Crossflow Shell and Tube Heat Exchanger Optimization in openMDAO

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To an optimist, the glass is half full. To a pessimist, it is half empty. To an engineer, the glass is twice as big as it needs to be.

– Various Sources

Contents

Nomenclature

ΔP_s	Major pressure loss on shell-side (Pa)
ΔP_t	Major pressure loss on tube-side (Pa)
ΔT_t	Tube-side outlet to inlet temperature differential (K)
ΔT_{LMTD}	Log mean temperature difference between fluids (K)
$\dot{m}_s$	Mass flow rate of shell-side fluid (kg/s)
$\dot{m}_t$	Mass flow rate of tube-side fluid (kg/s)
$\dot{Q}$	Heat transfer rate (W)
$\dot{V}_s$	Volumetric flow rate on the shell-side (m^3/s)
$\dot{V}_t$	Volumetric flow rate on the tube-side (m^3/s)
ϵ	Absolute roughness of inner tube surface (m)
μ_s	Dynamic viscosity of fluid on shell-side ($Pa \cdot s$)
μ_t	Dynamic viscosity of fluid on tube-side ($dimensionless$)
$\phi_{tube,i}$	Tube inner diameter (m)
$\phi_{tube,o}$	Tube outer diameter (m)
ψ_i	Geometry factor for inline shell-side pressure drop ($dimensionless$)
ψ_s	Geometry factor for staggered shell-side pressure drop ($dimensionless$)
ρ_s	Density of fluid on shell-side (m)
A	Total surface area of heat transfer (m^2)
a	Longitudinal tube spacing normalization SL/ϕ_i ($dimensionless$)
$A_{flow,s}$	The flow area on the shell-side between tube rows (m^2)
b	Transverse tube spacing normalization ST/ϕ_i ($dimensionless$)
C_{max}	Maximum heat capacity rate of shell or tube fluid ($W/kg \cdot K$)
C_{min}	Minimum heat capacity rate of shell or tube fluid ($W/kg \cdot K$)
$c_{P,s}$	Specific heat capacity at constant pressure of shell-side fluid ($J/kg \cdot K$)
$c_{P,t}$	Specific heat capacity at constant pressure of tube-side fluid ($J/kg \cdot K$)
C_r	Ratio of minimum to maximum heat capacity rate ($dimensionless$)
D_{core}	Depth of heat exchanger core (m)
e	Heat exchanger effectiveness [0...1]
f	Darcy friction factor ($dimensionless$)
$F_{a,i}$	Shell geometetry arrangement factor for in-line tube banks ($dimensionless$)
$F_{a,s}$	Shell geometetry arrangement factor for staggered tube banks ($dimensionless$)
h_s	Convective heat transfer coefficient of shell-side (W/m^2K)
h_t	Convective heat transfer coefficient of tube-side (W/m^2K)
H_{core}	Height of heat exchanger core (m)
k_s	Shell fluid conductivity ($W/m \cdot K$)
k_{tube}	Thermal conductivity of tube material ($W/m \cdot K$)
$L_{char,s}$	Characteristic length of shell-side (m)
L_{tube}	Tube length (m)
n	Percentage penalty on overall heat transfer coefficient [0...1]
N_{tubes}	Total number of tubes in heat exchanger ($integer$)
NL	Number of tube rows in longitudinal direction (parallel to shell flow) ($integer$)
NT	Number of tube rows in transverse direction (perpendicular to shell flow) ($integer$)
NTU	Number of transfer units ($dimensionless$)
$Nu_{D,s}$	Shell-side Nusselt number ($dimensionless$)
$Nu_{D,t}$	Tube-side Nusselt number ($dimensionless$)

