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CFD METHODS IN NATURAL CIRCULATION: SOME HISTORICAL ASPECTS BACKGROUND AND NUMERICS

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CFD METHODS IN NATURAL CIRCULATION: SOME HISTORICAL ASPECTS, BACKGROUND AND NUMERICS

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Abstract

This paper firstly summarizes some aspects of the early development of numerical techniques as applied to Fluid Dynamics, emphasizing work done in the last forty years. This is done in relation to nuclear installations or integral test facility experiments aimed at validating numerical models and techniques. Secondly, some theoretical aspects on numerical techniques formulation are introduced, aimed at giving a basis to the discussion of their application to natural circulation (NC) flow stability. Finally, a somewhat detailed introduction to the application of numerical techniques and computational fluid dynamics (CFD) in NC flows is presented in relation to installations of interest for Nuclear Energy.

Keywords: natural circulation, unstable flows, upwind differencing, stability, numerical diffusion and discretization

1. INTRODUCTION

This presentation is aimed at considering several aspects of numerical techniques giving the background to the computation of Fluid Dynamics as applied to the CFD of NC. It will be shown that there is plenty of consolidated literature and concepts on numerical methods since 30 years ago and that CFD is not a new activity in relation to NC and the thermal hydraulics of Nuclear Safety. In fact, many outstanding people contributed to this subject in the last decades. To justify this assertion, a brief account of early contributions is also presented. The present boom of CFD activity in NC and on separate effects in nuclear installations is a consequence of the needs of a re-emerging activity. In this way, Nuclear Safety benefits from well-developed techniques in other areas of computational mechanics. Although some spectacular CFD results may be found at thermal-hydraulics fora and in open (www) sources, not so many are already published in regular journals. Most publications deal with the needs and challenges posed by the physics and with clarifying the degree of detail required by nuclear safety.

It is useful to introduce two possible definitions in this context:

a) A numerical technique is an incremental (or discrete) way of representing a differential equation (that is part of a physical model in NC and,
b) CFD is a discipline that allows solving conservation equations using adequate discrete representations at a desired level of resolution, implying more than a numerical technique. CFD implies pre-processing to define the representation of the computational domain in discrete volumes and post-processing of the results obtained from the numerical technique adopted to show in different graphical ways the flow patterns and the scalar fields (like temperature and pressure).

Obviously, numerical techniques applications are not a new activity in relation to the thermal-hydraulics of all the flow stages of transients in nuclear installations (NC among others). In Authors´ view, it was the work at Los Alamos Scientific Laboratory, which, now more than 30 years ago in those days of "open" exchange of scientific information, opened the way to "widespread" numerical modeling in Fluid

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Dynamics. See, e.g. [1], summarizing work done up to 1981 at LANL. Many outstanding people contributed to this activity in the last forty years, however, again in Authors view, LANL pioneered in this subject and its most relevant people were: Francis H. Harlow, J. Fromm, C.W. Hirt, D.L. Liles, J. Mahaffy, A.A. Amsdem, J.R. Travis, J.P. Shanon, J. Pryor and B.J. Daly, among others. Perhaps, codes like PIC, MAC, SMAC, SOLA, SOLA-SURF, SOLA-DF, SOLA-VOF, SALE-3D, SOLALOOP, K-FIX, along with their detailed documentation, permitted some other people abroad the USA to contribute to the art. Freshpersons may be tempted to consider that the state of the art forty years ago was rather crude (instead of this, computers were not powerful enough), however contributions like the one by P. Roache [[2]] giving an important and comprehensive review and recommendations on numerical techniques and CFD by 1972, may solve this question. People at LLNL also contributed significantly by these years; see e.g. the papers by Noh [3] and Schulz [4]. Interested readers should browse the late 60´s and the 70´s issues of the Journal of Computational Physics. At the same time, other people pioneered in Europe, like B. Spalding, M. Wolfshtein and S. Patankar at Imperial College, R. Peiret at ONERA and many others. Some people that contributed to the development from the numerical analysis side will be mentioned in what follows, because the list is too long. The names of R. Courant, K.O. Friedrichs, D. Hilbert, J. von Neumann, P.D. Lax, R.D. Richtmyer, G.I. Marchuk (in Russia) and W.F. Ames must also be mentioned. It must be stressed that the Finite Element Method was starting to be applied to solve the Navier-Stokes equations. From the physical point of view, the Drift-Flux theory of two-phase flow, as developed by Zuber and Findlay in 1956 and by M. Ishii in his 1975 book, was the two-phase fluid model that allowed generating results of Nuclear Safety significance through its implementation in the TRAC code and other hydrodynamics codes at LASL. Many other people contributed significantly in this field, like J.M. Delhaye, N. Zuber, R. Lahey, M. Giot, F.H Moody, G.B. Wallis, R.E. Henry, J.A. Bouré, D.C. Groeneveld, G. Yadigaroglu and simply too many others to be cited here.

Before continuing, an appropriate conceptual excerpt from [[5]] may be introduced here: "In as much as we can simulate reality, we can use the computer to make predictions about what will occur in a certain set of circumstances… …Finite-difference techniques can create an artificial laboratory for examining situations which would be impossible to observe otherwise, but we must always remain critical of our results... …Finite differencing can be an extremely powerful tool, but only when it is firmly set in a basis of physical meaning. In order for a finite-difference code to be successful, we must start from the beginning, dealing with simple cases and examining our logic each step of the way." The importance of this assertion must be emphasized today, given the advancement of CFD applications and the relatively easy access to sophisticated CFD tools. The philosophy of merging physical intuition and numerical properties has been always inspiring for CFD practitioner and code developers. This tradition still persists and a recent example may be found in [6].

