = Re.to("“).magnitude Pr = Pr.to("“).magnitude Pr_s = Pr_s.to("“).magnitude

bands = [
    (1e3, 2e3, {"inline": (0.90, 0.40), "staggered": (1.04, 0.40)}),
    (2e3, 4e3, {"inline": (0.52, 0.50), "staggered": (0.71, 0.50)}),
    (4e3, 1e5, {"inline": (0.27, 0.63), "staggered": (0.35, 0.60)}),
    (1e5, 2e6, {"inline": (0.021, 0.84), "staggered": (0.022, 0.84)}),
]
C = None; m = None
for Re_min, Re_max, table in bands:
    if Re_min <= Re < Re_max:
        C, m = table["staggered" if arrangement == "staggered" else "inline"]
        break
if C is None:
    raise ValueError(f"Re={Re:.0f} outside Zukauskas bands")
n = 0.36 if Pr <= 10.0 else 0.25
s = 0.25
nu = C * (Re**m) * (Pr**n) * ((Pr / max(Pr_s, 1e-12))**s)
return Q_(nu, ""), Q_(m, "")

def nu_churchill_bernstein(Re: Q_, Pr: Q_) -> Q_: Re = Re.to("“).magnitude Pr = Pr.to("“).magnitude a = 0.3 b = (0.62 * Re $\cdot$ 0.5 * Pr(1/3)) / (1 + (0.4/Pr)(2/3)) c = (1 + (Re/282000.0)(5/8))(4/5) return Q_(a + b * c, “)

def nu_gnielinski(Re: Q_, Pr: Q_, mu_ratio: Q_, L: Q_, D: Q_) -> Q_: Re = Re.to("“).magnitude Pr = Pr.to("“).magnitude L = L.to("meter").magnitude D = D.to("meter").magnitude if Re < 2300.0: Gz = Re * Pr * (D / max(L, 1e-12)) return Q_(3.66 + (0.0668 * Gz) / (1 + 0.04 * Gz**2/3), “) f = (0.79 * log(Re) - 1.64) ** -2 num = (f/8) * (Re - 1000.0) * Pr den = 1 + 12.7 * (f/8) $\cdot$ 0.5 * (Pr(2/3) - 1) Nu = num / max(den, 1e-12) mu_ratio = mu_ratio.to("“).magnitude return Q_(Nu * (mu_ratio ** 0.11), “)

def compute_nusselt(w:WaterStream, stage: HXStage, T_wall: Q_) -> Q_:

if stage.kind == "single_tube":
    L = stage.spec["outer_diameter"]
    Aflow = stage.spec["cold_flow_A"]
    umax = stage.spec.get("umax_factor")
    Re = reynolds_number(w, Aflow, L, umax)
    Pr = pr(w)
    return nu_churchill_bernstein(Re, Pr)

if stage.kind == "tube_bank":
    L = stage.spec["outer_diameter"]
    Aflow = stage.spec["cold_flow_A"]
    umax = stage.spec.get("umax_factor")
    Re = reynolds_number(w, Aflow, L, umax)
    Pr = pr(w)
    Pr_s = pr_s(w, T_wall)

```

```

N_rows = stage.spec["N_rows"]
ST = stage.spec["ST"]
SL = stage.spec["SL"]
arrangement = stage.spec["arrangement"]
Nu, m = nu_zukauskas_bank(Re, Pr, Pr_s, arrangement)
Nu *= bank_row_factor(N_rows)
Nu *= spacing_factor(L, ST, SL, arrangement, m)
return Nu

if stage.kind == "reversal_chamber":
    L = stage.spec["outer_diameter"]
    Aflow = stage.spec["cold_flow_A"]
    umax = stage.spec.get("umax_factor")
    Re = reynolds_number(w, Aflow, L, umax)
    Pr = pr(w)
    Rc = stage.spec["curvature_radius"]
    Nu = nu_churchill_bernstein(Re, Pr)
    return Nu * bend_factor_external(L, Rc)