Pr_s	Shell-side Prandtl number evaluated at average fluid temperature (*dimensionless*)
Pr_t	Tube-side Prandtl number evaluated at average fluid temperature (*dimensionless*)
$Pr_{s,w}$	Shell-side Prandtl number evaluated at the wall temperature (*dimensionless*)
R_{tube}	Thermal resistance of the tube wall (m^2K/W)
$Re_{D,s}$	Shell-side Reynolds number (*dimensionless*)
$Re_{D,t}$	Tube-side Reynolds number (*dimensionless*)
SL	Longitudinal center to center tube distance (parallel to shell flow direction) (m)
ST	Transverse center to center tube distance (perpendicular to shell flow direction) (m)
$T_{in,s}$	Shell inlet temperature (K)
$T_{in,t}$	Tube inlet temperature (K)
$T_{out,s}$	Shell outlet temperature (K)
$T_{out,t}$	Tube outlet temperature (K)
U	Overall heat transfer coefficient (W/m^2K)
V_s	Fluid velocity on shell-side between tube rows (m/s)
V_t	Fluid velocity on tube-side (m/s)
V_{fluid}	Volume of fluid in all tubes (m^3)
V_{tube}	Volume of tube construction material in heat exchanger core (m^3)
W	Wet mass of heat exchanger core (kg)

1 Introduction

This case study explores geometry optimization of crossflow shell-and-tube heat exchangers using the openMDAO framework. All code is available at https://github.com/Finn-Arcadi/HEOpt.

2 openMDAO Model

The design variables are the shell and tube outlet temperatures, and in both the longitudinal and transverse directions the number and spacing of tubes. Figure 2 summarizes the inputs to the model, and Figure 3 shows the geometry parameters. All variables are treated as continuous, and after optimization the tube counts are rounded up and re-evaluated for a final performance metric.

The layout geometries are shown in Figure 3, and the structure of the openMDAO model is summarized in Figure 4 in the appendix.

2.1 Solvers

The heat transfer area is computed by iteration using the NonlinearBlockGS solver, operating in a subgroup. The Darcy friction factor is solved implicitely nonlinear NewtonSolver and linear DirectSolver, operating in the main group. The model is optimized by the SLSQP driver.

2.2 Optimization Examples

Four optimizations are compared to validate the Nusselt number coefficients; two in-line cases, and two staggered cases, either with high or low effectiveness, in order to examine the model at a range of Reynolds numbers.

A fifth case is included that relaxes the depth constraint on the core, allowing the optimizer to achieve a lower overall mass.

Global values across simulations are shown in tables 1 and 2. A glycol-water mix is specified on the tube side, and dry air is used on the shell-side. The library CoolProp is used for these estimates, allowing for a range of other fluids to be set easily.

Table 1: Global Inputs

Parameter	**Value**
Heat transfer target	20,000 W
Shell inlet temperature	35 C
Tube inlet temperature	75 C
Overall heat transfer coeff. penalty	0 %
Shell reference pressure	101,325 Pa
Tube reference pressure	210,000 Pa
Relative humidity (shell-side)	0 %
Glycol percentage (tube-side)	50 %
Tube absolute roughness[1]	5 µm
Tube material density[1]	7850 kg/m^3
Tube thermal conductivity[1]	25 W/mK

Table 2: Global Constraints

Parameter	**Value**
Core length (tube)	45.7 cm
Core height (transverse)	30.5 cm
Core depth (longitudinal)	7.6 cm
Tube-side pressure drop	68.9 kPa
SL/D (a)	1.25 - 3
ST/D (b)	1.25 - 5
Max tube-side temperature change	10 C
Tube wall thickness[2]	>0.127 mm
Tube outer diameter [2]	3.175 - 12.7 mm

[1] Typcical values for stainless steel

[2] Dimensions based on stock materials from McMaster-Carr

2.3 Results

The high-flow (HF) cases used a shell-side pressure limit of 1000 Pa and a minimum effectiveness of 0.5, while the low-flow (LF) cases used 150 Pa and 0.75, respectively. A final low-flow example is included, showing that increasing the allowable core depth to 5in (12.7cm) allows for a lower mass design via a higher ST/D ratio.

Table 3: Results

Design	**Mass (kg)**	**L (cm)**	**H (cm)**	**D (cm)**	**a**	**b**	**NL**	**NT**
LF 20kW Staggered	6.16	43.6	18.3	7.93	1.25	1.34	20	43
LF 20kW Inline	6.37	43.0	21.4	7.93	1.25	1.50	20	45
HF 20kW Staggered	3.14	43.4	9.1	7.93	1.25	1.30	20	22
HF 20kW Inline	3.17	43.8	10.2	7.93	1.25	1.46	20	22
LF 20kW Inline 5in	4.97	45.0	14.1	12.7	1.25	2.11	32	21

A comparison is shown in figure 1 focussing on the Nusselt number estimation, comparing against data from Zukauskas [3]

