



## **A NEW COMPUTATIONAL ALGORITHM FOR THERMAL-HYDRAULICS ANALYSIS OF INDUSTRIAL PLANTS**

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***Abstract.** This work presents an original algorithm using a numerical solution scheme of a physical model representing the thermal-hydraulic behavior of an industrial plant. This model is described by one direction equation in the preferred flow direction. A homogeneous fluid slip model in thermal dynamic equilibrium is assured. The algorithm presents a totally implicit and iterative scheme in time, when no reverse flow occurs. It is recurrent in space, producing a marching algorithm in space. Results are presented for two test cases. The first one was compared to RELAP5/MOD3.2 results. The second case was compared to an analytical solution. Both results showed low absolute errors, no numerical diffusion and real time processing.*

***Key words:** Algorithm, Thermal-hydraulics, Numerical scheme*

### **1. INTRODUCTION**

The development of codes for thermal-hydraulic analysis of industrial plants is of paramount importance, primarily to assist safety analysis and to simulate physical process, thus allowing a better operational performance of the system. These codes generate thermal-hydraulics parameters of fluid flow from the solution of mathematical equations which describe the physical model representing the process to be simulated. These

parameters must be as close as possible to the desired result. Solution of these equations in differential form requires a great deal of computational effort, usually not compatible to the purpose of real time simulations. In view of this, numerical solution schemes have been proposed, that guarantee stability and convergence, reducing as much as possible numerical diffusion. Given the large effort in the development of computational tools and of numerical analysis methods, various thermal-hydraulic analysis codes have recently been made, showing new solution methods.

This work presents the numerical scheme of a new computational algorithm, which was motivated by the development of a code that would generate precise results in real time, as described in Lapa (1998).

The method presents, as an original characteristics, a numerical scheme fully implicit and iterative in time, as long as reverse flow does not occur, and recurrent in space. That is to say, cell parameters are calculated as a function of the previous cell, where they are already known, establishing a marching algorithm in space. This peculiarity warrants convergence and fast computation.

## 2. THE PHYSICAL MODEL

### 2.1 Homogeneous model with slip

We have adopted the homogeneous slip model in this work. This model assumes that liquid and vapor phases flow independently, with constant average velocities, not necessarily equal. It was assumed thermodynamic equilibrium between phases, although a simulation which relaxes this hypothesis has been presented by Singhal & Srikantiah (1991).

The slip velocity is obtained via algebraic equations expressed in terms of the relative velocity, which depends on empirically obtained factor. In this work, relative velocity is obtained by the drift mode, as described in Delhaye *et al.* (1981).

This model has the advantage of working with only three equations and yet produce satisfactory results. The modeling of the physical problem starts with one dimensional equations in the direction of preferential flow, as detailed below.

### 2.2 Local balance equations

The equations derived from the model are detailed in Lapa (1998). We note that this model assumes thermodynamic equilibrium and because of that, terms that represent volume changes are neglected, a valid assumption for moderate compressible process with subsonic velocities.

a) Mass conservation equation

$$\frac{\partial \hat{\rho}}{\partial t} + \nabla \cdot \left( \hat{\rho} \hat{u} \right) = 0 \quad (1)$$

b) Energy conservation equation

$$\frac{\partial}{\partial t} \left( \hat{\rho} \hat{H} - \hat{P} \right) + \nabla \cdot \left[ \hat{\rho} \hat{H} \hat{u} + \hat{\alpha} (1 - \hat{\alpha}) \left( \frac{\hat{\rho}_l \hat{\rho}_v}{\hat{\rho}} \right) (\hat{H}_v - \hat{H}_l) \hat{u} \right] = -\nabla \cdot \hat{q} \quad (2)$$

c) Momentum conservation equation

$$\frac{\partial}{\partial t} \left( \hat{\rho} \hat{u} \right) + \nabla \cdot \left[ \hat{\rho} \hat{u} \otimes \hat{u} + \hat{\alpha} (1 - \hat{\alpha}) \left( \frac{\hat{\rho}_l \hat{\rho}_v}{\hat{\rho}} \right) \hat{u} \otimes \hat{u} \right] = -\nabla \hat{P} + \nabla \hat{\tau} + \hat{\rho} \hat{g} \quad (3)$$

