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CUBIC HERMITE INTERPOLATION FUNCTION IN SUPERCRITICAL HEAT EXCHANGER MODELING

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Abstract. *Most heat exchangers may be fairly accurately modeled using an analytical approach, generally presented in Heat Transfer textbooks as the Logarithmic Mean Temperature Difference and the efficiency-NTU methods (for design and analysis problems, respectively), with subtle adaptations when there is phase change involved. Concerning about the environmental impact of CFC and HFC working fluids in heating and refrigeration, and also the possibility of a better matching between heat source and working fluid temperatures in power generation has attracted attention to the possibility of using supercritical cycles, mostly using* CO_2 *as working fluid. Above the critical temperature and/or pressure (point) the working fluid does not experience a phase change between liquid and vapor, it changes continuously its properties but, when the temperature and pressure get near the critical point, much more intensely than it changes in single phase fluids below the critical point. The intense variations of fluids properties accompanied by temperature (and less noticeable pressure) variations are much more difficult to model analytically than those observed in single phase or conventional two-phase heat exchangers, and so emerges the need for fully numerical approaches based on some sort of finite difference or approximate spectral methods. Since the computational demands of a one-dimensional discretization are not extremely high, the usual second and first-order accurate ones (central differences and upwind differences) are considered satisfactory and really an optimal balance between complexity and performance. The present paper shows that the use of fourth-order accurate cubic Hermite polynomials as interpolation functions does not increase the complexity too much and greatly improves the convergence of a control volume based finite element method for supercritical heat exchanger modeling. The results of the use of Hermite cubic (spline) interpolation function are compared with those of more conventional approaches and also other not so usual. To perform this comparison a test problem is solved using some different approaches, starting the use of an interpolation function based in analytical solution, not dismissing the classical linear interpolation, but then comparing the Hermite cubic spline interpolation function fourth order of convergence with the accuracy provided by other cubic polynomials.*

Keywords: *Interpolation function, Heat exchanger, Supercritical* CO_2

1. INTRODUCTION

The present work was motivated by conversations about heat exchanger modeling in which it was posed the question if polynomials of third degree used to describe the properties profiles along the pipes/channels inside these heat exchangers would be as useful in numerical simulation as they are in fitting experimental data. The title and the abstract above may suggest that the paper would start presenting Hermite (cubic splines) interpolation functions and then compare these interpolation functions with other alternatives. But the aforementioned conversations evolved in a less straight way and this paper kept almost the same order in that they occurred. So the Hermite interpolation will appear only after some previous exploration of what now appear to be less promising alternatives. Initially is discussed an interpolation based in an analytical solution (that seemed deserving a trial since analytical solutions are so much used in the heat exchangers design), in the sequence appears the Lagrange cubic interpolation functions and at the end of the paper a curious experiment with cubic polynomials in their canonical form.

As the discussion evolved, it became focused on supercritical heat exchangers, where the intensity of the supercritical fluid property variations precludes the use of analytical solutions. The supercritical heat exchanger problem and the basic algorithm used to test the diverse interpolation procedures compared here are presented by Utamura *et al.* (2008). The algorithm is based in mass and enthalpy steady state balances (momentum may be added, but it is not needed here) over control volumes whose lengths are calculated (one by one, in a marching procedure) to allow a given heat transfer rate q between the hot and the cold fluids (this q is a grid spacing[1], that leads to a spatial grid of **varying** heat exchanger segment **lengths** L_k). The total heat exchanger length would be $L_{\text{total}} = \sum_{k=1}^{n} L_k$, but, as the complete algorithm explanation cannot be properly reproduced here, for lack of space, even the subscript k will be omitted in the remaining of this paper. What will be presented in the following sections are the different ways of calculating these heat exchanger segment lengths (from now on simply denoted by L) resulting from the use of different interpolation functions.

1.1 The test case

The problem in which the solving ability of different interpolations are compared is one of those presented by Utamura *et al.* (2008). It is essentially the design of a supercritical counterflow heat exchanger: in the left side CO_2 enters at temperature $T_g(0) = 118$ ºC, pressure $P_g = 115$ bar and a mass flow of $\dot{m}_g = 57{,}8$ kg/h, while in the right side enters H_2O at $T_f(L_{\text{total}}) = 7$ ºC, pressure $P_f = 2{,}5$ bar and a mass flow of $\dot{m}_f = 48$ kg/h. The required total heat transfer is $n\,q = 4{,}63$ kW (since q is the heat rate in each heat exchanger segment, there being n of them in total).

