SIMULATION OF THERMAL SYSTEMS USING A GENERALIZED COMPUTATIONAL ALGORITHM

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Abstract. *The present algorithm consists in a simulation program with modular characteristics. The modules are composed for specific routines related with the components of the system. The input data file composes of the working fluids, the characteristics of each component and the known variables. Based on the index of mass rate vectors, the indexes of mass rate are generated upstream and downstream of each node. The conservation laws are used to compose, automatically, the system of equations, which are solved by Newton Raphson method for multiple equations and unknowns.*

Keywords: *Thermal Systems, Generalized Computational Algorithm, Newton Raphson Method.*

1. INTRODUCTION

The expression "Simulation of Thermal Systems" presumes knowledge of the performance characteristics of all components as well as equations for thermodynamic properties of the working substances.

The simulation of thermal systems can be applied to heating and cooling plants and it consists of calculation of all operating variables such as temperatures, pressures, specific energy and fluid flow rates at a given time. The equations for performance characteristics of the components and thermodynamic properties, along with energy and mass balances, form a set of simultaneous equations relating the operating variables. The mathematical description of system simulation is that of solving the simultaneous equations, many of which may be nonlinear.

Several users need to simulate thermal system, such as chemical and process industries, air conditioning engineers and thermal power plants. Evans *et. al.* (1968) has shown that chemical and industries process have used generalized programs for several years. Several programs have been developed in the industry. Examples of these programs are: *PACER* (Purdue-Dartmouth), *MAEBE* (University of Tennessee), *COPE* (Esso Research and Engineering), *CHEOPS* (Shell Oil), *PEDLAN* (MobilOil) and *FLEXIBLE FLOWSHEET* (M. W. Kellogg).

Stoecker (1971) developed a generalized program for steady state system simulation. However, the program of this author does not generate the system of equations by specifics routines. Reynolds (1979) developed equations to compute the physical and thermodynamic properties of fluids. Klein and Alvarado (1993) developed the program *EES* (Engineering Equation Solver) for the solution of a set of algebraic equations and thermophysical property

functions useful for engineering calculations. Nevertheless, this program do not generate the system of equations.

This work shows the computational algorithm used to simulate, in steady-state, any thermal system. The algorithm composes by specific subroutines that compute physical and thermodynamic properties and others subroutines, that apply the conservation laws, are used to form, automatically, the system of equations, which are solved by Newton-Raphson method for multiple equations and unknowns.

This paper concludes presenting a simulation of a thermal system (regenerative cycle) to compute its variables.

2. DATA FILE CONSTRUCTION

The system of equations is generated through the following data file (See Fig. 1) and the nomenclature of the data file inputs is defined in Table 1.

$$
\begin{aligned}
&n_n \quad n_p \quad n_c \\[6pt]
&npk \quad inpk_1 \quad pk_1 \quad inpk_2 \quad pk_2 \ \ldots \ inpk_n \quad pk_n \\
&ntk \quad intk_1 \quad tk_1 \quad intk_2 \quad tk_2 \ \ldots \ intk_n \quad tk_n \\
&nqk \quad inqk_1 \quad qk_1 \quad inqk_2 \quad qk_2 \ \ldots \ inqk_n \quad qk_n \\[6pt]
&z_{n1} \quad z_{n2} \ \cdots \ z_{nn} \\[6pt]
&unp_1 \quad dnp_1 \quad Dp_1 \quad Lp_1 \quad Sk_1 \quad rp_1 \\
&unp_2 \quad dnp_2 \quad Dp_2 \quad Lp_2 \quad Sk_2 \quad rp_2 \\
& \cdot \\
& \cdot \\
& \cdot \\
&unp_n \quad dnp_n \quad Dp_n \quad Lp_n \quad Sk_n \quad rp_n \\[6pt]
&efc_1 \quad \dot{W}_{c_1} \quad \dot{Q}_{c_1} \quad isob_1 \quad isot_1 \quad isos_1 \quad isoh_1 \\[6pt]
&efc_2 \quad \dot{W}_{c_2} \quad \dot{Q}_{c_2} \quad isob_2 \quad isot_2 \quad isos_2 \quad isoh_2 \\
&\phantom{efc_2 \quad \dot{W}_{c_2}} \cdot \\
&\phantom{efc_2 \quad \dot{W}_{c_2}} \cdot \\
&\phantom{efc_2 \quad \dot{W}_{c_2}} \cdot \\
&efc_n \quad \dot{W}_{c_n} \quad \dot{Q}_{c_n} \quad isob_n \quad isot_n \quad isos_n \quad isoh_n \\[6pt]
&unc_1 \quad dnc_1 \quad nuc_2 \quad ndc_2 \ldots unc_n \quad dnc_n
\end{aligned}
$$