The following relations apply to Eqs. (1-3):

$$\begin{aligned} \hat{u}_{\sim R} &= \hat{u}_{\sim v} - \hat{u}_{\sim l} \quad , \quad \hat{\rho} = \hat{\alpha} \hat{\rho}_v + (1 - \hat{\alpha}) \hat{\rho}_l \quad , \quad \hat{\rho} \hat{H} = \hat{\alpha} \hat{\rho}_v \hat{H}_v + (1 - \hat{\alpha}) \hat{\rho}_l \hat{H}_l \quad , \\ \hat{u}_{\sim} &= \frac{\left( \hat{\alpha} \hat{\rho}_v \hat{u}_v + (1 - \hat{\alpha}) \hat{\rho}_l \hat{u}_l \right)}{\hat{\rho}} \quad , \quad H_v = H_v(P, T) \quad , \quad H_l = H_l(P, T) \quad (4.a-f) \\ \hat{\alpha} &\bullet \text{ void fraction,} \quad \hat{u}_{\sim R} \bullet \text{ slip velocity,} \quad \text{index : } v \bullet \text{ vapor, } l \bullet \text{ liquid.} \end{aligned}$$

The following simplifications are assumed: preferential flow directions, average values for areas and volumes of scalar quantities.

These local equations are substituted by equations with only one dimensional dependence, on the preferential hydraulic direction of flow and these equations are then spatially integrated using the classical Divergence Theorem. The plant is then divided in to components and the spatial integration takes into account the geometric configuration of the plant. The one dimensional equations are valid on a local basis, to the right or to the left of the points of singularities (which indicate presence of a valve or pump), as described below.

### 2.3 Spatially integrated equations taking into account the presence of singularities

These equations present products of variables which must then be linearized, e. g., state equations. Linearization is performed using Taylor Series Expansion to first order, as shown in Lapa (1998). Index **k** means time step and index **n** indicates internal iteration for each time step, in case this iteration is derived.

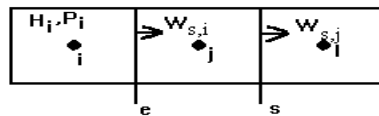


Figure 1 – representation of three consecutive components, each having one input/output (centered mesh)

a) Mass conservation equation

$$\begin{aligned} & \frac{\Delta T^k}{V_j} W_{s,j}^{k+1,n+1} + \frac{\partial \rho}{\partial H} \Big|_{(H_j^{k+1,n}, P_j^{k+1,n})} H_j^{k+1,n+1} + \frac{\partial \rho}{\partial P} \Big|_{(H_j^{k+1,n}, P_j^{k+1,n})} P_j^{k+1,n+1} = (\rho_j^k - \rho_j^{k+1,n}) + \\ & = \frac{\partial \rho}{\partial H} \Big|_{(H_j^{k+1,n}, P_j^{k+1,n})} H_j^{k+1,n} + \frac{\partial \rho}{\partial P} \Big|_{(H_j^{k+1,n}, P_j^{k+1,n})} P_j^{k+1,n} + \frac{\Delta T^k}{V_j} (W_{s,i}^{k+1,n+1} - G_j^{k+1,n}) \end{aligned} \quad (5)$$

$G_j = G_j(H_j, P_j)$  is the term that accounts for the possible leaks in component **j**. This term is obtained via empirical relations as shown in Mc Fadden *et al* (1998).

$V_j \rightarrow$  volume of component **j**.