2. INTERPOLATION FUNCTION BASED IN AN ANALYTIC SOLUTION

The enthalpy balances for a counterflow heat exchanger in which the properties of the fluid streams and of the heat exchanger are known functions of a longitudinal coordinate along the exchanger may be expressed as the following system of linear[2] ordinary differential equations (ODEs)

$$\begin{cases} C_g(x)\dfrac{\mathrm{d}T_g(x)}{\mathrm{d}\,x} = U'(x)[T_f(x) - T_g(x)] \\[2ex] C_f(x)\dfrac{\mathrm{d}T_f(x)}{\mathrm{d}\,x} = U'(x)[T_f(x) - T_g(x)]) \end{cases} \tag{1}$$

where $C_f(x) = \dot{m}_f c_{p\,f}(x)$ is the varying heat capacity of f fluid stream (to fluid g, $C_g(x)$ is defined analogously) and

$$U'(x) = \frac{\mathrm{d}\,[UA(x)]}{\mathrm{d}x} \tag{2}$$

is a coefficient of heat transfer by unity length of the heat exchanger. It should be noticed that usually the specific heat is not a known function of the position, but a function of the temperature, rendering the problem nonlinear, but the hypothesis adopted here may be useful in an approximation to that nonlinear problem.

Subtracting the second from the first equation in the system given in Eq. (1) one gets[3]

$$\frac{\mathrm{d}[\Delta T(x)]}{\mathrm{d}\,x} = \frac{U'(x)}{C_g(x)}\left[\frac{C_g(x)}{C_f(x)} - 1\right]\Delta T(x) \tag{3}$$

that may be solved by separating the variables and integrating. So

$$\int_{\Delta T_0}^{\Delta T(x)} \frac{\mathrm{d}[\Delta T]}{\Delta T} = \ln\left[\frac{\Delta T(x)}{\Delta T_0}\right] = \int_{x_0}^{x} \frac{U'(x)}{C_g(x)}\left[\frac{C_g(x)}{C_f(x)} - 1\right]\mathrm{d}x \tag{4}$$

Assuming that the heat exchanger properties vary linearly with x and defining, for a subdomain of length L, the nondimensional coordinate $\xi = (x - x_0)/L$ one gets those properties expressed as

$$U'(\xi) = U'_0 + U''\xi \qquad C_g(\xi) = C_{g_0} + C'_g\xi \qquad C_f(\xi) = C_{f_0} + C'_f\xi \tag{5}$$

The integral than becomes

$$\ln\left[\frac{\Delta T(x)}{\Delta T_0}\right] = L\int_0^{\xi} \frac{U'_0 + U''\xi}{C_{g_0} + C'_g\xi}\left[\frac{C_{g_0} + C'_g\xi}{C_{f_0} + C'_f\xi} - 1\right]\mathrm{d}\xi \tag{6}$$

and the obtained profile of temperature difference between the streams is

$$\begin{aligned} \Delta T(\xi) =& \Delta T_0\,(1 + \xi\,C'_f/C_{f_0})^{\frac{L}{C'_f}\left(U'_0 - \frac{C_{f_0}U''}{C'_f}\right)} \\ & \times (1 + \xi\,C'_g/C_{g_0})^{\frac{L}{C'_g}\left(\frac{C_{g_0}U''}{C'_g} - U'_0\right)} \exp\left[\left(\frac{1}{C'_f} - \frac{1}{C'_g}\right)L\,U''\xi\right] \end{aligned} \tag{7}$$

[1]This spacing q generates two grids (different only by an offset) of uniformly spaced enthalpies h_g and h_f.
[2]The ODEs are linear, even if the coefficients C_g, C_f and U' are high order polynomials of the independent variable x, as long as these coefficients do not depend on the unknown functions (T_g and T_f).
[3]For a heat exchanger of parallel currents the sign of the first term inside the brackets in Eq. (3) would become negative.

For the parallel flow heat exchanger, analogously

$$\ln\left[\frac{\Delta T(x)}{\Delta T_0}\right] = -L\int_0^{\xi} \frac{U_0' + U''\xi}{C_{g_0} + C_g'\xi}\left[\frac{C_{g_0} + C_g'\xi}{C_{f_0} + C_f'\xi} + 1\right] \mathrm{d}\xi \tag{8}$$

and the obtained profile of temperature difference between the streams is

$$\begin{aligned}\Delta T(\xi) =& \Delta T_0\,(1 + \xi\, C_f'/C_{f_0})^{\frac{L}{C_f'}\left(\frac{C_{f_0}U''}{C_f'} - U_0'\right)} \\ & \times (1 + \xi\, C_g'/C_{g_0})^{\frac{L}{C_g'}\left(\frac{C_{g_0}U''}{C_g'} - U_0'\right)} \exp\left[-\left(\frac{1}{C_f'} + \frac{1}{C_g'}\right) L\, U''\xi\right]\end{aligned} \tag{9}$$