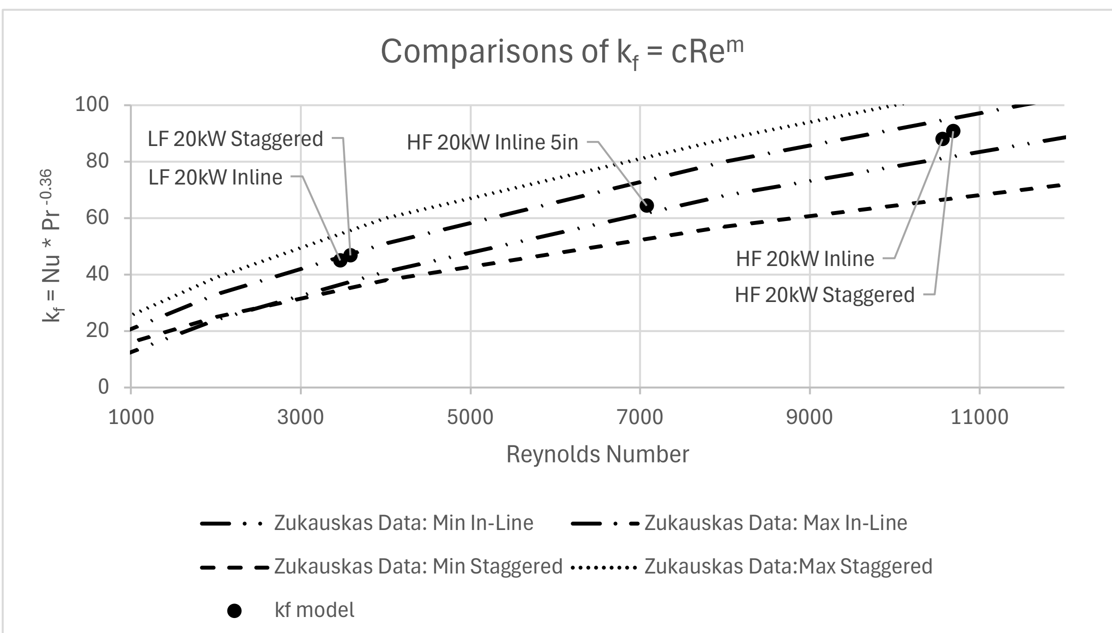

Figure 1: Nusselt Number Validation

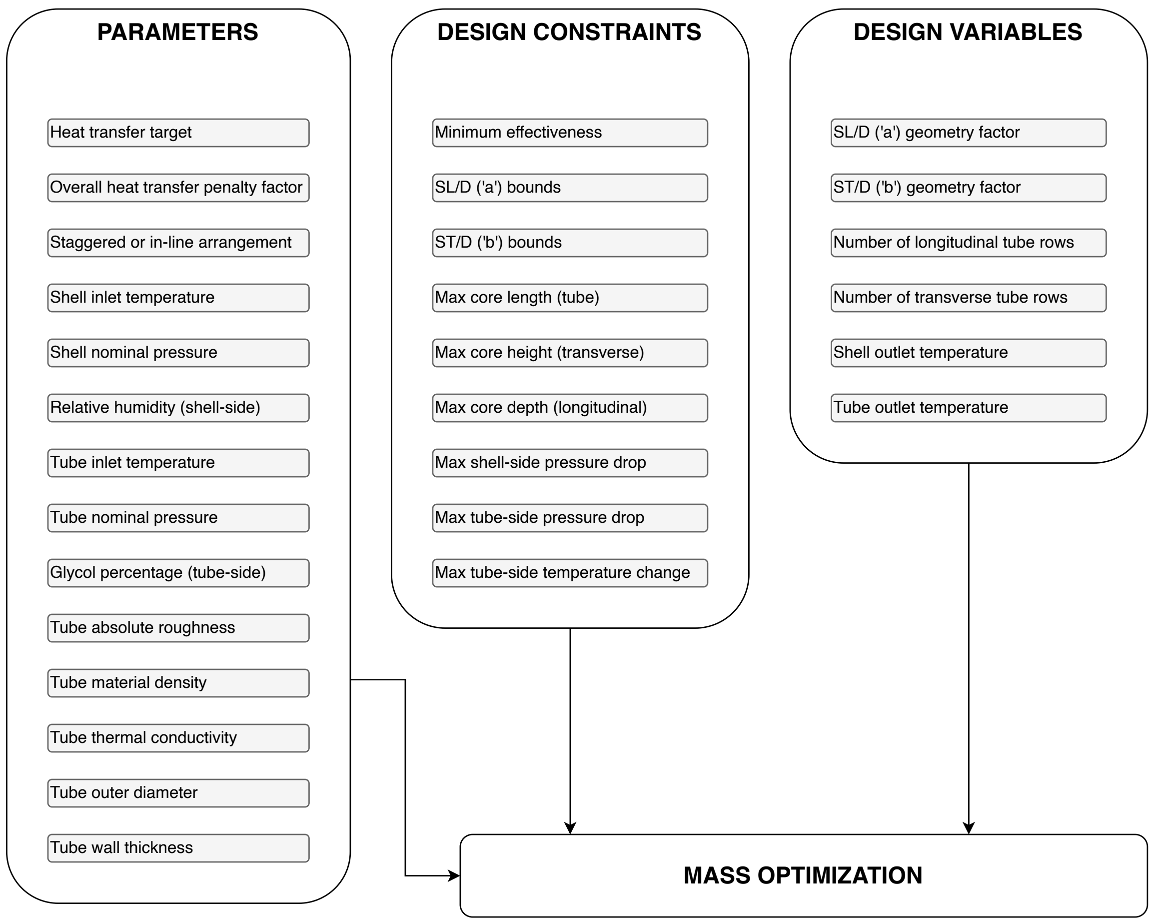

Figure 2: Optimization Parameters

3 Background Theory

The steps for calculation of the tube layouts shown in figure 3 are as follows:

1. Calculate flow rates in the shell and tube.
2. Calculate parameters for the LMTD method and NTU methods.
3. Calculate heat transfer coefficients with some initial guesses for core geometry.
4. Calculate the required area for target heat transfer.
5. Itterate the core geometry and recalculate heat transfer coefficieints until required area and actual area converge.
6. Check heat transfer with NTU method.
7. Calculate shell and tube major pressure loss.

3.1 Flow Rates

Using the first law, the mass flow rate of both fluids will be solved for, treating outlet temperatures as a design variables:

$$\dot{m}_t = \frac{\dot{Q}}{c_{P,t}\left(T_{in,t} - T_{out,t}\right)} \tag{1}$$

$$\dot{m}_s = \frac{\dot{Q}}{c_{P,s}\left(T_{out,s} - T_{in,s}\right)} \tag{2}$$

3.2 LMTD Method