b) Energy conservation equation

$$\begin{aligned} & \frac{V_j}{\Delta T^k} \left( \rho_j^{k+1,n} + \frac{\partial \rho}{\partial H} \Big|_{(H_j^{k+1,n+1}, P_j^{k+1,n+1})} H_j^{k+1,n} \right) H_j^{k+1,n+1} - \sum_{\substack{s,j \\ W_{s,j} < 0}} W_{e,j}^{k+1,n+1} H_l^{k+1,n} + \\ & + \frac{V_j}{\Delta T^k} \left( 1 - \frac{\partial \rho}{\partial P} \Big|_{(H_j^{k+1,n+1}, P_j^{k+1,n+1})} H_j^{k+1,n} \right) P_j^{k+1,n+1} - \sum_{\substack{e,j \\ W_{e,j} \geq 0}} (H_j^{k+1,n} W_{e,j}^{k+1,n+1}) \\ & + \sum_{\substack{s,j \\ W_{s,j} \geq 0}} (H_j^{k+1,n} W_{s,j}^{k+1,n+1} + W_{s,j}^{k+1,n} H_j^{k+1,n+1}) = Q_j^{k+1,n+1} + \frac{V_j}{\Delta T^k} (\rho_j^k H_j^k - P_j^k) + \\ & + \sum_{\substack{s,j \\ W_{s,j} \geq 0}} (H_j^{k+1,n} W_{s,j}^{k+1,n} - H W_{s,j}^{k+1,n}) - \sum_{\substack{s,j \\ W_{s,j} < 0}} THB_{s,l}^{k+1,n} + H_j^{k+1,n} G_j^{k+1,n} \\ & + \frac{V_j}{\Delta T^k} \left[ \frac{\partial \rho}{\partial H} \Big|_{(H_j^{k+1,n+1}, P_j^{k+1,n+1})} (H_j^{k+1,n})^2 + \frac{\partial \rho}{\partial P} \Big|_{(H_j^{k+1,n+1}, P_j^{k+1,n+1})} P_j^{k+1,n} H_j^{k+1,n} \right] + \\ & + \sum_{\substack{e,j \\ W_{e,j} \geq 0}} (W_{e,j}^{k+1,n} H_i^{k+1,n} + H W_{e,j}^{k+1,n} + THB_{e,i}^{k+1,n}) + \sum_{\substack{e,j \\ W_{e,j} < 0}} (H_j^{k+1,n} W_{e,j}^{k+1,n} + H W_{e,j}^{k+1,n}) \end{aligned} \quad (6)$$

c) Momentum conservation equation

The concept of staggered mesh applied to the momentum conservation equation was reformulated in order to include the component ahead of the component being analysed. This idea can be better explained by referring to figure 2.

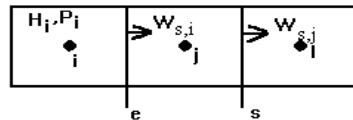


Figure 2 – component with only one input and one output

The momentum conservation equation becomes:

$$\begin{aligned} & \left( -A_{e,j}^k W_{e,j}^{k+1} - B_i^k W_i^{V,k+1} \right) - P_i^{k+1} + P_j^{k+1} + B_j^k W_j^{V,k+1} + b_{e,j}^k + \\ & + \beta_{e,l} \left[ -P_j^{k+1} - B_j^k W_j^{V,k+1} - b_{e,l}^k + A_{e,l}^k W_{e,l}^{k+1} + B_l^k W_l^{V,k+1} \right] = 0 \end{aligned} \quad (7)$$

where the real number  $\beta_{e,l}$  was introduced as an optimization parameter, in order to the marching matrix be as well conditioned as possible.

$$\begin{aligned} A_{e,j}^{k+1,n} &= \frac{L_{i,s} + L_{j,e}}{A_{e,j} \Delta T^k} (1 + T_e^{k+1,n}) + \left[ \frac{-(\varrho_j^{k+1,n} - \varrho_i^{k+1,n})}{(\varrho_j^{k+1,n} A_{e,j})^2} + 2 \left( \frac{C_{e,j}}{\varrho_{e,j}} \right)^{k+1,n} \right] |W_{e,j}^{k+1,n}|, \\ B_j^{k+1,n} &= \frac{(W_j^v)^{k+1,n}}{\varrho_j^{k+1,n} [(A_j^v)^{k+1,n}]^2}, \quad B_i^{k+1,n} = \frac{(W_i^v)^{k+1,n}}{\varrho_i^{k+1,n} [(A_i^v)^{k+1,n}]^2}, \\ b_{e,j}^{k+1,n} &= \frac{1}{2} \left[ \frac{[(W_j^v)^{k+1,n}]^2}{\varrho_j^{k+1,n} [(A_j^v)^{k+1,n}]^2} - \frac{[(W_i^v)^{k+1,n}]^2}{\varrho_i^{k+1,n} [(A_i^v)^{k+1,n}]^2} \right] + \left( \frac{C_{e,j}}{\varrho_{e,j}} \right)^{k+1,n} |W_{e,j}^{k+1,n}| W_{e,j}^{k+1,n} + T_{v_R,e}^{k+1,n} - T_{v_R,s}^{k+1,n} + \\ & + g \left[ (Y_i - Y_j) + (HEAD_{e,j})^{k+1,n} \right] \varrho_{e,j}^{k+1,n} - \frac{(\varrho_j^{k+1,n} - \varrho_i^{k+1,n})}{2(\varrho_{e,j}^{k+1,n} A_{e,j})^2} |W_{e,j}^{k+1,n}| W_{e,j}^{k+1,n} + \frac{(L_{i,s} + L_{j,e})}{A_{e,j} \Delta T^k} W_{e,j}^{k+1,n} \end{aligned} \quad (8.a-d)$$