Figure 1- Data File.

Table 1. Nomenclature of the inputs in Data File.

Data File Inputs	Nomenclature
Number of nodes	n_n
Number of pipes	n_p
Number of components	n_c
Number of known pressures	npk

Node index indicating the location where the pressure n is known	$inpk_n$
Known pressure n	pk_n
Number of known temperatures	ntk
Node index indicating the location where the temperature n is known	$intk_n$
Known temperature n	tk_n
Number of known mass quality	nqk
Known mass quality n	qk_n
Node index indicating the location where the mass quality is known	$inqk_n$
Node n level	z_{nn}
Upstream node of the piping n	unp_n
Downstream node of the piping n	dnp_n
Diameter of the pipe n	Dp_n
Length of the pipe n	Lp_n
Sum of all factors of located loss	Sk_n
Roughness of pipe n	rp_n
Efficiency of the component n	efc_n
Power of the component n	$\dot{W}_{c_n}$
Rate of heat transfer of the component n	$\dot{Q}_{c_n}$
If the transformation in the component n is isobaric	$isob_n$
If the transformation in the component n is isotherm	$isot_n$
If the transformation in the component n is isoentropic	$isos_n$
If the transformation in the component n is isoenthalpic	$isoh_n$
Number of points of the characteristic curve of the component n	npc_n
If $(efc_n > 1)$ then $npc_n = efc_n$ and read x_1 y_1 , x_2 y_2 , ... , x_n y_n	------
Coordinate in the x direction of the characteristic curve	x_n
Coordinate in the y direction of the characteristic curve	y_n
Upstream node of the component n	unc_n
Downstream node of the component n	dnc_n

Based on the index of mass rate vectors, the indexes of mass flow rate are automatically generated upstream and downstream of each node.

3. SYSTEM OF EQUATIONS

The system of equations for a generic thermal system is given as follows:

Conservation of mass:

$$\sum \dot{m}_{un_1} - \sum \dot{m}_{dn_1} = 0 \qquad (1.1)$$

$$\sum \dot{m}_{un_2} - \sum \dot{m}_{dn_2} = 0 \qquad (1.2)$$

$$.$$
$$.$$
$$.$$

$$\sum \dot{m}_{un_n} - \sum \dot{m}_{dn_n} = 0 \qquad (1.n_n)$$

The subscripts un_n and dn_n indicate, respectively, the upstream and downstream positions of the node n and $\dot{m}$ represents the mass flow rate.

Energy equation:

$$\dot{Q}_{c_1} - \dot{W}_{c_1} - [\sum \dot{m}_{dc_1} (h_{dc_1} + \frac{V_{dc_1}^2}{2} + z_{dc_1} \cdot g) - \sum \dot{m}_{uc_1} (h_{uc_1} + \frac{V_{uc_1}^2}{2} + z_{uc_1} \cdot g)] = 0 \qquad (1.n_n+1)$$

$$\dot{Q}_{c_2} - \dot{W}_{c_2} - [\sum \dot{m}_{dc_2} (h_{dc_2} + \frac{V_{dc_2}^2}{2} + z_{dc_2} \cdot g) - \sum \dot{m}_{uc_2} (h_{uc_2} + \frac{V_{uc_2}^2}{2} + z_{uc_2} \cdot g)] = 0 \quad (1.n_n+2)$$