Two examples of different scales of space and time scale resolution, published more than 25 year ago, will be shown in what follows, aimed at demonstrating the origin of the techniques and its propagation. The first one is taken from [7], showing the results of a LBLOCA, computed using 13500 computing cells and a two-fluid model, as implemented in the SALE-3D code. The second one is taken from [8], considering NC flow in a container partially filled with a solid and computed with far more modest resources that allowed 1331 fluid computing cells with an in-house developed code that was a SOLA extension to 3D.

In the following paragraphs it will be evident that the main interest will be on one-dimensional (1D) NC flows. Then, it is on interest pointing out the need of making efforts in the appropriate modelling of 1D flows fluid dynamics. This may seem a somewhat old-fashioned proposal at this time, when multidimensional CFD modelling governs the trends in the analysis of NC and separate effects in Nuclear Safety related issues. It also seems that the application of CFD to NC has at least two decades of delay with regard to other fields in computational mechanics.
The reason for this delay may be because:

a) Scaling laws usually "force" to almost 1D integral test facilities representations of real life installations, with pre-established flow patterns;
b) A huge effort was focused on the development of a representative physical data base (amenable to 1D analysis) and separate effects on the other side (like plume analysis, non-symmetric flow distribution, particular aspects of reactor components behavior, etc.) affordable through detailed computational techniques;

c) Code assessment for safety analysis also imposed and still imposes a great effort for 1D;
d) Time scales to solve problems in realistic way (as a compromise between cell Courant number limitation for fast transients using semi-implicit methods and time inaccuracies, i.e. damping, for implicit methods impose large number of time steps to span long time transients (e.g. in SBLOCAs);
e) Ill-posedness of the governing equations "precluded" the search for detailed convergence of solutions, leading to coarse grid computations and stabilization of flow solvers solutions by numerical means;
f) Computers were not fast, cheap and widely available and not too many were interested in paying for detailed analyses, neither were asking too much for them, given the nuclear industry stagnation.

There is another aspect that is somewhat redundant with the previous paragraph. As stated in [9], "Sometimes, scaling leads to the adoption of the 1-D approximation; this may, in turn, hide important aspects of the system physics. A simple example of this situation consists in keeping the height of the system unchanged to get the same buoyancy; then, if the system is scaled accordingly to the power/volume ratio, the cross section area of the volume will be reduced; this leads to a much smaller pipe diameter that makes the 1-D representation reasonable, at the cost of eliminating the possibility of fluid internal recirculation... ...A workaround for this situation is providing paths for recirculation, in the form of additional, interconnected components; however, this solution may impose the flow pattern in the system and the balance between these aspects is a challenge to any practitioner in natural circulation modelling".

In the Authors´ opinion 1D, thermal hydraulics system codes will be used at least for a decade or more, coupled with 3D modules for the core and/or for some specific components where separate effects analysis is the goal. Then, in the following paragraphs, some basic aspects of numerical techniques as applied to simple 1D problems of physical significance will be reviewed.

2. THE BASIS OF DISCRETE FORMULATIONS FOR CONSERVATION EQUATIONS

It is important to start with a general formulation of a discrete approximation of a parabolic problem, because it gives the basis for almost all discrete formulations of the Navier-Stokes equations. The approach to be followed is the classic one, as may be found in Marchuk [10] and in Mitchell and Griffiths [11]. The theory related to operators (linear ones, to be strict) may be found in classic books.

Let us assume that **L** is a linear differential operator relating a dependent variable **u** to the space coordinate **x** and time **t**. The linearity of **L** does not pose an essential limitation, due to the possibility of linearizing the problem. Considering a 1D problem is just for convenience.

Then, the differential problem may be formulated as follows:

$$\frac{\partial u}{\partial t} = L\left(t, x, \frac{\partial^k}{\partial x^k}\right) u, \quad k = 1, K \tag{1}$$

If u is expanded in terms a Taylor series around **t** in terms of a time increment **Δt**, then:

$$u(t+\Delta t, x) = u(t,x) + \frac{1}{1!}\frac{\partial u}{\partial t}\Delta t + \frac{1}{2!}\frac{\partial^2 u}{\partial t^2} + HOT \tag{2}$$

where HOT means terms of higher order in **Δt**. This is a two-level time discrete formulation, implying also that L is independent of t, a reasonable assumption for many practical applications.
Now, equation (2) may be written in operator form as:

$$u(t+\Delta t) = \exp\left(\Delta t \frac{\partial}{\partial t}\right) u(t,x) = \exp(\Delta t \cdot L)\, u(t,x) \tag{3}$$

Although typical of the finite differences method, equation (3) opens the way to all the different approximations for two-level time discretizations. For example, by a suitable operator pre-multiplication of equation (3), leads to:

$$\exp(-\frac{\Delta t}{2}\cdot L)\,u(t+\Delta t)=\exp(\frac{\Delta t}{2}\cdot L)\,u(t,x) \tag{4}$$

which is a time centered (Crank-Nicholson) approximation.