if stage.kind == "economiser":
    D = stage.spec["inner_diameter"]
    if "tube_length" in stage.spec:
        L = stage.spec["tube_length"]
    elif "inner_length" in stage.spec:
        L = stage.spec["inner_length"]
    else:
        raise KeyError(f"{stage.name}: economiser missing both 'tube_length' and 'inner_length'")
    Aflow = stage.spec["cold_flow_A"]
    T_bulk = WaterProps.T_from_Ph(w.P, w.h)
    umax = stage.spec.get("umax_factor")
    Re = reynolds_number(w, Aflow, D, umax)
    Pr = pr(w)
    mu_ratio = _mu_ratio(w, T_bulk, T_wall)
    return nu_gnielinski(Re, Pr, mu_ratio, L, D)

raise ValueError(f"unknown stage kind: {stage.kind}")

def mu_ratio(w: WaterStream, T_bulk: Q, T_wall: Q) -> Q: mu_b = WaterProps.mu_from_PT(w.P, T_bulk) mu_w = WaterProps.mu_from_PT(w.P, T_wall) return mu_b / mu_w

def bend_factor_external(D: Q, Rc: Q) -> Q:
    if Rc <= 0 or D <= 0:
        return 1.0
    phi = 1.0 + 0.10 * sqrt(D / Rc)
    return Q(phi, "")

def spacing_factor(D: Q, ST: Q, SL: Q, arrangement: str, m_exp: Q) -> Q: if arrangement == "staggered": denom_T = ST - D denom_L = SL - (0.5 * D) vmax_ratio = (ST / denom_T) * (SL / denom_L) vmax_ratio = vmax_ratio0.5 else: vmax_ratio = ST / (ST - D) m_exp = m_exp.to("").magnitude phi = vmax_ratio m_exp return phi

def bank_row_factor(N_rows: Q) -> Q: n = N_rows.to("").magnitude f = 1.0 - 0.30 * exp(-0.30 * n) return Q(f, "")

def h_water_singlephase(w: WaterStream, stage: HXStage, T_wall) -> Q: Nu = compute_nusselt(w, stage, T_wall) k = WaterProps.k_from_Ph(w.P, w.h) if stage.kind in ("single_tube", "tube_bank", "re-

```

```

versal_chamber"): Dh = stage.spec["outer_diameter"] else: Dh = stage.spec["inner_diameter"] return (Nu
* k / Dh).to("W/m^2/K")

def h_water_boil_cooper(P: Q, qpp: Q_, Rp: Q_) -> Q_: p_r = (P.to("MPa") / P_CRIT_WATER).magnitude
Rp_um = Rp.to("micrometer").magnitude q_kWm2 = qpp.to("kW/m^2").magnitude h_kWm2K = 55.0
* (p_r0.12) * ((Rp_um))-0.55) * (MW_WATER-0.5) * (q_kWm20.67) return Q_(h_kWm2K,
"kW/m^2/K").to("W/m^2/K")

def water_htc(w: WaterStream, stage: HXStage, T_wall: Q_, qpp: Q_) -> tuple[Q_, bool]: if
stage.spec["pool_boiling"]: Rp = stage.spec["roughness_cold_surface"] h_nb = _h_water_boil_cooper(w.P,
qpp, Rp) return h_nb, True

boiling = _is_boiling(w.P, w.h, T_wall)
if boiling:
    h_lo = _h_liquid_only(w, stage, T_wall)
    h_nb = _h_water_boil_cooper(w.P, qpp, stage.spec["roughness_cold_surface"])
    T_sat = WaterProps.Tsat(w.P)
    mu_l = WaterProps.mu_from_PT(w.P, T_sat)
    A = stage.spec["cold_flow_A"]
    Dh = stage.spec["cold_Dh"]
    G = _mass_flux(w, A)
    h_lv = WaterProps.h_g(w.P) - WaterProps.h_f(w.P)
    x = WaterProps.quality_from_Ph(w.P, w.h)
    Re_lo = (G * Dh / mu_l).to("")
    S = _chen_S_factor(qpp, G, h_lv, Re_lo)
    if x is not None:
        F = _chen_F_factor(w.P, x)
    else:
        F = 1
    h_c = F * h_lo + S * h_nb
else:
    h_c = _h_water_singlephase(w, stage, T_wall)
return h_c, boiling