The heat transfer may be calculated via the log mean tempreature difference:

$$\dot{Q} = UA\Delta T_{LMTD} \tag{3}$$

where

$$\Delta T_{LMTD} = \frac{\Delta T_{max} - \Delta T_{min}}{ln(\frac{\Delta T_{max}}{\Delta T_{min}})} \tag{4}$$

$$\Delta T_{max} = T_{in,t} - T_{out,s} \tag{5}$$

$$\Delta T_{min} = T_{out,t} - T_{in,s} \tag{6}$$

Later, we will use this to solve for the required area of the heat exchange surface.

3.3 NTU Method

The NTU method is used to verify the results of the LMTD method.

$$C_{min} = min(\dot{m}_t c_{P,t}, \dot{m}_s c_{P,s},) \tag{7}$$

$$C_{max} = max(\dot{m}_t c_{P,t}, \dot{m}_s c_{P,s},) \tag{8}$$

$$C_r = \frac{C_{min}}{C_{max}} \tag{9}$$

C_r will always be less than 1, and is the ratio of the two heat capacity rates C_min and C_max, used to calculated the effectiveness:

NTU is then calculated as:

$$NTU = \frac{UA}{C_{min}} \tag{10}$$

The effectiveness is the ratio of actual heat transfer to the maximum possible heat transfer:

$$e = \frac{\dot{m}_t c_{P,t}(T_{in,t} - T_{out,t})}{\dot{m}_s c_{P,s}(T_{in,t} - T_{in,s})} \tag{11}$$