The temperature difference between streams is very interesting to plot, but for use in the Utamura *et al.* (2008) marching algorithm the really useful formula is that obtained from Eq. (6) or Eq. (8) for the length of the subdomain in each this temperature difference varies from a known temperature difference ΔT_0 to another ΔT_1. These are

$$\begin{aligned}L \;=\; & \ln\left(\frac{\Delta T_1}{\Delta T_0}\right) \Big/ \left[\frac{1}{C_f'}\left(U_0' - \frac{C_{f_0}U''}{C_f'}\right)\ln\left(1 + \frac{C_f'}{C_{f_0}}\right)\right. \\ & \left. + \frac{1}{C_g'}\left(\frac{C_{g_0}U''}{C_g'} - U_0'\right)\ln\left(1 + \frac{C_g'}{C_{g_0}}\right) + \left(\frac{1}{C_f'} - \frac{1}{C_g'}\right)U''\right]\end{aligned} \tag{10}$$

for the counterflow heat exchanger and

$$\begin{aligned}L \;=\; & \ln\left(\frac{\Delta T_1}{\Delta T_0}\right) \Big/ \left[\frac{1}{C_f'}\left(\frac{C_{f_0}U''}{C_f'} - U_0'\right)\ln\left(1 + \frac{C_f'}{C_{f_0}}\right)\right. \\ & \left. + \frac{1}{C_g'}\left(\frac{C_{g_0}U''}{C_g'} - U_0'\right)\ln\left(1 + \frac{C_g'}{C_{g_0}}\right) - \left(\frac{1}{C_f'} + \frac{1}{C_g'}\right)U''\right]\end{aligned} \tag{11}$$

for the parallel flow heat exchanger.

3. SOME FINITE ELEMENTS METHOD (FEM) LIKE APPROACHES

In this section the enthapy balances are rewritten with emphasis in their nonlinear character. Then some aspects of the Finite Elements Method (Zienkiewicz *et al.*, 2013), nominally, the way in which the interpolation functions are built and integrated, will be employed.

3.1 Enthalpy formulation

As a library of thermodynamic properties of fluids is essential in the solution of the nonlinear problem[4], to write the enthalpy balance in terms of enthalpy may be a good idea. So doing

$$\begin{cases}\dfrac{\mathrm{d}h_g(x)}{\mathrm{d}\,x} = \dfrac{U'(h_g(x), P_g(x), h_f(x), P_f(x))}{\dot m_g}\left[T_f(h_f(x), P_f(x)) - T_g(h_g(x), P_g(x))\right] \\ \dfrac{\mathrm{d}h_f(x)}{\mathrm{d}\,x} = \dfrac{U'(h_g(x), P_g(x), h_f(x), P_f(x))}{\dot m_l}\left[T_f(h_f(x), P_f(x)) - T_g(h_g(x), P_g(x))\right]\end{cases} \tag{12}$$

To make this problem solvable additional equations involving the pressures P_f and P_g would be needed, and this more general problem is mentioned here only to emphasize the hypothesis that will be assumed (and not mislead the reader to illusions about the generality of the approach that will be taken here). Assuming that U' is independent of the unknown variables and that the pressures in each stream are constants one gets

$$\begin{cases}\dfrac{\mathrm{d}h_g(x)}{\mathrm{d}\,x} = \dfrac{U'}{\dot m_g}\left[T_f(h_f(x)) - T_g(h_g(x))\right] \\ \dfrac{\mathrm{d}h_f(x)}{\mathrm{d}\,x} = \dfrac{U'}{\dot m_f}\left[T_f(h_f(x)) - T_g(h_g(x))\right]\end{cases} \tag{13}$$

[4]The EES (Klein and Alvarado, 2002) software was used in the computations presented here

that is the problem really solved in the Utamura *et al.* (2008) test case. Again introducing the non dimensional coordinate and integrating

$$\begin{cases} h_g(\xi) - h_g(0) = L \displaystyle\int_0^{\xi} \frac{U'}{\dot{m}_g} [T_f(h_f(\xi)) - T_g(h_g(\xi))] \, \mathrm{d}\xi \\ h_f(\xi) - h_f(0) = L \displaystyle\int_0^{\xi} \frac{U'}{\dot{m}_l} [T_f(h_f(\xi)) - T_g(h_g(\xi))] \, \mathrm{d}\xi \end{cases} \tag{14}$$

3.2 Lagrange polynomial interpolation functions

In a typical finite element method a set of p + 1 shape functions $\mathcal{N}_i(\xi)$ normalized Lagrange polynomials of degree p) are used to write

$$h_g(\xi) = \sum_{i=1}^{p+1} \mathcal{N}_i(\xi) h_g(\xi_i) \qquad \text{and} \qquad h_f(\xi) = \sum_{i=1}^{p+1} \mathcal{N}_i(\xi) h_f(\xi_i) \tag{15}$$

with

$$\xi_i = (i-1)/p \qquad\qquad i = 1, 2, ..., p+1 \tag{16}$$

Then the required integrals are performed by Gaussian quadrature, generally using $(p+1)/2$ integration points (that is exact for a polynomial of degree p) leading to the system of $2p+1$ nonlinear equations