Note that the term  $\Delta T$  in the denominator of the expression for the input flow of component “i” ( $W_{e,i}$ ), is identical to the output flow rate of component “j” ( $W_{s,j}$ ). Numerical results were obtained supposing a  $\beta_{e,l}$  value in the range 1 - 2, in such a way that, depending on the flow conditions in the previous time step, the coefficient in  $W_{s,j}$  be greater than the coefficient in  $W_{s,i}$ . The value  $\beta_{e,l} = 1,5$  gave the best results for the tests done. Determination of  $\beta$  optimum will be done in future work.

### 3. PROPOSED ALGORITHM

#### 3.1 Marching scheme on hydraulic segment

One can observe that the output variables of the component “i”, preceding the component being analysed are identical, that is:  $W_{e,j}^{k+1,n+1} = W_{s,i}^{k+1,n+1}$ ,  $A_{e,j} = A_{s,i}$ .

Once the balance equations are deduced for a node **j**, one can make a matrix representation for this node as follows:

$$M_j X_j = b_j \quad (9)$$

It should be noted, on the independent terms, the presence of variables:  $W_{e,i}^{k+1,n+1}$ ,  $W_{s,i}^{k+1,n+1}$ ,  $H_i^{k+1,n+1}$  e  $P_i^{k+1,n+1}$ . However, applying mass conservation to volume “i”:

$$\begin{aligned}
W_{e,i}^{k+1,n+1} = & W_{s,i}^{k+1,n+1} + \frac{V_i}{\Delta T_k} \left\{ \frac{\partial \rho}{\partial H} \Big|_{(H_i^{k+1,n}, P_i^{k+1,n})} H_i^{k+1,n+1} + \frac{\partial \rho}{\partial P} \Big|_{(H_i^{k+1,n}, P_i^{k+1,n})} P_i^{k+1,n+1} \right\} + \\
& - \frac{V_i}{\Delta T_k} \left\{ (\rho_i^k - \rho_i^{k+1}) + \frac{\partial \rho}{\partial H} \Big|_{(H_i^{k+1,n}, P_i^{k+1,n})} H_i^{k+1,n} + \frac{\partial \rho}{\partial P} \Big|_{(H_i^{k+1,n}, P_i^{k+1,n})} P_i^{k+1,n} - G_i^{k+1,n} \right\}
\end{aligned} \tag{10}$$

It is possible to eliminate the flow rate  $W_{e,i}^{k+1,n+1}$  and thus rewrite node **j** system as

$$M_j X_{\sim j}^{k+1,n+1} = B_j Y_{\sim i}^{k+1,n+1} + f_{\sim j}^{k+1,n} \tag{11}$$

The system described by Eq. (11) is a 4x4 system, where each line represents, respectively, equation of mass conservation, energy conservation, momentum conservation and continuity of mass flow rates at component interfaces. This system leads to a marching scheme, once the terms associated with previous component are known. But this does not happen. In this form, the equations for conservation of mass, energy and momentum are linearized and the pressure associated with next component is taken at previous time step, as it happens also to the output flow rate of the same component. This loss of implicit character of the algorithm is regained by iterating on the linearized equations, and the starting values of previous time step. This assures that the starting point is as close as possible of the real value. With the iteration matrix being fixed during iteration for each fixed “n”, the system can be represented by:

$$A^k \text{col} [W_{s,j}^{k+1,n} \ H_j^{k+1,n} \ P_j^{k+1,n} \ W_{e,j}^{k+1,n}] = B^k \text{col} [W_{s,j-1}^{k+1,n} \ H_{j-1}^{k+1,n} \ P_{j-1}^{k+1,n} \ W_{e,j-1}^{k+1,n}] + \tilde{b}^{0,k} + \tilde{b}^{1,k+1,n} \tag{12}$$

When there is no reverse flow, the scheme is totally implicit. When reversion of flow occurs, stability is lost and a Courant number based time step control is triggered. Also, when the iterative process used to recover implicitness is diverging, the time step is halved and the whole process is reinitialized for a new time step.