def mass_flux(w: WaterStream, Aflow: Q) -> Q_: return (w.mass_flow / Aflow).to("kg/m^2/s")

def h_liquid_only(w: WaterStream, stage: HXStage, T_wall: Q) -> Q_: D_h = stage.spec["cold_Dh"]
if stage.kind == "economiser": if "tube_length" in stage.spec: L = stage.spec["tube_length"] else:
raise KeyError(f"{{stage.name}}: missing 'tube_length' or 'inner_length' for liquid-only boiling model")
else: L = stage.spec["inner_length"] A = stage.spec["cold_flow_A"] T_sat = WaterProps.Tsat(w.P)
mu_l = WaterProps.mu_from_PT(w.P, T_sat) k_l = WaterProps.k_from_PT(w.P, T_sat) cp_l =
WaterProps.cp_from_PT(w.P, T_sat) G = _mass_flux(w, A) Re_lo = (G * D_h / mu_l).to(" ")
Pr = prandtl_number(cp_l, mu_l, k_l).to("") mu_ratio = (mu_l / WaterProps.mu_from_PT(w.P,
T_wall)).to(" ")
if stage.kind == "economiser":
    Nu = nu_gnielinski(Re_lo, Pr, mu_ratio, L, D_h)
elif stage.kind == "tube_bank":
    Pr_s = prandtl_number(cp_l, WaterProps.mu_from_PT(w.P, T_wall), WaterProps.k_from_PT(w.P, T_wall))
    Nu, m = nu_zukauskas_bank(Re_lo, Pr, Pr_s, stage.spec["arrangement"])
    Nu *= bank_row_factor(stage.spec["N_rows"])
    Nu *= spacing_factor(D_h, stage.spec["ST"], stage.spec["SL"], stage.spec["arrangement"], m)
else:
    Nu = nu_churchill_bernstein(Re_lo, Pr)

return (Nu * k_l / D_h).to("W/m^2/K")

```

```

def martinelli_Xtt(P: Q: float) -> float: T_sat = WaterProps.Tsat(P) rho_l = WaterProps.rho_from_Px(P, Q_(0.0, ""))
rho_g = WaterProps.rho_from_Px(P, Q_(1.0,""))
mu_l = WaterProps.mu_from_PT(P, T_sat)
mu_g = WaterProps.mu_from_PT(P, T_sat)
mu_ratio = (mu_l / mu_g).to("").magnitude
rho_ratio = (rho_g / rho_l).to("").magnitude
return ((1 - x) / x) ** 0.9 * (mu_ratio ** 0.1) * (rho_ratio ** 0.5)

def chen_S_factor(qpp: Q, G: Q_, h_lv: Q_, Re_lo: Q_) -> Q_: Re = max(1.0, Re_lo.to("").magnitude)
S = 1.0 / (1.0 + 2.53e-6 * (Re ** 1.17))
return Q_(max(0.1, min(S, 1.0)), "")

def chen_F_factor(P: Q, x: float) -> Q_: Xtt = martinelli_Xtt(P, x)
F = 1.0 + 0.12 * (max(1e-6, 1.0 / Xtt) ** 0.8)
return Q(min(5.0, max(1.0, F)), "")

=====
FILE: config/air.yaml =====
T: { value: 300.0, unit: kelvin }
P: { value: 101325, unit: Pa }
composition: O2: { value: 0.23067, unit: dimensionless }
N2: { value: 0.755866, unit: dimensionless }
Ar: { value: 0.01287, unit: dimensionless }
CO2: { value: 0.000594, unit: dimensionless }
H2O: { value: 0.0, unit: dimensionless }

=====
FILE: config/drum.yaml =====
inner_diameter: { value: 4.5, unit: m }
length: { value: 5.0, unit: m }
wall_thickness: { value: 0.05, unit: m }
conductivity: { value: 40, unit: W/m/K }
surfaces: inner: roughness: { value: 5, unit: micrometer }
emissivity: { value: 0.80, unit: dimensionless }
fouling_thickness: { value: 0.0001, unit: m }
fouling_conductivity: { value: 0.2, unit: W/m/K }