$$\begin{cases} h_g(\xi_j) - h_g(0) = \dfrac{L\,U'}{\dot{m}_g} \overline{\Delta T}_j & j = 2, 3..., p \\ h_f(\xi_j) - h_f(0) = \dfrac{\dot{m}_g}{\dot{m}_l} [h_g(\xi_j) - h_g(0)] & j = 2, 3..., p \\ q = L\,U' \, \overline{\Delta T}_{p+1} \\ h_g(1) - h_g(0) = \dfrac{q}{\dot{m}_g} \\ h_f(1) - h_f(0) = \dfrac{\dot{m}_g}{\dot{m}_l} [h_g(1) - h_g(0)] \end{cases} \tag{17}$$

for the 2p + 1 unknowns

$$h_g(\xi_i) \text{ and } h_l(\xi_i), \text{ for } i = 2, 3, ..., p+1 \qquad \text{and} \qquad L \tag{18}$$

since $h_g(0)$, $h_l(0)$ and q are given data.

The fractions of mean temperature differences over the heat exchanger segment are calculated (requiring p odd) as follows

$$\begin{aligned} \overline{\Delta T}_j &= \int_0^{\xi_j} \left[T_f\left(\sum_{i=1}^{p+1} \mathcal{N}_i(\xi) h_f(\xi_i) \right) - T_g\left(\sum_{i=1}^{p+1} \mathcal{N}_i(\xi) h_g(\xi_i) \right) \right] \mathrm{d}\xi \\ &\approx \frac{j-1}{p} \sum_{m=1}^{\frac{p+1}{2}} \left[T_f\left(\sum_{i=1}^{p+1} \mathcal{N}_i(\xi_{m,j}) h_f(\xi_i) \right) - T_g\left(\sum_{i=1}^{p+1} \mathcal{N}_i(\xi_{m,j}) h_g(\xi_i) \right) \right] w_m \end{aligned} \tag{19}$$

It is important to notice that in the literature the finite elements are formulated using local coordinates with range $-1 \leq \eta \leq 1$ (not from $0 \leq \xi \leq 1$ as here). This means that a transformation $\eta = 2\xi - 1$ is required to map a coordinate used here to that normally used in the shape functions. For the interesting case of $p = 3$ the Lagrange ones become, in the coordinate system of this document

$$\begin{aligned} &\mathcal{N}_1(\xi) = \tfrac{9}{2}(1-\xi)\left(\tfrac{2}{3}-\xi\right)\left(\tfrac{1}{3}-\xi\right) \\ &\mathcal{N}_2(\xi) = \tfrac{27}{2}\,\xi\,(1-\xi)\left(\tfrac{2}{3}-\xi\right) \\ &\mathcal{N}_3(\xi) = \tfrac{27}{2}\left(\xi-\tfrac{1}{3}\right)\xi\,(1-\xi) \\ &\mathcal{N}_4(\xi) = \tfrac{9}{2}\left(\xi-\tfrac{2}{3}\right)\left(\xi-\tfrac{1}{3}\right)\xi \end{aligned} \tag{20}$$

The corresponding two points Gaussian integration, uses the weights and integration points

$$w_1 = w_2 = \frac{1}{2} \qquad \text{and} \qquad \xi_{m,j} = \left(1 + \frac{2m-3}{\sqrt{3}}\right)\frac{j-1}{2p} \tag{21}$$

Yet a different a coordinate transformation was needed, to map the integration interval $0 \leq \xi \leq \xi_j = (j-1)/p$ to the standard interval $-1 \leq \eta \leq 1$. It was

$$\eta = \frac{2\,p\,\xi}{j-1} - 1 \tag{22}$$

3.3 Temperature formulation

Trying to avoid computational difficulties found in the enthalpy formulation, the specific heat definition was used to obtain a formulation in which the temperature are primary unknowns (and not calculated in function of enthalpy (a demanding task for the fluid properties library functions). There is not enough space in this paper for presenting in details this temperature formulation that is completely parallel to the presented for enthalpy, only the equations analogous to Eq. (14) are shown here

$$\begin{cases} T_g(\xi) - T_g(0) = L\displaystyle\int_0^\xi \frac{U'}{\dot{m}_g\, c_{p_g}}[T_f(\xi) - T_g(\xi)]\,\mathrm{d}\xi \\ T_f(\xi) - T_f(0) = L\displaystyle\int_0^\xi \frac{U'}{\dot{m}_f\, c_{p_f}}[T_f(\xi) - T_g(\xi)]\,\mathrm{d}\xi \end{cases} \tag{23}$$

The computational stability really improved (less iterations and less carefully specified initial guess were demanded for the solution of the problem) using this temperature formulation and the Lagrange interpolation functions. The accuracy, however, even degraded a little bit and so the Hermite interpolation functions were tested in the next subsection using again the enthalpy formulation.