A fully implicit approximation may be obtained again by pre-multiplication of equation (3), in the form:

$$\exp(-\Delta t\cdot L)\,u(t+\Delta t)=u(t,x) \tag{5}$$

Another important aspect of the formulation shown as equation (3), is that it allows for considering problems in multidimensional space coordinates as a succession of 1D problems. Suppose for the moment that the space operator **L** may be written as the sum of three operators $\mathbf{L_1}$, $\mathbf{L_2}$, $\mathbf{L_3}$, each one depending on **x, y, z**. Then, taking for example equation (5), it may be written that:

$$\exp(-\Delta t\cdot L_1)\exp(-\Delta t\cdot L_2)\exp(-\Delta t\cdot L3)\,u(t+\Delta t)=u(t,x) \tag{6}$$

Equation (6) may be split by suitable definitions, in the sequence of 1D problems as follows:

$$\exp(-\Delta t\cdot L_1)\,u^{*} = u(t,x)$$

$$\exp(-\Delta t\cdot L_2)\,u^{**} = u^{*}$$

$$\exp(-\Delta t\cdot L_3)\,u(t+\Delta t) = u^{**}$$

This approach, of fully implicit type in time is known as D´Yakonov splitting technique and this and many other of similar types have been used since the mid of the 60´s. What is important to understand is that intermediate values do not necessarily coincide with the time interpolation of **u** at intermediate times. This subject will be resumed later when be considering general types of operators.

Now it becomes necessary to fix some ideas on the approximation of **L**. To accomplish this task, the approximations of [11] to space derivatives are in order.

Considering the expansion:

$$u(x\pm\frac{1}{2}\Delta x)=u(x)\pm\frac{1}{1!}\frac{\partial u}{\partial x}\frac{\Delta x}{2}+\frac{1}{2!}\frac{\partial^2 u}{\partial x^2}\frac{\Delta x^2}{4}+\cdots\ ,$$

and the definition of the centered space operator

$$\delta\left[u(x)\right]=\ u(x+\frac{1}{2}\Delta x)\text{ - }u(x-\frac{1}{2}\Delta x)\ ,$$

it follows that:

$$\frac{\partial u}{\partial x}=\frac{2}{\Delta x}\cdot\sinh^{-1}(\frac{\delta_x}{2})=\frac{1}{\Delta x}(\delta_x+\mathrm{HOT})$$

Then, considering now that (**Δt, Δx**) are constant along the plane (**t, x**) and **t=n·Δt; x = i· Δx**, equation (1) may be written in exact difference form as:

$$u_i^{n+1}=\exp\left[\Delta t\cdot L\left(i\cdot\Delta x,n\cdot\Delta t,\frac{2}{\Delta x}\cdot\sinh^{-1}(\frac{\delta_x}{2}),\left(\frac{2}{\Delta x}\cdot\sinh^{-1}(\frac{\delta_x}{2})\right)^2\right),\cdots\right]u_i^n \tag{7}$$

Please note that the power of an operator is understood as its iterative application. In equation (7), u_i^n is the exact value of **u(t+Δt, x+)**. All finite difference equations come from truncation of this expression.

DETAILED STUDIES OF REACTOR COMPONENTS

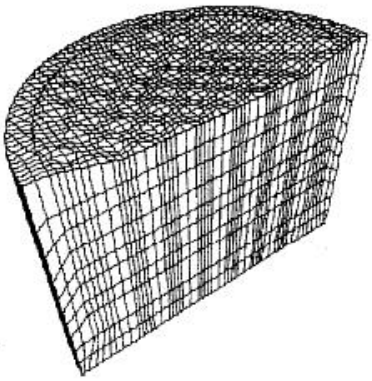


Fig. 7. Perspective view of the fluid-dynamics computing mesh for the upper plenum, which is created from a block of cells 52 cells wide, 26 cells deep, and 10 cells high. The front of the mesh lies on the symmetry plane that cuts through the midlines of the outlet pipes.

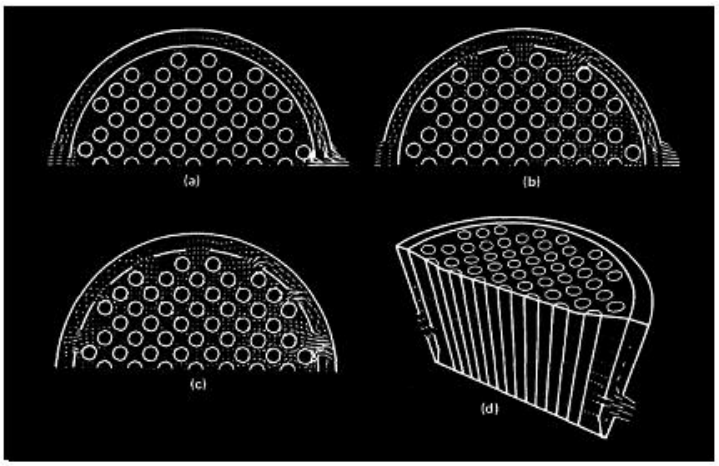
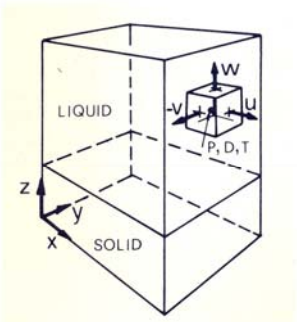


Fig. 8. Calculated velocity vectors showing the flow of water during a depressurization resulting from a break in the outlet pipe on the right. Shown are the vectors at (a) a horizontal level near the bottom of the outlet pipes, (b) at the horizontal level of the sets of three large holes in the plenum cylinder, (c) at the horizontal level of the sets of seven large holes in the plenum cylinder, and (d) across the vertical symmetry plane.