Via system triangularization, vector  $X_j^{k+1,n}$  is made explicit, and one associates cell “i” to “j-1”. Then, considering two consecutive cells “j” and “j+1”, one has:

$$X_{\sim j+1}^{k+1,n+1} = D_{j+1} Y_{\sim j}^{k+1,n+1} + G_{\sim j+1}^{k+1,n} \tag{13}$$

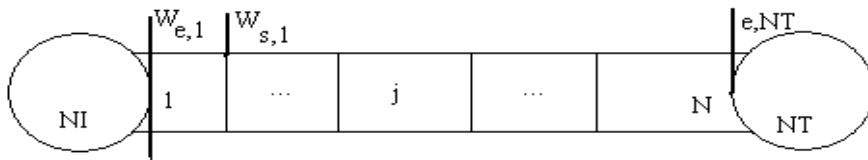


Figure 3 – hydraulic segment starting at node “NI” ending at node “NT”

The hydraulic segment represented in figure 3 is subdivided into components, numbered in sequential order. The starting segment is node component 1.

Thus, the system represented by Eq. (13), when applied to cell 1, becomes:

$$\begin{bmatrix} W_{s,j}^{k+1,n+1} \\ H_j^{k+1,n+1} \\ P_j^{k+1,n+1} \\ W_j^{k+1,n+1} \end{bmatrix} = \begin{bmatrix} C_j^{1,1} & C_j^{1,2} & C_j^{1,3} & C_j^{1,4} \\ C_j^{2,1} & C_j^{2,2} & C_j^{2,3} & C_j^{2,4} \\ C_j^{3,1} & C_j^{3,2} & C_j^{3,3} & C_j^{3,4} \\ C_j^{4,1} & C_j^{4,2} & C_j^{4,3} & C_j^{4,4} \end{bmatrix} \begin{bmatrix} W_{s,1}^{k+1,n+1} \\ H_1^{k+1,n+1} \\ P_1^{k+1,n+1} \\ W_{e,1}^{k+1,n+1} \end{bmatrix} + \begin{bmatrix} F_{W_s}^{k+1,n+1} \\ F_H^{k+1,n+1} \\ F_P^{k+1,n+1} \\ F_{W_e}^{k+1,n+1} \end{bmatrix} \quad (14)$$

Once the conditions at node N1 are known, which is treated as implicit, and applying the previous equation for  $j = 1$ , one has:

$$\begin{aligned} C_1^{1,1} = C_1^{2,2} = C_1^{3,3} = C_1^{4,4} = 1 \quad \text{and} \\ C_1^{1,2} = C_1^{1,3} = C_1^{1,4} = C_1^{2,1} = C_1^{2,3} = C_1^{2,4} = C_1^{3,1} = C_1^{3,2} = C_1^{3,4} = C_1^{4,1} = C_1^{4,2} = C_1^{4,3} = 0 \end{aligned}$$

with  $C_j^{m,n}$  ;  $m, n = 1,2,3,4$ , for node  $(j+1) > 2$  given by numerical formulae as follows,

$$C_{j+1}^{m,n} = \sum_{z=1}^4 D_{j+1}^{m,z} C_j^{z,n} \quad \text{where } m, n = 1,2,3,4 \quad (15)$$

and the independent terms given by:

$$\begin{bmatrix} F_{j+1}^{W_s} \\ F_{j+1}^H \\ F_{j+1}^P \\ F_{j+1}^{W_{Se}} \end{bmatrix} = \begin{bmatrix} D_{j+1}^{1,1} & D_{j+1}^{1,2} & D_{j+1}^{1,3} & D_{j+1}^{1,4} \\ D_{j+1}^{2,1} & D_{j+1}^{2,2} & D_{j+1}^{2,3} & D_{j+1}^{2,4} \\ D_{j+1}^{3,1} & D_{j+1}^{3,2} & D_{j+1}^{3,3} & D_{j+1}^{3,4} \\ D_{j+1}^{4,1} & D_{j+1}^{4,2} & D_{j+1}^{4,3} & D_{j+1}^{4,4} \end{bmatrix} \begin{bmatrix} F_j^{W_s} \\ F_j^H \\ F_j^P \\ F_j^{W_s} \end{bmatrix} + \begin{bmatrix} G_{j+1}^{W_s} \\ G_{j+1}^H \\ G_{j+1}^P \\ G_{j+1}^{W_s} \end{bmatrix} \quad (16)$$

The described system has the characteristic of being implicit with respect to integration in time and also has the peculiarity of obtaining the information associated with the component “j”, referred to previous component “i”, at the same time step level of integration. This fact makes the marching scheme unique and accounts for its fast performance in obtaining the solution of the system.

Matrix  $D_{j+1}$  contains the variations in the thermal-hydraulic parameters, between a given control volume and the next one. Applying this fact successively, one obtains a recurrence relation, Eq. (15), which allows generating  $C_j^{m,n}$ . This matrix contains the relationship among successive components and so, the variables of interest for each cell of the hydraulic segment become functions of the starting node, which is implicitly treated. One should note that this matrix is calculated only once for each iteration, thus reducing drastically the calculation time and each iteration is “activated” to regain the implicit character of the method.

This “implicitness” of the scheme is only lost when reverse flow occurs at the output of the component of interest, as explained above, in view of the donor cell concept used in the energy equation. In this case the donor component becomes the next component to the component of interest, and variables yet to be known appear in the equations, which forces values of these variables at previous time step values to be taken, in order to avoid iteration.

To solve this problem, considering the system as linearized, one applies the principle of superposition.

#### 4. NUMERICAL EXPERIMENTS AND RESULTS

Plant number 1 – This loop contains a pump and a valve, which are considered as singularities in the horizontal plan.

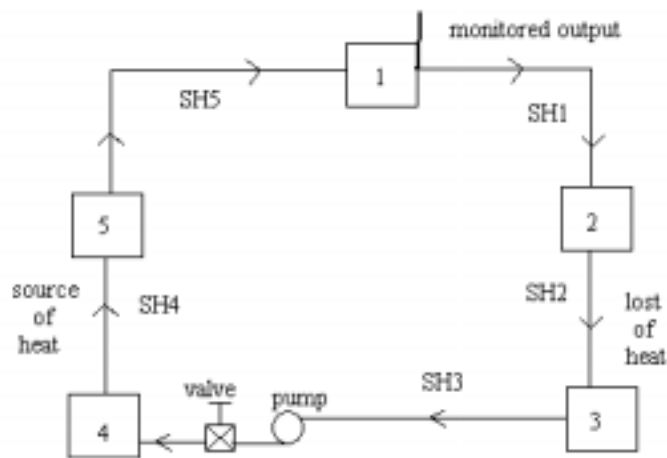


Figure 4 – plant number 1

a) Operational condition data

- nominal flow rate = 40,0 Kg/s
- nominal temperature = 240,0 °C
- nominal pressure = 1,20E+07 N/m<sup>2</sup>

- pump transient: pump suffers a motor torque change in 5,0s. This change can be described by a first order polynomial