=====
FILE: config/flue_canteramodel.yaml =====
units: length: cm time: s quantity: mol activation-energy: cal/mol

phases: - name: gas_mix thermo: ideal-gas transport: mixture-averaged kinetics: none elements: [C, H, O, N, S, Ar] species: [CO2, H2O, SO2, O2, N2, Ar, CH4, C2H6, C3H8, C4H10, H2S] state: T: 300 K P: 1 atm X: "N2:1.0"

species: # CO2 - name: CO2 composition: { C: 1, O: 2 } thermo: model: NASA7 temperature-ranges: [200.0, 1000.0, 6000.0] data: # 200–1000 K - [ 2.35677352, 8.98459677e-03, -7.12356269e-06, 2.45919022e-09, -1.43699548e-13, -4.83719697e+04, 9.90105222, ] # 1000–6000 K - [ 3.85796028, 4.41437026e-03, -2.21481404e-06, 5.23490188e-10, -4.72084164e-14, -4.87591660e+04, 2.27163806, ]

transport:
  model: gas
  geometry: linear
  well-depth: 244.0 # K
  diameter: 3.763 # angstrom
  dipole: 0.0 # Debye
  polarizability: 2.650 # angstrom^3
  rotational-relaxation: 2.1 # Zrot at 298 K

# H2O - name: H2O composition: { H: 2, O: 1 } thermo: model: NASA7 temperature-ranges: [200.0, 1000.0, 6000.0] data: - [ 4.19864056, -2.03643410e-03, 6.52040211e-06, -5.48797062e-09, 1.77197817e-12, -3.02937267e+04, -8.49032208e-01, ] - [ 3.03399249, 2.17691804e-03, -1.64072518e-07, -9.70419870e-11, 1.68200992e-14, -3.00042971e+04, 4.96677010, ] transport: model: gas geometry: nonlinear diameter: 2.641 well-depth: 809.1 polarizability: 0.0 rotational-relaxation: 4.0 acentric-factor: 0.344

# SO2 - name: SO2 composition: { S: 1, O: 2 } thermo: model: NASA7 temperature-ranges: [200.0, 1000.0, 6000.0] data: - [ 4.88475400, -2.17239500e-03, 6.74313500e-06, -5.71253000e-09, 1.67180000e-12, -3.05629240e+04, 2.29262800, ] - [ 4.88475400, -2.17239500e-03, 6.74313500e-06, -5.71253000e-09, 1.67180000e-12, -3.05629240e+04, 2.29262800, ] transport: model: gas geometry: nonlinear diameter: 4.11 well-depth: 335.0 polarizability: 0.0 rotational-relaxation: 1.0 acentric-factor: 0.256

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```

# ----- O2 ----- - name: O2 composition: { O: 2 } thermo: model: NASA7
temperature-ranges: [200.0, 1000.0, 6000.0] data: - [ 3.78245636, -2.99673416e-03, 9.84730201e-06,
-9.68129509e-09, 3.24372837e-12, -1.06394356e+03, 3.65767573, ] - [ 3.28253784, 1.48308754e-03, -
7.57966669e-07, 2.09470555e-10, -2.16717794e-14, -1.08845772e+03, 5.45323129, ] transport: model:
gas geometry: linear diameter: 3.458 well-depth: 107.4 polarizability: 1.6 rotational-relaxation: 3.8
acentric-factor: 0.0222

# ----- N2 ----- - name: N2 composition: { N: 2 } thermo: model: NASA7
temperature-ranges: [200.0, 1000.0, 6000.0] data: - [ 3.53100528, -1.23660987e-04, -5.02999433e-07,
2.43530612e-09, -1.40881235e-12, -1.04697628e+03, 2.96747468, ] - [ 2.95257626, 1.39690040e-03, -
4.92631603e-07, 7.86010367e-11, -4.60755321e-15, -9.23948688e+02, 5.87188762, ] transport: model:
gas geometry: linear diameter: 3.621 well-depth: 97.53 polarizability: 1.76 rotational-relaxation: 4.0
acentric-factor: 0.040