Figure 1 Early CFD results, relevant to LBLOCA studies, from [7]



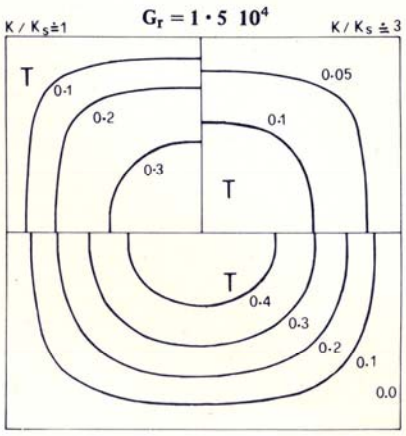


Fig. 6.– Composición de salidas de computadora en la interfase. (Composition of computer outputs for isotherms in the interface).

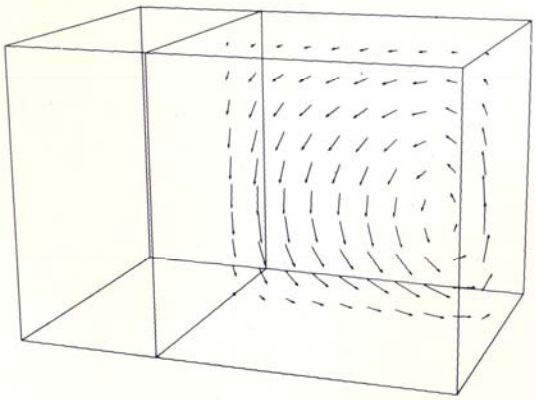


Fig. 3.– Gráfico de vectores velocidad para Gr = 1,5 × 10⁴, Pr = 3,5, t = 0,25, k_s/k = 1,05, para el recipiente en posición horizontal. Plano vertical y = 0,45. (Velocity vector plot for Gr = 1.5 × 10⁴; Pr = 3.5; t = 0.25; k_s/k = 1.05, for container in horizontal position. Vertical plane, y = 0.45).

Figure 2 Early CFD results, relevant to NC in a heated container, from [8]

In order to get practical working approximations in a computational plane, subdivided in a finite grid, equation (7) must be truncated to different orders of approximation. As Mitchell and Griffiths [11] point out, that there is no best way to obtain a difference equation. Many times the ones used are based on intuition and a desired property of the resulting scheme. A simple equation to illustrate the process of approximation is the heat transport equation. In this case, it may be written that:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \tag{8}$$

Then, equation (7) becomes:

$$u_i^{n+1} = \exp\left[\Delta t \cdot L\left(\alpha\left(\frac{2}{\Delta x} \cdot \sinh^{-1}\left(\frac{\delta_x}{2}\right)\right)^2\right)\right] u_i^n$$

Truncating this equation to first order, results:

$$u_i^{n+1} = \Delta t \cdot \left(1 + \Delta t \cdot \alpha \frac{4}{\Delta x^2} \cdot \frac{\delta_x^2}{4}\right) u_i^n = u_i^n + \Delta t \cdot \alpha \frac{\delta_x^2 u_i^n}{\Delta x^2}$$

Finally,

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{\delta_x^2 u_i^n}{\Delta x^2} \tag{9}$$

This is the simplest approximation to the heat diffusion equation, explicit in time and space, known as the finite difference Euler´s approximation to equation (8).

3. THE ORDER OF DISCRETE APPROXIMATIONS

In this paragraph, the concept of numerical (or artificial) viscosity will be introduced. The need to stabilize numerical solutions by artificial, numerical means was introduced by Von Neumann and Richtmyer in 1950 [12]. Many papers in the 60´s refer to this pioneering contribution as its sole reference. This implies both the originality of the papers themselves and the importance of [12]. In dealing with the problem of shock waves, said Authors introduced a non-physical, numerically dissipative term proportional to the gradients of the velocity, using it at the zones of large gradients and setting it to zero at "normal" zones.

The linear, 1D scalar advection-diffusion equation is paradigmatic in showing the effects of appropriate control of the truncation error of a discrete approximation. In coping with truncation error, it must be remembered that it is a necessary consequence of getting useful working approximations to conservation equations. Truncation error cannot be avoided in real life. For example, considering again Equation (9), it may be shown by Taylor´s series expansion around $t=n.\Delta t$, $x=n.\Delta x$ that it is an $\boldsymbol{O}(\Delta t, \Delta x^2)$ approximation to the original differential equation (8). Perhaps one of the more influencing papers in the clarification of the effects of truncation error is due to Hirt [13] in 1968. He introduced the concept that the equation really solved by the numerical scheme is the one obtained by adding the terms arising from the truncation error. The lowest order terms of the Taylor´s expansion must be the original differential equations. The remaining ones are the truncation error. Numerical consistency forces these additional terms tend to zero when the discretization intervals tend to zero in some way. Hirt was able to show how the additional terms of even order in Δx could lead to unphysical behavior, by assimilating these terms to the so-called "artificial viscosity" or "numerical viscosity" because they were proportional to some power of the space and time intervals. It is now interesting to consider explicitly the example of [13].
The linear advection-advection equation is:

$$\frac{\partial u}{\partial t} + C \cdot \frac{\partial u}{\partial x} = \alpha \frac{\partial^2 u}{\partial x^2} \tag{10}$$