$$\vdots$$

$$\dot{Q}_{c_n} - \dot{W}_{c_n} - [\sum \dot{m}_{dc_n} (h_{dc_n} + \frac{V_{dc_n}^2}{2} + z_{dc_n} \cdot g) - \sum \dot{m}_{uc_n} (h_{uc_n} + \frac{V_{uc_n}^2}{2} + z_{uc_n} \cdot g)] = 0 \quad (1.n_n+n_c)$$

$$p_{up_1} - p_{dp_1} - K_1 \cdot \dot{m}_1^2 = 0 \qquad\qquad (1.n_n+n_c+1)$$

$$p_{up_2} - p_{dp_2} - K_2 \cdot \dot{m}_2^2 = 0 \qquad\qquad (1.n_n+n_c+2)$$

$$\vdots$$

$$p_{up_n} - p_{dp_n} - K_{n_p} \cdot \dot{m}_{n_p}^2 = 0 \qquad\qquad (1.n_n+n_c+n_p)$$

The subscripts are defined in Table 2.

Table 2. Nomenclature of the subscripts.

Subscripts	Nomenclature
Component n	c_n
Downstream of the component n	dc_n
Upstream of the component n	uc_n
Upstream of the pipe n	up_n
Downstream of the pipe n	dp_n

where $\dot{Q}$ is the rate of heat transfer and $\dot{W}$ is the power. The rate of heat transfer $\dot{Q}$ and the power $\dot{W}$ are adjusted, respectively, based on the characteristic curve of each component, as follow:

$$\dot{Q}_{c_n} = A_n \cdot \dot{m}_n^2 + B_n \cdot \dot{m}_n + C \qquad\qquad (2.1)$$

$$\dot{W}_{c_n} = E_n \cdot \dot{m}_n^2 + F_n \cdot \dot{m}_n + G \qquad\qquad (2.2)$$

Considering $n_n + n_c + n_p = n$, the equations (1) to (n) can be written in implicit form as follows:

$$F_1(V_1, V_2, ..., V_n) = 0 \qquad\qquad (3.1)$$

$$F_2\left(V_1, V_2, ..., V_n\right) = 0 \tag{3.2}$$

$$.$$
$$.$$
$$.$$

$$F_n\left(V_1, V_2, ..., V_n\right) = 0 \tag{3.n}$$

Considering the initial guessed values for the variables as: $V_1^0, V_2^0, ..., V_n^0$, the Taylor-series expansion for (Eqs. 3.1-3.n) generate the set of simultaneous equations as follow (Stoecker, 1980):

$$\left(V_1^0 - V_1\right)\frac{\partial F_1}{\partial V_1} + \left(V_2^0 - V_2\right)\frac{\partial F_1}{\partial V_2} + ... + \left(V_n^0 - V_n\right)\frac{\partial F_1}{\partial V_n} = 0 \tag{4.1}$$

$$\left(V_1^0 - V_1\right)\frac{\partial F_2}{\partial V_1} + \left(V_2^0 - V_2\right)\frac{\partial F_2}{\partial V_2} + ... + \left(V_n^0 - V_n\right)\frac{\partial F_2}{\partial V_n} = 0 \tag{4.2}$$

$$.$$
$$.$$
$$.$$

$$\left(V_1^0 - V_1\right)\frac{\partial F_n}{\partial V_1} + \left(V_2^0 - V_2\right)\frac{\partial F_n}{\partial V_2} + ... + \left(V_n^0 - V_n\right)\frac{\partial F_n}{\partial V_n} = 0 \tag{4.n}$$

where $\dfrac{\partial F_i}{\partial V_j}$ represents the partial derivative of the function i regarding to variable j. These partial derivatives are calculated numerically.

