Supporting Information: Model formulation and optimization of the mechanical variables for heat exchanger design

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The model for design of shell and tube HE is formulated as a MINLP optimization problem already presented by Ravagnani and Caballero¹.

Only the mechanical aspects are considered in this paper, since thermo fluid variables were obtained for each modeling cell regarding temperature distribution.

For the mechanical variables of the heat exchanger, Table 1 containing the respective values for tube was constructed according to the TEMA standards. This table contains two types of external diameter for the tubes (19.05 and 25.4 *mm*), two types of geometric arrangement, three options for pitch (23.79, 25.4 and 31.75 *mm*), five types of number of tube passes, 1, 2, 4, 6, or 8, and 21 different types of shell and tube bundles diameter, ranged from 0.205 *m* and 0.173 *m* to 1.524 *m* and 1.473 *m*, respectively, with 565 rows.

To find D_s , D_3 , D_2 , a_{rr} , pt, N_{tp} and n_b , the following equations are used (Eqs. 1 - 8):

$$D_{s} = \sum_{i=1}^{565} D_{si} ynt(i) \tag{1}$$

Table 1: Tube counting table

D (m)	D (m)	D (m)		104 (mg)	Number of tube passes				
D_s (m)	D_3 (m)	D_2 (m)	a_{rr}	<i>pt</i> (m)	1	2	4	6	8
		0.01905	\triangle	0.02379	38	32	26	24	18
		0.01905		0.02540	32	26	20	20	
0.20500	0.17325	0.01905	\triangle	0.02540	37	30	24	16	
		0.02540		0.03175	21	16	16	14	
		0.02540	\triangle	0.03175	22	18	16	14	
		0.01905	\triangle	0.02379	62	56	47	42	36
		0.01905		0.02540	52	52	40	36	
0.2543	0.22276	0.01905	\triangle	0.02540	61	52	48	48	
		0.02540		0.03175	32	32	26	24	
		0.02540	\triangle	0.03175	37	32	28	28	
:	:	÷	:	:	:	:	:	:	÷
		0.01905	\triangle	0.02379	2704	2660	2556	2526	2489
		0.01905		0.02540	2241	2214	2167	2142	2110
1.42240	1.3716	0.01905	\triangle	0.02540	2588	2545	2446	2409	2373
		0.02540		0.03175	1420	1400	1371	1333	1307
		0.02540	\triangle	0.03175	1638	1605	1549	1501	1472
1.52400	1.47300	0.01905	Δ	0.02379	3399	3343	3232	3195	3162
		0.01905		0.02540	2587	2556	2510	2485	2460
		0.01905	\triangle	0.02540	2987	2945	2827	2798	2770
		0.02540		0.03175	1639	1615	1587	1553	1522
		0.02540	\triangle	0.03175	1889	1851	1797	1761	1726

$$D_3 = \sum_{i=1}^{565} D_{3i} ynt(i) \tag{2}$$

$$D_2 = \sum_{i=1}^{565} D_{2i} ynt(i) \tag{3}$$

$$a_{rr} = \sum_{i=1}^{565} a_{rri} ynt(i)$$
 (4)

$$pt = \sum_{i=1}^{565} pt_i ynt(i)$$
 (5)

$$N_{tp} = \sum_{i=1}^{565} N_{tpi} ynt(i)$$
 (6)

$$n_b = \sum_{i=1}^{565} n_{bi} ynt(i) \tag{7}$$

$$\sum_{i=1}^{565} ynt(i) = 1 \tag{8}$$

Five kinds of tube length are considered (*L*):

$$N_L = \begin{bmatrix} 2.438 & 3.658 & 4.877 & 6.096 & 6.706 \end{bmatrix},$$

$$L = 2.438y_1^L + 3.658y_2^L + 4.877y_3^L + 6.096y_4^L + 6.706y_5^L$$
(9)

$$\sum_{i=1}^{5} y_i^L = 1. {(10)}$$

Baffle spacing (l_s) is defined between D_s and $D_s/5$:²

$$\frac{D_s}{5} \le l_s \le D_s,\tag{11}$$

and, then, the number of baffles (N_{bf}) is:

$$N_{bf} = \frac{L}{l_s} - 1. ag{12}$$

Tube inside diameter (D_1) is obtained for different values of tube external diameter (D_2) and BWG (Birmingham Wire Gage), factor used by TEMA to define wall tube thickness. For the considered D_2 values there are two sets of D_1 values (Table 2).

Table 2: Determination of tube inside diameter for different values of tube external diameter

$D_2 = 0$).01905m	$D_2 = 0.02504m$			
BWG	$D_1(m)$	BWG	$D_1(m)$		
10	0.0122	8	0.0170		
11	0.0129	9	0.0179		
12	0.0135	10	0.0186		
13	0.0142	11	0.0193		
14	0.0148	12	0.0199		
15	0.0154	13	0.0206		
16	0.0157	14	0.0212		
17	0.0161	15	0.0217		
18	0.0166	16	0.0221		
		17	0.0225		
		18	0.0229		

$$BWG_1 = \sum_{j=1}^{9} y_{1j}^{bwg} BWG_j^1 \tag{13}$$

$$\sum_{j=1}^{9} y_{1j}^{bwg} \le 1 \tag{14}$$

$$BWG_2 = \sum_{j=1}^{11} y_{2j}^{bwg} BWG_j^2 \tag{15}$$

$$\sum_{j=1}^{11} y_{2j}^{bwg} \le 1 \tag{16}$$

$$BWG = BWG_1 + BWG_2 \tag{17}$$

For the heat load (Q), as hot fluid flows in shell side:

$$Q = M_s C_{ps} (T_{si} - T_{so}) \tag{18}$$

or

$$Q = M_t C_{pt} (T_{to} - T_{ti}). (19)$$

For the log mean temperature difference, the Chen approximation was used³:

$$LMTD = \left(\frac{t_1 t_2 (t_1 + t_2)}{2}\right)^{\frac{1}{3}},\tag{20}$$

$$t_1 = T_{so} - T_{ti} \tag{21}$$

$$t_2 = T_{si} - T_{to}. (22)$$

For F_t determination, the correlation proposed by Blackwell and Haydu⁴ was used. Finally, the objective function is defined as an area minimization problem:

$$A = n_b \pi D_2 L. \tag{23}$$

References

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