If centered approximations are used for the space derivatives, then:

$$\frac{\partial u}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2} + C \cdot \frac{\partial u}{\partial x} = \alpha \frac{\partial^2 u}{\partial x^2} + O(\Delta t^2, \Delta x^2)$$

This is a hyperbolic equation, instead of the original parabolic one. The analysis of its domain of dependence and the need to keep a positive diffusion coefficient leads to the conditions needed to keep the solution stable, namely:

$$\alpha - C^2 \cdot \frac{\Delta t}{2} > 0 \qquad \frac{2\alpha}{\Delta t} \leq \left(\frac{\Delta x}{\Delta t}\right)^2 \tag{11}$$

Perhaps, the most interesting result for this equation comes from considering α=0 and using a non centered approximation for the space derivative. In this case:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -C \cdot \frac{u_i^n - u_{i-1}^n}{\Delta x}; \qquad C > 0 \tag{12}$$

Following the same procedure as before, it may be found that:

$$\frac{\partial u}{\partial t} + C \cdot \frac{\partial u}{\partial x} = \frac{C \cdot \Delta x}{2} \cdot \left(1 - \frac{C\Delta t}{\Delta x}\right) \cdot \frac{\partial^2 u}{\partial x^2} + O(\Delta t^2, \Delta x^2) \tag{13}$$

where:

$$C_{OU} = \frac{C \cdot \Delta t}{\Delta x}$$

is the cell Courant number. As may be observed in Equation (13), the diffusion coefficient comes directly from the discretization parameters and the advection velocity. Keeping this coefficient positive implies keeping the cell Courant number less or equal to unity. C_{OU}>1 implies that the fluid transverses more that a space interval (a computing cell) in one time interval. This is not allowed on physical grounds. Violating this condition leads to growing oscillations (physically sound growing oscillations!). In [13], the more important case of non-linear problems is analyzed in the same way. Some aspects of the two-dimensional case will be considered later.

The explicit time, centred space approximation given by (12) constitutes the "Forward time, upwind space" approximation to the scalar wave equation or, in short, the FTUS method. This is the simplest way to construct solutions in CFD. This is the usual approximation used in the CFD codes to stabilize calculations or to regularize ill-posed models like in RELAP5 [14], through the introduction of controlled numerical diffusion. Many other, quite sophisticated methods have been developed with this philosophy. The interested reader may consider the book by Laney [15]. Adequate discretization permits keeping low truncation error and allowing the computation of unstable flows.

The adequate treatment of truncation error has been show to allow the computation of solutions. It will be shown in what follows, this is a useful methodology to get linearized forms of the non-linear governing equations, with controlled truncation error. Important examples of this assertion may be found in [10]. In a practical case of direct application to Nuclear Safety, the SETS (for Stability-Enhanced, Two-Step) methodology [16] was developed to eliminate the C_{OU} limit restriction. On the same ground, one of the Authors (JCF and former collaborators) developed and applied a similar procedure to incompressible flows.

In what follows this will be exemplified, simply by showing how use this concept to linearize Burger´s like operators. Let:

$$\frac{\partial u}{\partial t} + L_1(u) + N(u) = 0$$

be the equation under analysis, where L1 is a linear operator and N is a nonlinear operator.

Let us assume that N is restricted to the form:

$$N(u) = L_2(u) \cdot A(u)$$

where $L_2(u)$ is linear in u and A is such that the algebraic problem resulting from the discrete approximation of the previous equations is also linear.

Burger's equation is a useful example; in this case:

$$A \equiv u, \quad L_1 = \frac{\partial^2}{\partial x^2}, \quad L_2 = \frac{\partial}{\partial x}$$

A Crank-Nicholson approximation may be written as:

$$\left[I + \frac{\Delta t}{2} L_1 + \frac{\Delta t}{2} A^* \cdot L_2 \right] U^{n+1} = \left[I - \frac{\Delta t}{2} L_1 - \frac{\Delta t}{2} A^* \cdot L_2 \right] U^n$$

where I is the identity operator and A* is an operator independent of time and a suitable approximation to A to be defined in what follows.

Expanding this expression in a Taylor series around n, we get:

$$\begin{aligned} & u + \Delta t \frac{\partial u}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 u}{\partial t^2} + \\ & + \frac{\Delta t}{2} L_1 + \frac{\Delta t}{2} A^* \cdot L_2 + \Delta t \cdot \frac{\Delta t}{2} \cdot \left[\frac{\partial L_1}{\partial t} + A^* \cdot \frac{\partial L_2}{\partial t} \right] + \\ & - u + \frac{\Delta t}{2} L_1 + \frac{\Delta t}{2} A^* \cdot L_2 = O\left(\Delta t^3\right) \end{aligned}$$

In order to obtain an estimation for we now ask: under which conditions is this equation an "exact", i.e., an $O(\Delta t^2, \Delta x^2)$ approximation to the solution of the original equation? The answer comes from subtracting the previous equation from the original one:

$$\frac{\partial u}{\partial t} + \frac{\Delta t}{2} \frac{\partial^2 u}{\partial t^2} + L_1 + A^* \cdot L_2 + \frac{\Delta t}{2} \cdot \left[\frac{\partial L_1}{\partial t} + A^* \cdot \frac{\partial L_2}{\partial t} \right] = O\left(\Delta t^2\right)$$

Derivation of the original differential equation and replacement leads to:

$$A^* \cdot L_2\left(u^{n+1/2}\right) = A\left(u^{n+1/2}\right) \cdot L_2\left(u^{n+1/2}\right)$$

Then,

$$A^* \equiv A\left(u^{n+1/2}\right)$$

which is the ***O***(2,2) expression searched. The numerical approximation to the intermediate time step may be obtained in different linear ways. Because of the CN formulation, terms involving additional diffusion terms do not arise. If A^* is evaluated as shown, then, the technique coincides with a predictor-corrector scheme based on the evaluation of "non-linear" coefficients evaluated at $t = n\Delta + \Delta t/2$. This result is well known. As may be observed from the above derivation, truncation error was used again in a convenient way.