The solution of the linear system (4.1) to (4.n) are the variables:

$$\Delta V_1 = V_1^0 - V_1 \tag{5.1}$$
$$\Delta V_2 = V_2^0 - V_2 \tag{5.2}$$

$$.$$
$$.$$
$$.$$

$$\Delta V_n = V_n^0 - V_n \tag{5.n}$$

The new guessed values for the variables are:

$$V_1^{new} = V_1^{old} - \Delta V_1 \tag{6.1}$$
$$V_2^{new} = V_2^{old} - \Delta V_2 \tag{6.2}$$

$$.$$
$$.$$
$$.$$

$$V_n^{new} = V_n^{old} - \Delta V_n \tag{6.n}$$

4. THE SOLUTION PROCEDURE

The procedure for solving the equations (4) to (6) is an iterative one in which the following steps are followed. The solution procedure is used to solve the non-linear set of equations (1.1) to (1.n). It is called Newton-Raphson method for multiple equations and unknowns.

The generalized computational algorithm is followed:

1. The input Data File is read
2. The indexes of mass rate are generated upstream and downstream of each node
3. The thermodynamic properties, where the states are defined, are calculated
4. All the variables of the system are guessed
5. The thermodynamic properties, after the states are known, are calculated
6. The state in the outlet of each component is defined based on the thermodynamic transformation (isothermic, isoenthalpic, isentropic and isobaric)
7. The residue equations F_1 to F_n are calculated
8. The partial derivatives are calculated
9. The non-linear system (1.1) to (1.n) is solved
10. The new guessed values for the variables are determined until convergence be reached.

5. THE CALCULATION PROCEDURE OF FLUID PROPERTIES

The thermodynamic properties of the working fluids for the saturated and superheated states are determined as follow:

$$u = \int_{T_0}^{T} C_v^0(T)dt + \int_0^{\rho} \frac{1}{\rho^2}\left[p - T\left(\frac{\partial p}{\partial T}\right)_\rho \right]d\rho + u_0 \tag{7}$$

where:

$\quad\quad u$ -   internal energy
$\quad\quad u_0$ -   reference value
$\quad\quad C_v^0$ -   Ideal gas specific heat
$\quad\quad \rho$ -   vapor density
$\quad\quad p$ -   pressure
$\quad\quad T$ -   temperature.

$$p = \rho RT + F(T,\rho) \tag{8}$$

where:

$\quad\quad R$ -   constant of the compressive substance
$\quad\quad F(T, \rho)$ -   function of the variables ρ , T and the working fluid.

The following equations determine the enthalpy and entropy:

$$h = u + pv \tag{9}$$

$$s = \int_{T_0}^{T} \frac{C_v^0(T)}{T} dt - R \ln \rho + \int_{0}^{\rho} \frac{1}{\rho^2} \left[\rho R - \left(\frac{\partial p}{\partial T} \right)_\rho \right] dp + s_0 \tag{10}$$

The latent heat (h_{lv}) is determined from Clapeyron equation, as:

$$h_{lv} = T v_{lv} \frac{dp_{sat}}{dT_{sat}} \tag{11}$$

The entropy and internal energy of vaporization are calculated as:

$$s_{lv} = \frac{h_{lv}}{T} \tag{12}$$

$$u_{lv} = h_{lv} - p_{sat} v_{lv} \tag{13}$$

The equation in the generalized form is determined as:

$$p = p(T, \rho) \tag{14}$$

The ideal gas specific heat is determined as a function of temperature:

$$C_v^0 = C_v^0(T) \tag{15}$$

The saturation pressure is:

$$p_{sat} = p_{sat}(T_{sat}) \tag{16}$$

The saturated liquid density is determined as:

$$\rho_l = \rho_l(T_{sat}) \tag{17}$$

The thermodynamic properties in the liquid region are determined as follow:

$$f = f_p + \left(f_{es} - f_{ps} \right) \left(\frac{\ln pc - \ln p}{\ln pc - \ln p_s} \right) \tag{18}$$