3.4 Hermite interpolation functions

As writing the Hermite interpolation (shape) functions (cubic splines) is harder than writing the Lagrange ones the standard non dimensional coordinate used in FEM $\eta = 2(x - x_0)/L - 1$, impliyng $-1 \leq \eta \leq 1$, will be used here to facilitate confrontation with the formulae found in literature

$$\begin{aligned} \mathcal{H}_{01}(\eta) &= 1 + [(1+\eta)^3 - 3(1+\eta)^2]/4 \\ \mathcal{H}_{11}(\eta) &= (\eta-1)^2(1+\eta)\,L/8 \\ \mathcal{H}_{02}(\eta) &= [3(1+\eta)^2 - (1+\eta)^3]/4 \\ \mathcal{H}_{12}(\eta) &= (\eta-1)(1+\eta)^2 L/8 \end{aligned} \tag{24}$$

the enthalpies now being expressed as

$$\begin{aligned} h_g(\eta) &= \sum_{i=0}^{1}\left[\mathcal{H}_{i1}(\eta)h_g^{(i)}(-1) + \mathcal{H}_{i2}(\eta)h_g^{(i)}(1)\right] \\ &= \sum_{i=0}^{1}\sum_{j=0}^{1}\mathcal{H}_{i(j+1)}(\eta)h_g^{(i)}(2j-1) \end{aligned} \tag{25}$$

$$h_f(\eta) = \sum_{i=0}^{1}\sum_{j=0}^{1}\mathcal{H}_{i(j+1)}(\eta)h_f^{(i)}(2j-1) \tag{26}$$

where the superscript (i) indicates the i-th spatial derivative. Therefore one gets the system of equations

$$\begin{cases} q = L\,U'\,\overline{\Delta T} \\ h_g(1) - h_g(-1) = \dfrac{q}{\dot{m}_g} \\ h_f(1) - h_f(-1) = \dfrac{\dot{m}_g}{\dot{m}_l}\,[h_g(1) - h_g(-1)] \\ h'_g(1) = \dfrac{L\,U'}{\dot{m}_g}\,[T_f(h_f(1)) - T_g(h_g(1))] \\ h'_f(1) = \dfrac{\dot{m}_g}{\dot{m}_l}\,h'_g(1) \end{cases} \tag{27}$$

with

$$\begin{aligned} \overline{\Delta T}_j &= \int_{-1}^{1}\left[T_f\left(\sum_{i=0}^{1}\sum_{j=0}^{1}\mathcal{H}_{i(j+1)}(\eta)h_f^{(i)}(2j-1)\right) - T_g\left(\sum_{i=0}^{1}\sum_{j=0}^{1}\mathcal{H}_{i(j+1)}(\eta)h_f^{(i)}(2j-1)\right)\right]\mathrm{d}\eta \\ &\approx \sum_{m=1}^{2}\left[T_f\left(\sum_{i=0}^{1}\sum_{j=0}^{1}\mathcal{H}_{i(j+1)}(\eta_m)h_f^{(i)}(2j-1)\right) - T_g\left(\sum_{i=0}^{1}\sum_{j=0}^{1}\mathcal{H}_{i(j+1)}(\eta_m)h_f^{(i)}(2j-1)\right)\right]w_m \end{aligned} \tag{28}$$

where

$$w_1 = w_2 = \frac{1}{2} \qquad \text{and} \qquad \eta_m = \frac{2m-1}{\sqrt{3}} \tag{29}$$

4. RESULTS

The performance of the different interpolation functions are compared here, in the solution of the problem described in the subsection 1.1. If the global coefficient of heat transfer U is constant along the heat exchanger lenght ($U'' = 0$) the product UA becomes proportional to the heat exchanger lenght (and is essentially the solution of the heat exchanger **design** problem). In the Figure 1 it is shown computations using various interpolation functions converging to this solution.