4. THERE IS MORE THAN TRUNCATION ERROR…

In the previous paragraph, the order of some discrete approximations has been discussed. There is another aspect that deserves attention when the coupling and type of dependent variables perturbations governs the dynamics of the solution. Depending on the type of perturbation, the wave velocity of a given numerical scheme must be considered. The discrete wave velocity is the velocity that a wave packet moves with, in relation to the fluid velocity. It is well known that the degree or delay of density (or temperature) perturbations with respect to fluid velocity is key to the appearance of instabilities. One of the most important references in this subject is the review by Threfethen [17], who showed how this property of a numerical scheme affects the transport velocity of a signal as a function of wave number and the discrete (finite-differences) approximation. Figure 1 is an illustration considering the linear advection of a scalar with two different waveforms, namely a wave packet and a smooth Gaussian. In both cases, the transport velocity is C = 1, the space interval is $\mathbf{\Delta x}$ = 1./160, the Courant number is C_{OU} = 0.4 and the total time of integration is t = 2. The numerical scheme is LEAPFROG, defined by -perhaps- the simplest numerical scheme of order ***O***(2,2), i.e.

$$\frac{u_i^{n+1} - u_i^{n-1}}{2\Delta t} = -C\frac{u_{i+1}^{n} - u_{i-1}^{n}}{2\Delta x} \tag{14}$$

The analysis for this behavior is simple and comes from considering that numerical schemes transports waves packets composed of waves of different frequency and wavelength with different velocities. The speed of propagation of the waves is dependent of κ., where κ is the wave number. Define ω as the angular wave frequency. If λ is the wavelength, the resolution is defined as m=λ/Δx. Additionally, by definition: θ = 2π / m.

Defining the group velocity as:

$$C_G = \frac{d\omega}{d\kappa}$$

and replacing each term of (14) by $\exp(\omega t - \kappa x)$, e.g.:

$$U_{i-1}^{n+1} = e^{j\left[\kappa\cdot(x-\Delta x) - \omega\cdot(t+\Delta t)\right]}$$

then:

$$\frac{C_G}{C} = 1 - \frac{1 - C_o^2}{2}\cdot\theta^2 \tag{15}$$

Using Equation (15) and the above mentioned discretization, the waves should be transported from x = 0.5 to x = 2.5. As it may be observed, this is fairly confirmed for the Gaussian wave perturbation (in Figure 2, the transport of a smooth Gaussian is not affected by the group velocity) and not for the same signal modulated by a sine wave having wave number 125.7 and a wave resolution of 8 points per wavelength. In this case, the group velocity is nearly 0.74, what results in the wave packet transport from x = 0.5 to x = 2. This property is valid also for multidimensional systems.