For a crossflow heat exchanger with both fluids unmixed it is given by:

$$e = 1 - e^{\frac{1}{C_r} \times NTU^{0.22} \times (e^{-C_r \times NTU^{0.78}} - 1)} \tag{12}$$

$$\dot{Q} = eC_{min}(T_{in,t} - T_{in,s}) \tag{13}$$

3.4 Overall Heat Transfer Coefficient

The overall heat transfer coefficient U is needed to calculate the required surface area of the heat exchanger, and is given by:

$$U = (1 - n)\left(\frac{1}{h_s} + \frac{1}{h_t} + R_{tube}\right)^{-1} \tag{14}$$

Here, n is a penalty on the overall heat transfer coefficient between 0 and 1, h_s is the shell-side convective heat transfer coefficient, h_t is the tube-side convective heat transfer coefficient, and R_{tube} is the thermal resistance of the tube wall.

The number of tubes in the shell flow direction NL and the number of tubes perpendicular to

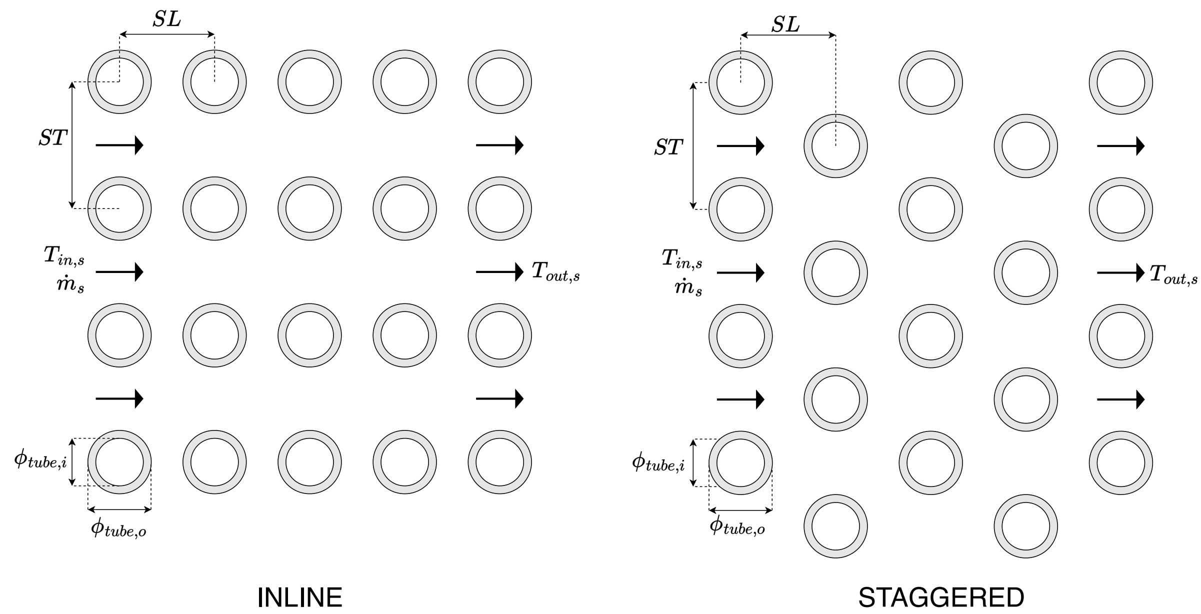

Figure 3: Tube Arrangements

the shell flow direction NT define total number of tubes N_{tubes}, used later for area calculation:

$$N_{tubes} = NL \times NT \tag{15}$$

Additionally, NL and NT have the following relationships to the overall core dimensions:

$$D_{core} = SL \times NL \tag{16}$$

$$H_{core} = ST \times NT \tag{17}$$

Where D_{core} and H_{core} are the depth and height of the core, respectively, and SL and ST the longitudinal and transverse tube spacings, respectively.

Non-dimensional geometry parameters a and b are also defined as follows and used for various correlations:

$$a = SL/\phi_{tube,o} \tag{18}$$

$$b = ST/\phi_{tube,o} \tag{19}$$

3.4.1 Tube Thermal Resistance

The tube thermal resistance is given as:

$$R_{tube} = \frac{ln(\frac{\phi_{tube,o}}{\phi_{tube,i}})}{2\pi k_{tube} L_{tube}} \tag{20}$$

Here, $\phi_{tube,o}$ is the tube outer diameter, $\phi_{tube,i}$ is the tube inner diameter, k_{tube} is the tube material thermal conductivity, and L_{tube} is the length of the tubes.