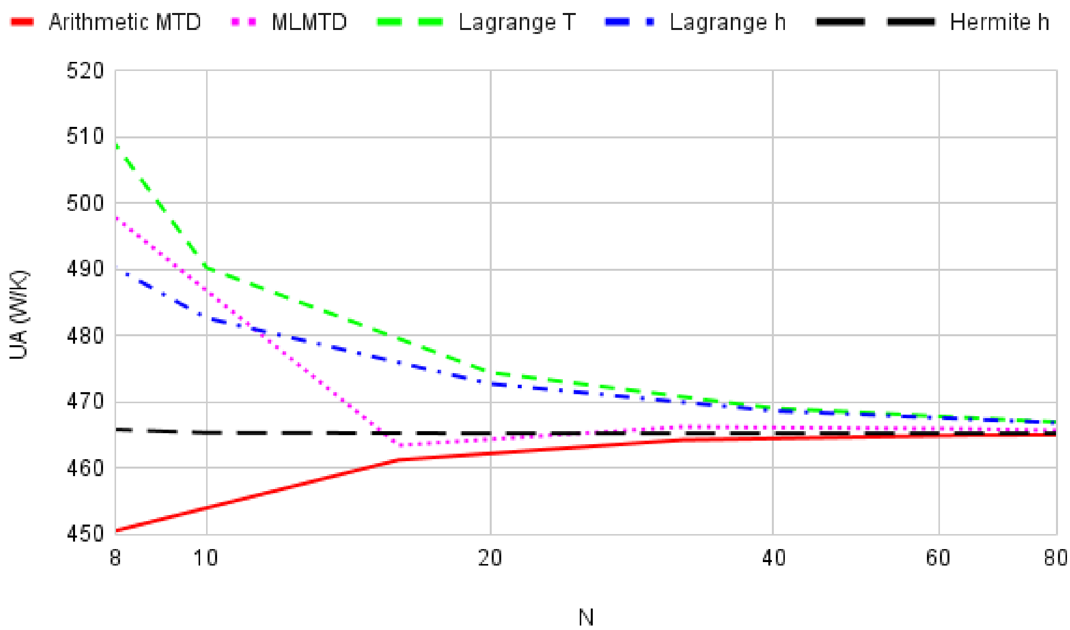

Figure 1. Convergence of the UA estimate as the number of heat exchanger segments n increases

In the Figure 1, the interpolation based in an analytical solution proposed in the section 2. is identified by the acronym MLMTD (for modified logarithmic mean temperature difference), in contrast to the calculation based on the original proposal of Utamura *et al.* (2008), identified as Arithmetic MTD (mean temperature difference).

No advantage of the more involved and computationally expensive MLMTD approach was visible in these results.The Grid Convergence Index (GCI) recommended by Celik (2008) went to 0,0 %, for both methods, with a 128 segments discretization. Interpolation functions based in analytical solutions of a simplified version of the problem to be solved are not a novelty: the Exponential Difference Scheme and the Power-Law Difference Scheme (PLDS) proposed by Patankar (1980) to approximate the former, are old examples of this. Also the fact that the MLMTD did not performed better than the simpler linear interpolation (Arithmetic MTD) is not a surprise: there is much criticism over the PLDS essentially for being more convoluted and less accurate than the linear interpolation (implied in the Central Difference Scheme – CDS), although the linear interpolation may produce undesirable oscillations and instability in some contexts of interest in the work of Patankar (1980).

The apparent order of accuracy (or convergence) of the approximations may be evaluated using the theory presented by Marchi and Silva (2002), that is essentially the same presented in the more widely known paper by Celik (2008). These apparent orders of accuracy may also be visualized as the angular coefficients of the log-log error graphs in the Fig. 2.

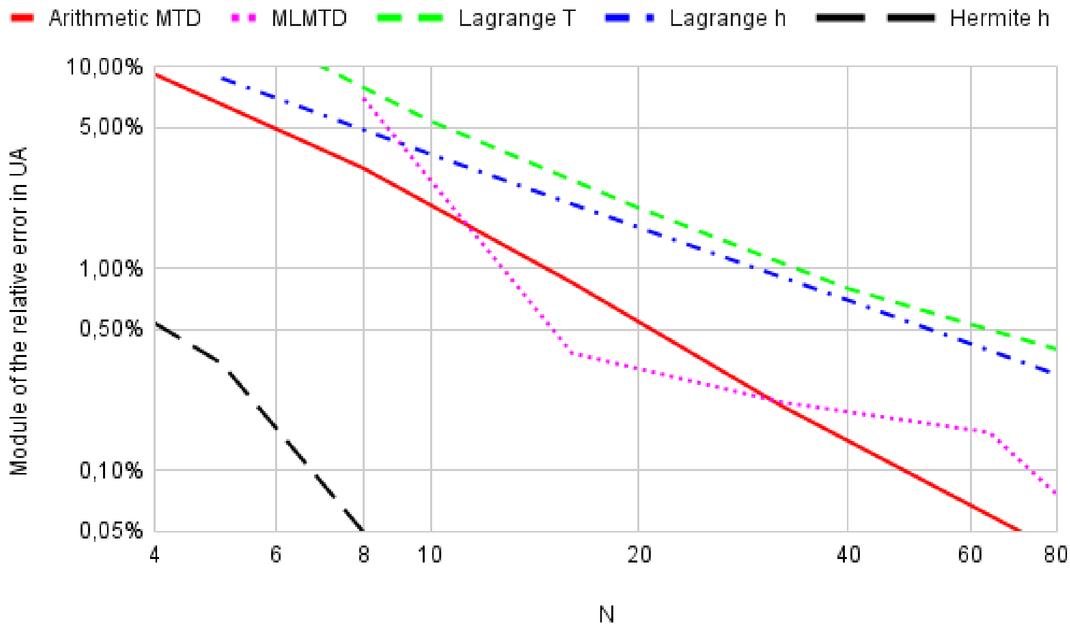

Figure 2. Low order of convergence obtained with Lagrange cubic interpolation compared with nearly second order of Utamura *et al.* (2008) Arithmetic MTD and of MLMTD and with almost fourth-order obtained with Hermite cubic spline

The apparent order of accuracy of the methods based in Lagrange polynomials falls between 2 and 1 (approaching 1,2 at the finer grids) and the GCI of the finest grids (that has 80 elements and so 241 nodes) are 0,2 % and 0,3 % for the formulations in T and in h respectively. But, with Hermite polynomials, finally some improvement in relation to the original method of Utamura *et al.* (2008) was obtained: the apparent order of accuracy was 3,9, the execution was fast and stable (in contrast to what was observed using Lagrange polynomials) and the CGI was below 0,01 % with a grid of just 20 elements (segments). With only 1 element the Hermite polynomials approach overestimated the UA in less than 1,25 %.