# ----- Ar ----- - name: Ar composition: { Ar: 1 } thermo: model: NASA7
temperature-ranges: [200.0, 1000.0, 6000.0] data: - [ 2.50000000, 0.00000000, 0.00000000, 0.00000000,
0.00000000, -7.45375000E+02, 4.37967491, ] - [ 2.50000000, 0.00000000, 0.00000000, 0.00000000,
-7.45375000E+02, 4.37967491, ] transport: model: gas geometry: atom diameter: 3.330 well-depth: 136.5
polarizability: 1.641 rotational-relaxation: 0.0 acentric-factor: 0.000

# ----- CH4 ----- - name: CH4 composition: { C: 1, H: 4 } thermo: model: NASA7
temperature-ranges: [200.0, 1000.0, 6000.0] data: - [ 5.14987613e+00, -1.36709788e-02, 4.91800599e-05,
-4.84743026e-08, 1.66693956e-11, -1.02466476e+04, -4.64130376e+00, ] - [ 7.48514950e-02, 1.33909467e-02,
-5.73285809e-06, 1.22292535e-09, -1.01815230e-13, -1.00095936e+04, 1.84373180e+01, ] transport: model:
gas geometry: nonlinear diameter: 3.746 well-depth: 141.4 polarizability: 2.6 rotational-relaxation: 13.0
acentric-factor: 0.011

# ----- C2H6 ----- - name: C2H6 composition: { C: 2, H: 6 } thermo: model:
NASA7 temperature-ranges: [200.0, 1000.0, 3500.0] data: # 200-1000 K - [ 4.29142492, -5.50154270e-
03, 5.99438288e-05, -7.08466285e-08, 2.68685771e-11, -1.15222055e+04, 2.66682316, ] # 1000-3500 K
- [ 1.07188150, 2.16852677e-02, -1.00256067e-05, 2.21412001e-09, -1.90002890e-13, -1.14263932e+04,
15.11561070, ] transport: model: gas geometry: nonlinear diameter: 4.302 # Å well-depth: 252.3 # K
polarizability: 4.226 # Å^3 rotational-relaxation: 1.5 acentric-factor: 0.099

# ----- C3H8 ----- - name: C3H8 composition: { C: 3, H: 8 } thermo: model:
NASA7 temperature-ranges: [200.0, 1000.0, 6000.0] data: - [ 5.40872872, -8.55221825e-03, 8.42178491e-05,
-1.00942683e-07, 3.86914479e-11, 9.42600956e+03, 3.62322504, ] - [ 5.75125882, 1.87605762e-02, -6.70191976e-
06, 1.07751871e-09, -6.43090885e-14, 7.97977293e+03, -4.91359355, ] transport: model: gas geometry: non-
linear diameter: 4.982 # Å well-depth: 266.8 # K polarizability: 5.921 # Å^3 rotational-relaxation: 1.0
acentric-factor: 0.1521

# ----- C4H10 ----- - name: C4H10 composition: { C: 4, H: 10 } thermo: model:
NASA7 temperature-ranges: [200.0, 1000.0, 6000.0] data: - [ 6.14474013, 1.64500242e-04, 9.67848789e-
05, -1.25486208e-07, 4.97846257e-11, -1.75989467e+04, -1.08058878, ] - [ 9.44547835, 2.57856620e-02, -
9.23613194e-06, 1.48631762e-09, -8.87891206e-14, -2.01383773e+04, -2.63477585e+01, ] transport: model:
gas geometry: nonlinear diameter: 5.206 well-depth: 350.9 polarizability: 0.0 rotational-relaxation: 1.0
acentric-factor: 0.20081

# ----- H2S ----- - name: H2S composition: { H: 2, S: 1 } thermo: model:
NASA7 temperature-ranges: [200.0, 1000.0, 6000.0] data: - [ 3.93234760, -5.02609050e-04, 4.59284730e-06,
-3.18072140e-09, 6.64975610e-13, -3.65053590e+03, 2.31579050, ] - [ 2.74521990, 4.04346070e-03, -1.63845100e-
06, 2.75202490e-10, -1.85920950e-14, -3.41994440e+03, 8.05467450, ] transport: model: gas geometry: non-
linear diameter: 3.60 # Å well-depth: 301.0 # K polarizability: 3.76 # Å^3 rotational-relaxation: 4.0
acentric-factor: 0.10