3.4.2 Shell-Side Heat Transfer

To calculate the shell side heat transfer coefficient, we will ultimately need to calculate the Nusselt number (the ratio of convective to conductive heat transfer). The Nusselt number is a function of the Reynolds number and the Prandtl number.

We first calculate the Reynolds number, for which we will need the shell fluid density ρ_s, velocity V_s, dynamic viscosity μ_s, and characteristic length $L_{char,s}$.

The hydraulic diameter of the flow cross section is used as the characteristic length:

$$L_{char,s} = \frac{4L_{tube}(ST - \phi_{tube,o})}{2(ST - \phi_{tube,o}) + 2L_{tube}} \quad (21)$$

Here, L_{tube} is the length of the tubes.

The shell-side flow velocity will be the velocity between the tubes, for which the flow area is required:

$$A_{flow,s} = (NT)(L_{tube})(ST - \phi_{tube,o}) \quad (22)$$

The volumetric flow rate of the shell fluid is given as:

$$\dot{V}_s = \frac{\dot{m}_s}{\rho_s} \quad (23)$$

The shell-side flow velocity is given as:

$$V_s = \frac{\dot{V}_s}{A_{flow,s}} \quad (24)$$

Finally, we may calculate the Reynolds number as:

$$Re_{D,s} = \frac{\rho_s V_s L_{char,s}}{\mu_s} \quad (25)$$

The Prandtl number is calculated as:

$$Pr_s = \frac{c_{P,s}\mu_s}{k_s} \quad (26)$$

where k_s is the shell fluid thermal conductivity.

There are various correlations to calculate the Nusselt number. Hausen [2] outlines a method to calculate an arrangement factor, F_a, for in-line or staggered tube banks. It is based on studies conducted by Grimison [1] and is valid for $1.25 < b < 3.0$ and $1.25 < a < 3.0$:

For inline tube banks, F_a is given by:

$$a_{fac} = \left(a + \frac{7.17}{a} - 6.52\right) \quad (27)$$

$$b_{fac} = \left(\frac{0.266}{(b-0.8)^2} - 0.12\right) \quad (28)$$

$$F_{a,i} = 1 + a_{fac} \times b_{fac} \times \left(\frac{1000}{Re_{D,s}}\right)^{0.5} \quad (29)$$

And used to calculate the Nusselt number in the form

$$Nu_{D,s,i} = 0.34 F_{a,i} Re_{D,s}^{0.61} Pr^{0.31} \quad (30)$$

and for staggered tube banks, it is given as:

$$F_{a,s} = 1 + 0.1a + 0.34/b \quad (31)$$

and used to calculate the Nusselt number as:

$$Nu_{D,s,s} = 0.35 F_{a,s} Re_{D,s}^{0.57} Pr_s^{0.31} \quad (32)$$

This method has problems for optimization because negative Nusselt numbers can be produced from equation 29 for various combinations of inputs.

Zukauskas [3] collected extensive data on the Nusselt number and presented a more robust set of calculations, dependent only on Reynolds number.

$$Nu_{D,s} = c Re_{D,s}^{m} Pr_s^{0.36} \left(\frac{Pr_s}{Pr_{s,w}}\right)^{0.25} \quad (33)$$

Empirical values for c and m are shown in tables 4 and 5. $Pr_{s,w}$ represents the Prandtl number at the wall conditions, and Pr the Prandtl number evaluated at the average fluid conditions, though in the present code that corrrection is ignored and the Prandl number is simply considered at the average shell temperature.

It is noted by Zukauskas that m decreases at values of a less than 1.5 and increases slightly at values of b less than 1.5, by a magnitude in either direction of up to about 10%. Finally, in the transitional flow case ($100 < Re < 1000$), correlations for the single-tube Nusselt numbers are substituted as they are shown to be good approximate values, noting that there is a slight underestimate in some cases for staggered banks.