Where:

f - Generalized property that can be u, h, s or ρ

f_p - Function of p and T calculated, respectively, by equation (5), (7), (8) and (13)

f_{ps} - Value of the saturation temperature, obtained by equation (14) and

f_{es} - This is the saturation value of f at temperature T, determined by:

a. Calculate $\dfrac{dp_{sat}}{dT_{sat}}$ from equation (11)

b. The saturated vapor properties u_v, h_v, s_v and ρ_v using the equations (7), (9), (10) and (14)

c. The saturated liquid density is determined by the equation (17)

d. h_{lv} and s_{lv} are calculated using equations (11) and (12)

e. The saturated liquid properties u_l , h_l , s_l and ρ_l are calculated by the subtractions u_v - u_{lv} , h_v - h_{lv}, s_v - s_{lv} and ρ_v - ρ_{lv}, respectively.

The equations (14), (15), (16) and (17) are adjusted by the least square method and data are available from Reynolds (1979). These equations are differentiated and integrated to obtain the thermodynamic properties. The thermodynamic properties, written in the implicit form, are determined by Newton Raphson method for multiple equations and unknowns.

The separated flow model, described by Collier (1972), is used to calculate the pressure gradient for two-phase flow, as follow. The properties of the two phases are: ρ_l, ρ_v, v_l, v_v. The vapor and liquid mass flow is defined as:

$$G_v = X\,G \ \text{ and } \ G_l = G - G_v \tag{19}$$

The mean velocities of vapor and liquid phases and the Reynolds number are:

$$V_{vs} = \frac{G_v}{\rho_v \cdot A}\,, \ V_{ls} = \frac{G_l}{\rho_l \cdot A}\,, \mathrm{Re}_{vs} = \frac{V_{vs} \cdot D}{v_v} \ \text{ and } \ \mathrm{Re}_{ls} = \frac{V_{ls} \cdot D}{v_l} \tag{20}$$

The friction factors for the vapor phase flow f_{vs} and liquid phase flow f_{lv} are calculated based on the Colebrook formula.

The pressure gradients on the vapor and liquid phases and the total pressure gradient are:

$$\left(\frac{\Delta p}{\Delta L}\right)_{vs} = \frac{\rho \cdot V_{vs}^2 \cdot f_{vs}}{2 \cdot D}\,, \ \left(\frac{\Delta p}{\Delta L}\right)_{ls} = \frac{\rho_l \cdot V_{ls}^2 \cdot f_{ls}}{2 \cdot D} \ \text{ and } \ \left(\frac{\Delta p}{\Delta L}\right) = \psi_v^2 \cdot \left(\frac{\Delta p}{\Delta L}\right)_{vs} \tag{21}$$

$$\text{where } \ \psi_v = \sqrt{1 + C \cdot \phi + \phi^2}\,, \ \phi = \frac{\left(\dfrac{\Delta p}{\Delta L}\right)_{ls}}{\left(\dfrac{\Delta p}{\Delta L}\right)_{vs}} \ \text{ and } C = 5.0 \tag{22}$$

6. NUMERICAL RESULTS

The regenerative cycle, shown in Figure 3, is used to analyze the output variables. In this thermal cycle, the nodes upstream and downstream of each component are randomly chosen.
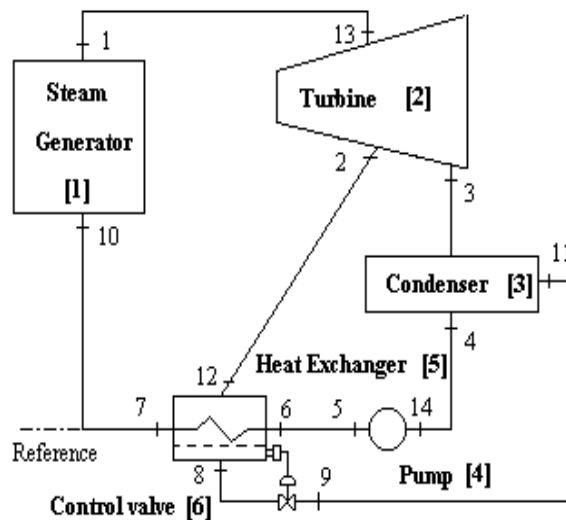

Figure 3 - Regenerative Cycle.