===== FILE: config/fuel.yaml =====
T: { value: 300.0, unit: kelvin } P: { value: 101325, unit: Pa } mass_flow: { value: 0.1, unit: kg/s }
composition: CH4: { value: 0.849546, unit: dimensionless } C2H6: { value: 0.061889, unit: dimensionless }
```

```

} C3H8: { value: 0.020597, unit: dimensionless } C4H10: { value: 0.005154, unit: dimensionless } H2S: { value: 0.000103, unit: dimensionless } N2: { value: 0.041293, unit: dimensionless } CO2: { value: 0.016418, unit: dimensionless } H2O: { value: 0.005, unit: dimensionless } Ar: { value: 0.0, unit: dimensionless }

===== FILE: config/operation.yaml =====
excess_air_ratio: { value: 1.05, unit: dimensionless } drum_pressure: { value: 10, unit: bar }

===== FILE: config/stages.yaml =====
HX_1: kind: "single_tube" pool_boiling: true inner_diameter: { value: 1.4, unit: m } inner_length: { value: 5.276, unit: m } wall_thickness: { value: 0.02, unit: m } conductivity: { value: 50, unit: W/m/K } surfaces: inner: roughness: { value: 50, unit: micrometer } emissivity: { value: 0.80, unit: dimensionless } fouling_thickness: { value: 0.0001, unit: m } fouling_conductivity: { value: 0.20, unit: W/m/K } outer: roughness: { value: 20, unit: micrometer } emissivity: { value: 0.80, unit: dimensionless } fouling_thickness: { value: 0.0001, unit: m } fouling_conductivity: { value: 0.20, unit: W/m/K }

K: hot_inlet: 0.5 hot_outlet: 0.0 hot_bend: 0.0

cold_inlet: 0.0
cold_outlet: 0.0
cold_bend: 0.0

HX_2: kind: "reversal_chamber" pool_boiling: true inner_diameter: { value: 1.6, unit: m } inner_length: { value: 0.8, unit: m } curvature_radius: { value: 0.8, unit: m } wall_thickness: { value: 0.02, unit: m } conductivity: { value: 50, unit: W/m/K } surfaces: inner: roughness: { value: 50, unit: micrometer } emissivity: { value: 0.80, unit: dimensionless } fouling_thickness: { value: 0.0001, unit: m } fouling_conductivity: { value: 0.20, unit: W/m/K } outer: roughness: { value: 20, unit: micrometer } emissivity: { value: 0.80, unit: dimensionless } fouling_thickness: { value: 0.0001, unit: m } fouling_conductivity: { value: 0.20, unit: W/m/K }

K: hot_inlet: 0.0 hot_outlet: 0.0 hot_bend: 0.3

cold_inlet: 0.0
cold_outlet: 0.0
cold_bend: 0.0

HX_3: kind: "tube_bank" pool_boiling: true inner_diameter: { value: 0.076, unit: m } inner_length: { value: 4.975, unit: m } tubes_number: { value: 118, unit: dimensionless } arrangement: "staggered" N_rows: { value: 6, unit: dimensionless } ST: { value: 0.11, unit: m } SL: { value: 0.11, unit: m } baffle_spacing: { value: 0.45, unit: m } baffle_cut: { value: 0.25, unit: dimensionless } bundle_clearance: { value: 0.010, unit: m } wall_thickness: { value: 0.0029, unit: m } conductivity: { value: 50, unit: W/m/K } surfaces: inner: roughness: { value: 50, unit: micrometer } emissivity: { value: 0.80, unit: dimensionless } fouling_thickness: { value: 0.0001, unit: m } fouling_conductivity: { value: 0.20, unit: W/m/K } outer: roughness: { value: 20, unit: micrometer } emissivity: { value: 0.80, unit: dimensionless } fouling_thickness: { value: 0.0001, unit: m } fouling_conductivity: { value: 0.20, unit: W/m/K }