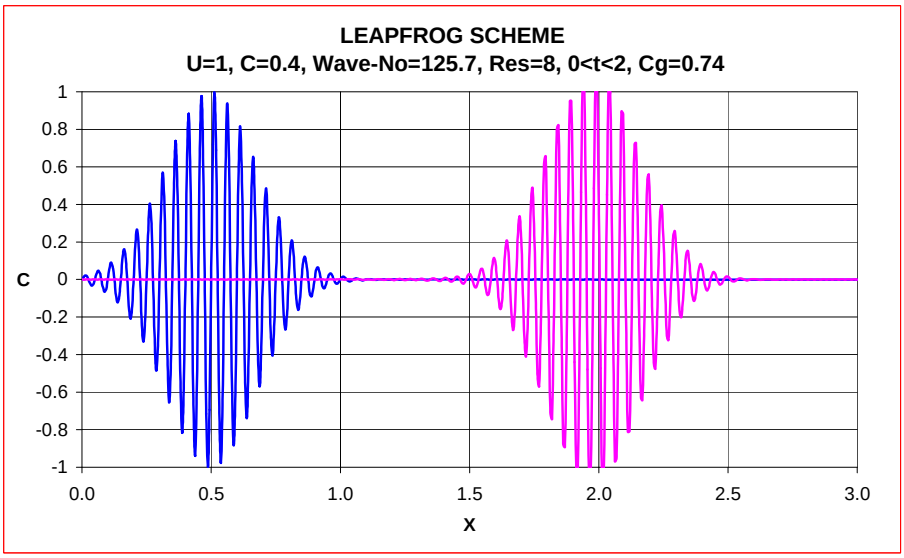


Figure 1 The transport of a wave packet under LEAPFROG

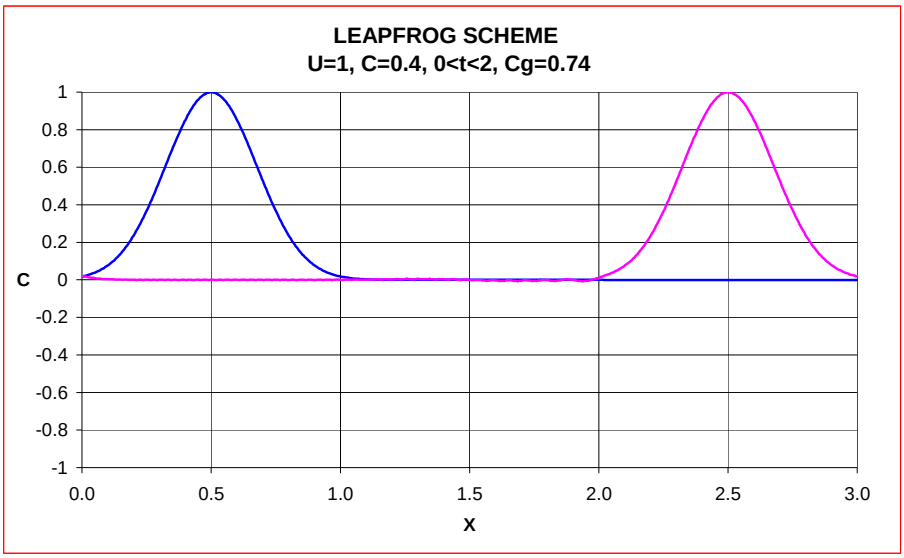


Figure 2 The transport of a smooth Gaussian wave under LEAPFROG

The above means that there is more than truncation error to be considered in assessing the quality of a solution. In fact, a simple conclusion is that the transport of the wave packet is correct, but its velocity (the group velocity) lags the phase velocity (that is also different from the fluid velocity) by 25%. Then, depending on the type of perturbations, there is a possibility of getting unexpected results regarding the computation of onset of instabilities of NC flows.

5. THE MEANING AND CONTROL OF NUMERICAL, NON-PHYSICAL SOLUTION OSCILLATIONS

In many cases of practical significance, the computed solution is stable but shows oscillations. Not necessarily, this is due to some intrinsic (physical) properties of the solution but, apart from being unexpected, these oscillations are spurious. The 1-D, linear, steady-state, advection-diffusion equation solution is another paradigmatic example of this. This equation may be written as:

$$P_e \cdot \frac{dU}{dx} - \frac{d^2U}{dx^2} = 0$$

$$U(0) = 0 \qquad U(1) = 1$$

were Pe is the Peclet number, defined as: Pe = C.L/α, where C is the advection velocity, L the length of the 1D domain and α is the mass diffusion coefficient. This equation constituted the so-called "though problem". Figure 5 shows the solution using centered differences for different Peclet numbers. Solid points indicate the exact solution. Hollow points indicate the exact, numerical, stable solution with non-growing oscillations. The oscillations (wiggles) are due to the non-appropriate boundary layer resolution at high Peclet numbers. Asymptotic analysis [18] or, more simply, introduction of upwinding eliminates the problem.

The existence of spurious oscillations in the solution of conservation equations may be the consequence of non-appropriate resolution of the boundary layer behavior of the solution, like in this case. Then, suppressing the oscillations may be non-conservative or, equivalently, allow computing a solution not showing all the important aspects of the physics. Work done in the 80´s served to clarify these aspects. P. Gresho at the LLNL contributed significantly to this subject. Perhaps, the most relevant reference in this subject was due to said Author [19]. However, an early discussion on the effects of discretization may be also be found in [13]. This last reference shows the effects of Δt in the incompressible flow of water under a sluice gate using the Marker and Cell (MAC) method and it is shown that the oscillations in the direction of the fluid velocity vectors can be attributed to the non-linear coupling of the momentum equations, particularly due to truncation errors involving velocity gradients. No upwinding was applied. Figure 6, taken from [13], illustrates these effects.

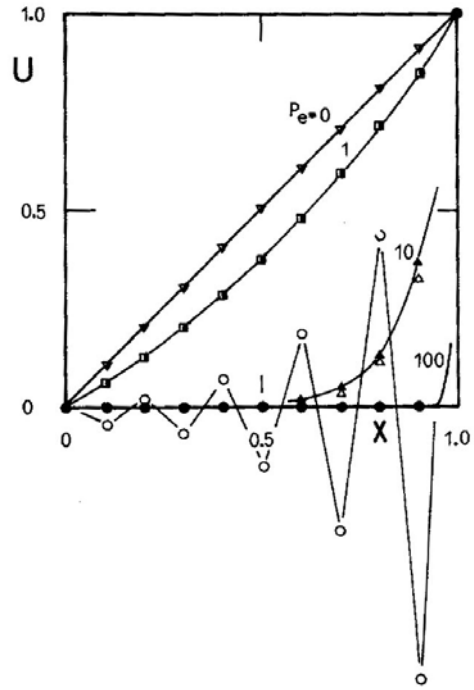


Figure 5 Spurious oscillations in the solution of the
1-D, linear, steady-state, advection-diffusion equation [18]

To conclude this paragraph it may be stated that non-growing oscillations in a computed solution may be an indication of non-appropriate discretization. Forcing their elimination may be a cause of losing information on the physics and at the same time, of making possible the calculation