Once obtained, the average Nusselt number may be used to calculate the convective heat transfer coefficient as:

$$h_s = \frac{Nu_{D,s} k_s}{\phi_{tube,o}} \quad (34)$$

Table 4: In-Line Coefficients

Reynolds Number	**c**	**m**
10 < Re < 100	0.8	0.4
100 < Re < 1000 (single tube values taken)	0.73	0.5
1000 < Re < 200,000	0.27	0.63
Re > 200,000	0.21	0.84

Table 5: Staggered Coefficients

Reynolds Number	**c**	**m**
10 < Re < 100	0.9	0.4
100 < Re < 1000 (single tube values taken)	0.73	0.5
1000 < Re < 200,000	$a/b < 2$: $0.3(a/b)^{0.2}$ $a/b > 2$: 0.4	0.6
Re > 200,000	$Pr > 1: 0.022$ $Pr = 0.7$: 0.019	0.84

3.4.3 Tube-Side Heat Transfer

The tube-side convective heat transfer coefficient is more straightforward to calculate and follows the same procedure. The characteristic length is simply the inner diameter of a tube in this case, the flow area is the cross-sectional area of a single tube and the velocity is the velocity inside a single tube.

The tube-side volumetric flow rate is given by:

$$\dot{V}_t = \frac{\dot{m}_t}{\rho_t} \tag{35}$$

And the tube-side velocity is:

$$V_t = \frac{\dot{V}_t}{N_{tubes}(\pi\phi_{tube,i}^2/4)} \tag{36}$$

The Reynolds number is then calculated as:

$$Re_{D,t} = \frac{\rho_t V_t \phi_{tube,i}}{\mu_t} \tag{37}$$

The Prandtl number is calculated as:

$$Pr_t = \frac{c_{P,t}\mu_t}{k_t} \tag{38}$$

The Nusselt number is calculated using the Dittus-Boelter equation for turbulent flow:

$$Nu_{D,t} = 0.023 Re_{D,t}^{0.8} Pr_t^n \tag{39}$$

Where n is 0.4 for heating and 0.3 for cooling of the fluid. Evaluation is performed at the average fluid temperature, as with the shell-side. A value for the Nusselt number of 4.36 is taken in the laminar regime assuming constant flux.

The tube-side convective heat transfer coefficient is then calculated as:

$$h_t = \frac{Nu_{D,t} k_t}{\phi_{tube,i}} \tag{40}$$

3.5 Area Estimate

Having calculated overall heat transfer coefficient, we may now estimate the required surface area of the heat exchanger using the LMTD method. Rearranging equation 3:

$$A = \frac{\dot{Q}}{U \Delta T_{LMTD}} \tag{41}$$

In order to calculate U, we had to assume geometry paraemters for the heat exchanger. Length of the core must now be solved iteratively to converge to the correct heat transfer rate.

$$L_{tube} = \frac{A}{N_{tubes}} \pi \phi_{tube,o} \tag{42}$$

3.6 Pressure Drop Estimates

On the tube-side, pressure loss is estimated via the Colebrook-White equation. Header losses are often significant but are not yet included.

On the shell side, the pressure drop will be estimated by an approach outlined by Hausen [2].

3.6.1 Tube-Side Pressure Drop

In turbulent conditions ($Re_{D,t} > 2300$), the Darcy friction factor is solved iteratively using the Colebrook-White equation:

$$\frac{1}{\sqrt{f}} = -2\log_{10}\left(\frac{\epsilon}{3.7\times\phi_{tube,i}} + \frac{2.51}{Re_{D,t}\sqrt{f}}\right) \tag{43}$$

Where ϵ is the absolute roughness of the tube inner surface in m. In laminar flow ($Re_{D,t} \leq 2300$), the friction factor is given as:

$$f = \frac{64}{Re_{D,t}} \tag{44}$$

This is also a good initial value for the iterative solution in turbulent flow.

Once the friction factor is known, the pressure drop across the core, as approximated by the pressure loss in a single tube at average velocity, is given by the Darcy-Weisbach equation:

$$\Delta P_t = f\frac{L_{tube}}{\phi_{tube,i}}\frac{\rho_t V_t^2}{2} \tag{45}$$

3.6.2 Shell-Side Pressure Drop

As presented by Hausen [2], the following is accurate for more than ten tube rows in the flow direction.

$$\Delta P_s = NL\psi\frac{\rho_s V_s^2}{2} \tag{46}$$

Here, ψ is an empirical factor that depends on the Reynolds number and the dimensionless tube spacings b and a. For an inline arrangement, it is given as:

$$\psi_i = Re_{D,s}^{-0.15\left[0.176+\frac{0.32b}{(a-1)^{0.43+1.13/b}}\right]} \tag{47}$$