K: hot_inlet: 0.5 hot_outlet: 1.0 hot_bend: 0.0

cold_inlet: 0.0
cold_outlet: 0.0
cold_bend: 0.0

HX_4: kind: "reversal_chamber" pool_boiling: true inner_diameter: { value: 1.6, unit: m } inner_length: { value: 0.8, unit: m } curvature_radius: { value: 0.8, unit: m } wall_thickness: { value: 0.02, unit: m } conductivity: { value: 50, unit: W/m/K } surfaces: inner: roughness: { value: 50, unit: micrometer } emissivity: { value: 0.80, unit: dimensionless } fouling_thickness: { value: 0.0001, unit: m } fouling_conductivity: { value: 0.20, unit: W/m/K } outer: roughness: { value: 20, unit: micrometer } emissivity: { value: 0.80, unit: dimensionless } fouling_thickness: { value: 0.0001, unit: m } fouling_conductivity: { value: 0.20, unit: W/m/K }

K: hot_inlet: 0.0 hot_outlet: 0.0 hot_bend: 0.3

```

```
cold_inlet: 0.0
cold_outlet: 0.0
cold_bend: 0.0
```

```
HX_5: kind: "tube_bank" pool_boiling: true inner_diameter: { value: 0.076, unit: m } inner_length: { value: 5.620, unit: m } tubes_number: { value: 100, unit: dimensionless } arrangement: "staggered" N_rows: { value: 6, unit: dimensionless } ST: { value: 0.11, unit: m } SL: { value: 0.11, unit: m } baffle_spacing: { value: 0.45, unit: m } baffle_cut: { value: 0.25, unit: dimensionless } bundle_clearance: { value: 0.010, unit: m } wall_thickness: { value: 0.0029, unit: m } conductivity: { value: 50, unit: W/m/K } surfaces: inner: roughness: { value: 50, unit: micrometer } emissivity: { value: 0.80, unit: dimensionless } fouling_thickness: { value: 0.0001, unit: m } fouling_conductivity: { value: 0.20, unit: W/m/K } outer: roughness: { value: 20, unit: micrometer } emissivity: { value: 0.80, unit: dimensionless } fouling_thickness: { value: 0.0001, unit: m } fouling_conductivity: { value: 0.20, unit: W/m/K }
```

```
K: hot_inlet: 0.5 hot_outlet: 1.0 hot_bend: 0.0
```

```
cold_inlet: 0.0
cold_outlet: 0.0
cold_bend: 0.0
```

```
HX_6: kind: "economiser" pool_boiling: false inner_diameter: { value: 0.0250, unit: m } tube_length: { value: 80, unit: m } n_tubes: { value: 120, unit: dimensionless } arrangement: "staggered" N_rows: { value: 26, unit: dimensionless } ST: { value: 0.075, unit: m } SL: { value: 0.08, unit: m } baffle_spacing: { value: 0.15, unit: m } baffle_cut: { value: 0.25, unit: dimensionless } bundle_clearance: { value: 0.010, unit: m } wall_thickness: { value: 0.0026, unit: m } conductivity: { value: 50, unit: W/m/K } surfaces: inner: roughness: { value: 20, unit: micrometer } emissivity: { value: 0.80, unit: dimensionless } fouling_thickness: { value: 0.0, unit: m } fouling_conductivity: { value: 0.20, unit: W/m/K } outer: roughness: { value: 50, unit: micrometer } emissivity: { value: 0.80, unit: dimensionless } fouling_thickness: { value: 0.0, unit: m } fouling_conductivity: { value: 0.20, unit: W/m/K } shell_inner_diameter: { value: 0.60, unit: m } # Gas side
```

```
K: hot_inlet: 0.5 hot_outlet: 1.0 hot_bend: 0.0
```

```
cold_inlet: 0.5
cold_outlet: 1.0
cold_bend: 0.3
```

```
===== FILE: config/water.yaml =====
enthalpy: { value: 440000, unit: J/kg } composition: H2O: { value: 1.0, unit: dimensionless }
```

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