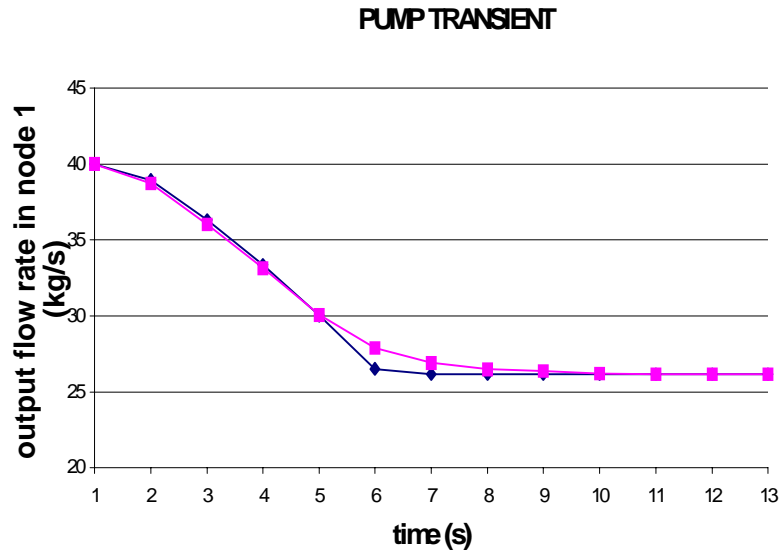
$$T = \begin{cases} At + B & \text{for } 0 \leq t \leq 5s \\ 5A + B & \text{for } t > 5s \end{cases}, \quad (7)$$

with  $A = -20,0 \text{ s}^{-1}$

Results for this case were compared to results from RELAP5/MOD3.2, as shown in Fig. 5.



b) Results for •  $t = 0,1s$  and 100 time steps (machine = 586DX / 166Hz / 64 Mb RAM)



- - NEW ALGORITHM (solution generation time = 9 s)
- - RELAP5/MOD3.2 (solution generation time = 140 s)

Figure 5 – power transient in plant number 1

Plant number 2 • open circuit, with 6 nodes, 3 pumps, 3 valves and 2 internal loops, as follows, in horizontal plan. The pump number 2 is closed. This case was chosen because an analytical solution is available for comparisons.

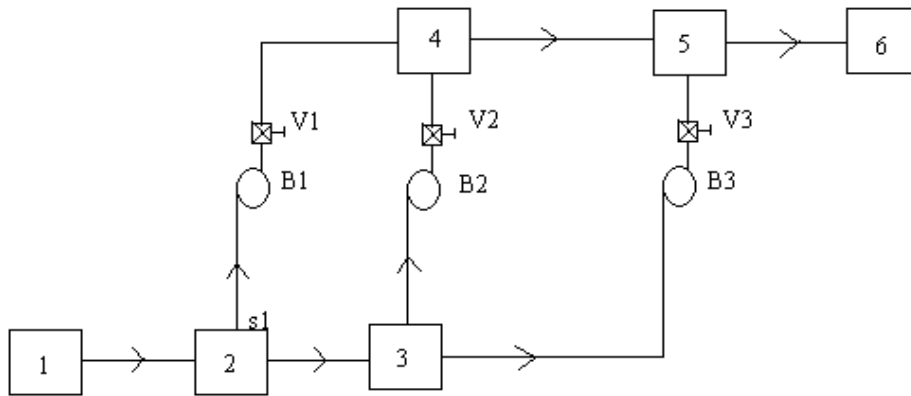


Figure 6 – plant number 2

a) Operational condition data

- nominal flow rate = 80 Kg/s
- nominal temperature = 270,0 °C
- nominal pressure = 1,45E+07 N/m<sup>2</sup>
- pressure loss coefficient of node 2 output **s1** = 3,0

Table 1 – plant number 2 results showing accuracy of the

<b>component</b>	<b>output flow rate (kg/s)</b> <b>• t = 0,1s</b>	<b>output flow rate (kg/s)</b> <b>• t = 0,01s</b>
Output 1 of node 2	39,998455	39,998533
Output 2 of node 2	40,001680	40,001608
Output of node 5 (output of internal loop)	80,000000	80,000047

#### 4. CONCLUSION

This new algorithm presents an original methodology to solve a complex thermal-hydraulic system. Its main characteristics are accuracy and fast solution generation, since the number of mathematical operation is much smaller than of other known algorithm. This allows development of real time simulators, with accuracy comparable to design codes.

The numerical results of plant number 1 were compared with the RELAP5/MOD3.2 code, confirming the accuracy of the scheme here proposed, as well as the fast solution generation. The numerical results of plant number 2 when compared with the exact analytical solution, obtained similar accuracy.

The novelty associated to the momentum equation,  $\beta$  weighting factor, introduces additional flexibility to be explored.

#### 5. SUGGESTION FOR FUTURE WORK

Extend the model to treat two phase flow with the 6 equation model to develop a complete thermal-hydraulic analysis code for industrial plants.

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