For a staggered arrangement, it is given as:

$$\psi_s = Re_{D,s}^{-0.16\left[1+\frac{0.47}{(a-1)^{1.08}}\right]} \tag{48}$$

3.7 Weight Estimate

For the wet weight of the heat exchanger we will need the volume of tube material:

$$V_{tube} = N_{tubes}L_{tube}\pi\left(\frac{\phi_{tube,o}^2 - \phi_{tube,i}^2}{4}\right) \tag{49}$$

as well as the inner fluid volume:

$$V_{fluid} = N_{tubes}L_{tube}\pi\left(\frac{\phi_{tube,i}^2}{4}\right) \tag{50}$$

The mass will then be:

$$W = \rho_{tube}V_{tube} + \rho_t V_{fluid} \tag{51}$$

4 Conclusion

The model presented for a cross-flow shell and tube heat exchanger is robust enough for optimization within a range of constraints, and shows valid results compared to available data.

There are also a number improvements that could be made. The shell-side Nusselt number calculation could be refined with corrections for the geometry factors a and b, as well as the correction term that evaluates the Prandtl number wall conditions.

Header and duct pressure loss analysis could be added to the model to broaden the scope of the system.

CFD analysis could be conducted to validate the heat transfer as well as the tube and shell pressure loss estimates.

Finally, other heat exchanger configurations could be added as options, such as plate-fin and tube-fin heat exchangers.

References

[1] E.D. Grimison. “Correlation and Utilization of New Data on Flow Resistance and Heat Transfer for Cross Flow of Gases Over Tube Banks.” In: *Transactions of the American Society of Mechanical Engineers* 59.7 (1937), pp. 583–594. ISSN: 0097-6822. DOI: 10.1115/1.4020557.

[2] H. Hausen. *Heat Transfer in Counterflow, Parallel Flow, and Crossflow.* McGraw-Hill, 1983. ISBN: 0-07-027215-8.

[3] A Žukauskas. “Heat Transfer from Tubes in Crossflow”. In: *Advances in Heat Transfer* 8 (1972), pp. 93–160.

A Code Reference

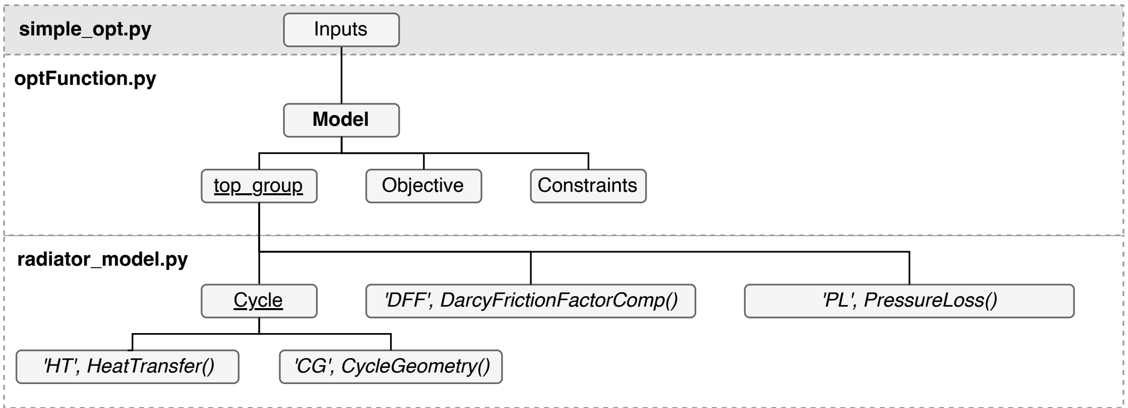

Figure 4: Model Hierarchy

simple_opt.py sets inputs and constraint variables and runs the optimization function.

optFunction.py structures the openMDAO problem and holds auxiliary classes. This is where objectives, constraints, and initial values are set.

radiator_model.py contains the core models themselves, packaged into openMDAO components and sub-groups.

The model depends on openMDAO and CoolProp, as well as Pypi's ht library to calculate a Nusselt number correction at low tube counts, based on Zukauskas' work.

- openMDAO, multidisciplinary optimization.
- CoolProp, large fluid property library.
- ht, general thermal library.