5. USING MINIMIZATION

5.1 A collocation approach

Probably the shortest path form the system of ODEs to the numerical solution of the problem is to assume that the temperatures can be expressed as polynomials, in its canonical form

$$T_g(\xi) = \sum_{i=1}^{p+1} a_{g_i} \xi^{i-1} \qquad \text{and} \qquad T_f(\xi) = \sum_{i=1}^{p+1} a_{f_i} \xi^{i-1} \tag{30}$$

in each heat exchanger segment, and then minimize a measure of the residual of expressions of the differential equations at n collocation points (usually equally spaced) along the segment. The residual of the global thermal balance is used to avoid a trivial solution with no heat exchange between the streams. The boundary conditions need to be enforced also (this is usually made by setting the independent term of the polynomials) and additional requirements (restrictions) may be imposed.

Keeping the focus on the design problem suggested by Utamura et al. (2008), the residuals to be minimized could be written (in terms of heat per length unit, in W/m)

$$
\begin{aligned}
R_{g_j} &= \frac{\dot{m}_g c_{p_g}}{L} \sum_{i=2}^{p+1} (i-1) a_{g_i} \left(\frac{j}{n+1} \right)^{i-2} - U' \sum_{i=1}^{p+1} (a_{f_i} - a_{g_i}) \left(\frac{j}{n+1} \right)^{i-1} \\
R_{f_j} &= \frac{\dot{m}_f c_{p_f}}{L} \sum_{i=2}^{p+1} (i-1) a_{f_i} \left(\frac{j}{n+1} \right)^{i-2} - U' \sum_{i=1}^{p+1} (a_{f_i} - a_{g_i}) \left(\frac{j}{n+1} \right)^{i-1} \\
R_{\text{global}} &= \frac{q}{U'} \sum_{i=1}^{p+1} \frac{a_{f_i} - a_{g_i}}{i}
\end{aligned}
\tag{31}
$$

and the problem stated as to find

$$
\begin{array}{ll}
\displaystyle \min_{L, a_{g_2}, a_{f_2}, \ldots, a_{g_{p+1}}, a_{f_{p+1}}} & \displaystyle R^2_{\text{global}} + \sum_{j=1}^{n} \left(R^2_{g_j} + R^2_{f_j} \right) \\
\text{s.t.} & a_{g_1} = T_{g_0} \\
 & a_{f_1} = T_{f_1} + \frac{q}{\dot{m}_f c_{p_f}}
\end{array}
\tag{32}
$$

for $p = 3$ the best result was obtained with $n = 3$ (many other n were tested, with $n = 0$ temperature profiles crossed each other, what is physically impossible) and it was an L 30 % below the exact. With $n = 2$ an L only 18 % above the exact was obtained, but the predicted temperature at the water inlet departed by 27 % (of the characteristic temperature difference of the problem) from its known value. To solve a series of minimization problems, one for each segment of a heat exchanger, seems to be a too difficult approach to be attempted in this study, but it is relatively easy to increase the order p of the polynomials. For $p = 4$ the best result was obtained with $n = 18$ and it was an L 19 % below the exact. This approach is very sensitive to the tolerance in the minimization and it was set to 1×10^{-8} to obtain these results (it is sensitive also to the initial guesses used).

It is worthy to emphasize the difference between this approach and an usual least squares problem where a distance between a function with unknown parameters and some known points is minimized. In the present approach no known solution points are available (except those given by the boundary/initial conditions). Here what is being minimized is the degree at which the trial functions with unknown parameters disobeys the differential equations system. As explained in the literature, the difference between a Point Collocation and a typical Ritz-Galerkin Finite Element Method resides essentially in how and where they measure this disobedience, using what test function (and this affects not only the rate at which the error will diminish with increasing the degrees of freedom of the tentative functions, but also the condition number of the matrices involved in the parameters estimation, and so the computational effort demanded by it).