The Figure 4 shows the input data file for the cycle shown in the Fig. 3.

```
14 6 6

2  2  1E6  3  0.005E6
3  1  600  7  90  5  33
2  8  0  4  0

5  4  4  3  0  0  0  -1  -1  5  3  0  5  0

7  10  0.2  500  0  1E-5
5   6   0.2  500  0  1E-5
9  11  0.2  10   0  1E-5
2  12  0.2  15   0  1E-5
1  13  0.2  15   0  1E-5
4  14  0.2  15   0  1E-5

0.9  0  3E6  0  1  1  1
0.8  3E6  0  1  1  0  1
0  0  -3E5  0  1  1  1
9  5  233  10 232   20 231   30 230   40 225   50 220   60 210  70 190  85 157
0  0  0  0  1  1  1
0  0  0  1  1  1  0

10  1  1    13  2  2    13  3  2    6  7  5    12  8  5    14  5  4

11  4  3    3  4  3    8  9  6
```

Figure 4 - Input data file for the cycle of Fig. 3.

The thermodynamic properties of each node are shown in Tab. 3 and the heat transfer rate and the power at each component are shown in Tab. 4.

Table 3. Thermodynamic properties.

Node	p MPa	T [°C]	s [KJ/Kg°K]	h [MJ/Kg]	ρ [Kg/m^3]
1	1,4597	600,0	7,850537	3,693896	3,6472
2	1,0000	554,1	7,908870	3,596024	2,6345
3	0,0050	86,21	8,697066	2,661534	0,0301
4	0,0050	32,86	0,473967	0,137166	994,54
5	1,5289	33,00	0,476377	0,139222	995,33
6	1,5174	33,00	0,476379	0,139212	995,33
7	1,5174	90,00	1,191911	0,378140	965,96
8	0,9988	179,8	2,137333	0,762297	887,08
9	0,0081	41,74	2,460843	0,762297	0,2284
10	1,4597	90,00	1,191969	0,378103	965,93
11	0,0050	41,74	8,447971	2,577670	0,0344
12	0,9988	554,1	7,909395	3,596034	2,6315
13	1,3745	600,0	7,878890	3,694553	3,4327
14	0,0339	32,86	4,743293	0,137235	994,61

Table 4 - Rate of heat transfer and power.

Component	$\dot{Q}$ [Watts]	$\dot{W}$ [Watts]
1	7,67592x10^7	0
2	0	2,20902x10^7
3	-5,82745x10^7	0

The Table 5 shows the mass rate indexes, the mass rate and the upstream and downstream nodes.

Table 5 - Mass rate indexes.

Mass rate index, its value [ton/h] and upstream and downstream nodes [node$_u$ - node$_d$]					
1	83,34 [7 -10]	**6**	83,34 [4 - 14]	**11**	7,026 [12 - 8]
2	83,34 [5 - 6]	**7**	83,34 [10 - 1]	**12**	83,34 [14 - 5]
3	7,026 [9 - 11]	**8**	7,026 [13 - 2]	**13**	7,026 [11 - 4]
4	7,026 [2 - 12]	**9**	76,31 [13 - 3]	**14**	76,31 [3 - 4]
5	83,34 [1 - 13]	**10**	83,34 [6 - 7]	**15**	7,026 [8 - 9]

7. CONCLUSIONS

The present algorithm calculates the operation variables for any thermal system, as such, the new values for the variables when the system operation is modified.

The Newton-Raphson technique, while a bit more complex, is quite powerful. To large systems, the number of equations becomes so large that the *n* x *n* matrix needed for solving the equations requires excessive memory space in the computer. Techniques for solving linear simultaneous equations that have sparse matrices are called for. Another approach is to break the system apart into smaller subsystems, which can be simulated individually and their results tied together by successive substitution.

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