5.2 Back to finite control volumes

A last numerical experiment was performed to understand better the possibilities and drawbacks of the direct minimization approach. It consisted in try to disguise the solution of the nonlinear algebraic system of equations obtained using the control volume enthalpy formulation and the canonical cubic polynomial as interpolation function as a minimization problem. The less difficult minimization problem so obtained was

$$\begin{aligned}
\min_{L} \quad & \left\{ \sum_{j=0}^{1} \left[T_g \left(\sum_{i=1}^{4} a_{gi} \xi_j^{i-1}, P_g \right) - T_f \left(\sum_{i=1}^{4} a_{fi} \xi_j^{i-1}, P_f \right) \right] w_j - \frac{q}{LU'} \right\}^2 \\
\text{s.t.} \quad & a_{g_1} = h_g(T_{g_0}, P_g) \\
& a_{f_1} = h_f(T_{f_1}, P_f) + \tfrac{q}{\dot{m}_f} \\
& a_{g_2} = \tfrac{LU'}{\dot{m}_g} [T_f(a_{f_1}, P_f) - T_{g_0}] \\
& a_{f_2} = \tfrac{\dot{m}_g}{\dot{m}_f} a_{g_2} \\
& \textstyle\sum_{i=1}^{4} a_{g_i} = h_g(T_{g_0}, P_g) + \tfrac{q}{\dot{m}_g} \\
& \textstyle\sum_{i=1}^{4} a_{f_i} = h_g(T_{f_1}, P_f) \\
& \textstyle\sum_{i=2}^{4} (a_{g_i}/i) = \tfrac{LU'}{\dot{m}_g} [T_{f_1} - T_g(h_g(T_{g_0}, P_g) - \tfrac{q}{\dot{m}_g}, P_g)] \\
& \textstyle\sum_{i=2}^{4} (a_{f_i}/i) = \tfrac{\dot{m}_g}{\dot{m}_f} \sum_{i=2}^{4} (a_{g_i}/i)
\end{aligned} \tag{33}$$

where, for the two point Gaussian quadrature,

$$w_0 = w_1 = \frac{1}{2} \qquad \text{and} \qquad \xi_j = \left(1 + \frac{j-1}{\sqrt{3}} \right) \Big/ 2 \tag{34}$$

and the a's are coefficients of polynomials representing the enthalpy

$$h_g(\xi) = \sum_{i=1}^{4} a_{g_i} \xi^{\,i-1} \qquad \text{and} \qquad h_f(\xi) = \sum_{i=1}^{4} a_{f_i} \xi^{\,i-1} \tag{35}$$

This lead to the same solution, 1,25 % above the exact , reported in the previous section when Hermite interpolation was used with just 1 heat exchanger segment. The instability of the above minimization problem, however, is much greater. Such that, to obtain any solution, it was necessary to use an initial guess very close to the searched minimum.

It must be noticed that that the **design** problem dealt with here seems particularly hard to solve directly by minimization. The **analysis** problem (given the heat exchanger properties and the difference between inlet temperatures, to calculate the rate of heat exchange) is easier. A remark on the additional difficulty introduced by the calculation of the temperature from given enthalpy, that demands by itself an iterative procedure, helps in understanding the difficulties associated with the last numerical experiment.

6. CONCLUSIONS

The main conclusion of the present work is the confirmation of a conjecture made at its beginning: that the accuracy or the Utamura *et al.* (2008) methodology for supercritical heat exchanger modeling could be improved using cubic polynomials to interpolate properties inside each heat exchanger segment. But the improvement was observed only when Hermite (spline) interpolations functions were used, and this was a surprise. Now it is easy to reason that the greater smoothness imposed by the spline interpolation functions makes the approximate solutions better than those obtained with the same number of segments but using interpolation functions with derivatives discontinuous between segments. At the start of the present work, however, this was by no means obvious to the authors, in spite of some previous successful experiences using splines in different contexts (Razzini *et al.*, 2020).

In the Numerical Methods literature (Li *et al.*, 2000), the possibility of reaching fourth order of accuracy in the solution of convection-diffusion problems through the use of cubic interpolation functions is discussed, but the Hermite interpolation functions are scarcely used in that context, probably because of the instability that arise at high Péclet numbers, as report Radu *et al.* (2015). Controlled artificial dissipation (Swanson *et al.*, 1998) may be used to alleviate such instability. No matter the performance of cubic Hermite interpolation functions in that problem [5], it seems that the practical advantage of the use of this interpolation in some heat exchanger design problems, demonstrated here, is relatively unknown, as no mention to it is found in the recently published books of Reddy and Gartling (2010) and of Roetzel *et al.* (2019).

Another development here presented is the derivation of an interpolation function, for use in nonlinear heat exchanger design problems, from the analytical solution of a related linear problem. The so derived interpolation function was shown to be accurate, but no more accurate (and more computationally expensive) than a much simpler linear interpolation.

[5] Mathematically quite different of the one dealt here, mostly because the diffusion in the flow direction is disregarded in the present work.

Finally, searching for less computationally demanding models, like those presented by Girault *et al.* (2011) and by Souraki *et al.* (2014)[6], for nonlinear heat exchangers, it was investigated the use of polynomials in its canonical form and minimization resources nowadays available at many software (even spreadsheets). It was concluded that such approach is much more viable today than it was some decades ago, but it is not yet competitive with the standard techniques based in writing a system of carefully chosen nonlinear equations as easy to solve as possible.

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9. RESPONSIBILITY NOTICE

[6]This paper presents another application of Hermite splines pretty relevant to Heat Transfer.