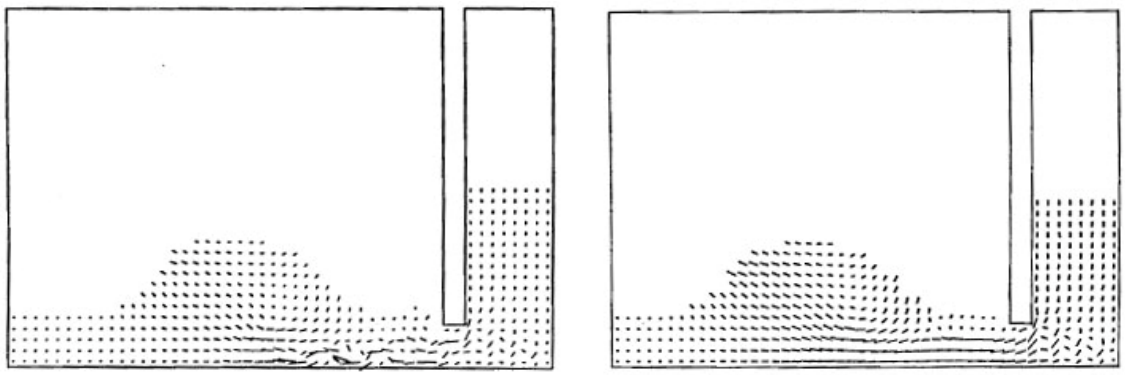


Figure 6a t=0.28 s, $\Delta t = 0.002$ s Figure 6b t=0.28 s, $\Delta t = 0.0001$ s

Figure 6 The effects of non-linear coupling in the solution of Navier-Stokes equations [13]

6. ONE-DIMENSIONAL vs MULTIDIMENSIONAL SIMULATIONS

In this paragraph, it will be considered why it is worth considering CFD approaches for CN, even in simple cases. This will be done through an example of how using well established, "natural" 1D laws in 1D TH loops leads to get non-conservative, wrong results. Later, it will be shown how to circumvent some difficulties associated with the use of 1D codes. The balance between pros and cons is left to the reader.

Let us consider the NC flow in a simple TH loop in unstable flow conditions, as analyzed in [20]. The loop [21], consists of a 23.2 mm I.D. glass pipe with rectangular layout see Figure 7, having 2.1 m vertical legs and equipped with 0.8 m long electrically heated and fluid cooled sections. The latter consists of a pipe-in-pipe heat exchanger, fed by relatively cold water, at prescribed flow rates.

The unstable test with a 420 W heater power will be consider for the sake of this paragraph purpose and the results were simulated using an in-house developed code and the thermal-hydraulics system code RELAP5. Based on previous experience, theoretical and experiments were expected to show the same trends. In order to assure coherence with the results obtained by the Authors of [21], the same friction relationship adopted in [22] was implemented in the in-house developed code TRANLOOP. It consists in taking the maximum out of the Poiseuille and the Colebrook-White relationships, resulting in a monotonous decreasing trend of the friction factor over the whole range of Reynolds numbers. In particular, in the case of smooth pipes, it results in assuming the transition from laminar to turbulent friction factor at a Reynolds number as low as about 1100.

The results obtained by TRANLOOP compared well with both the experimental measurements and the results of [22] using the ATHLET [23]code. In particular, the test case with 420 W heater power was found unstable with a period of flow reversal and amplitude of oscillations in temperatures similar to the ones observed in the experiment. This result was obtained making use of the low diffusion numerical scheme of [20] using both the “fine” and the “coarse” nodalization. On the other hand, in agreement with ATHLET, with the first order numerical scheme only the fine nodalization led to the prediction of unstable behavior, while the coarse one resulted in the calculation of stable conditions; this effect could be explained as a result of numerical diffusion. Figure 7 reports the trend calculated by TRANLOOP for loop flow, starting from a condition close to the steady-state and assigning an initial perturbation to flow rate.

In view of the good agreement obtained, it was decided to simulate the experiment using RELAP5. A somewhat detailed nodalization was set up. However, surprisingly enough, RELAP5 predicted a stable behavior for this condition. Given the similarity between the first order numerical method adopted in TRANLOOP and the semi-implicit scheme of RELAP5, when used for single-phase flow, it was not considered likely that the reason for such discrepancy could be a difference in the numerical diffusion introduced by the (similar) discretization. It was therefore hypothesized that this difference could be the result of the adoption of different friction laws in the two programs.

In order to verify this assumption, a calculation for the case with 420 W power was performed with TRANLOOP making use of the Churchill correlation [24], which has a more strict resemblance with the relationship adopted in RELAP5. In agreement with what was suspected, stable flow behavior was obtained just as it was observed in the corresponding RELAP5 calculation. This preliminary result stimulated a more systematic and in depth analysis of the problem, whose details may be found in [20].

Then, it was concluded that using the standard friction correlation, which considers in detail the transition from laminar to turbulent flow conditions, lead to stable NC flow conditions for this case operating in the transition Reynolds number regime. ***This result is non-conservative.*** Using the friction law as deduced from the experiments, lead to a correct prediction of flow conditions. Using appropriate closure correlations in NC simulations is a basic tenet. However, changing them may be not possible or not considered necessary. This is particularly true when there are not experiments to rely on or, more frequently, when designing a new experiment or installation.

Because of the above results, it was decided to apply a CFD approximation to predict the flow. It must be noted that, in this case, no macroscopic friction law is used in the CFD calculation. The CFD code chosen was FLUENT 6.0. A cross section of the grid adopted is shown in Figure 8. In total, the number of computing cells was in the order of 50000. The results obtained for this case are shown in Figure 9, that show the unstable behavior expected. In this sense, the use of the CFD approximation was rewarding.

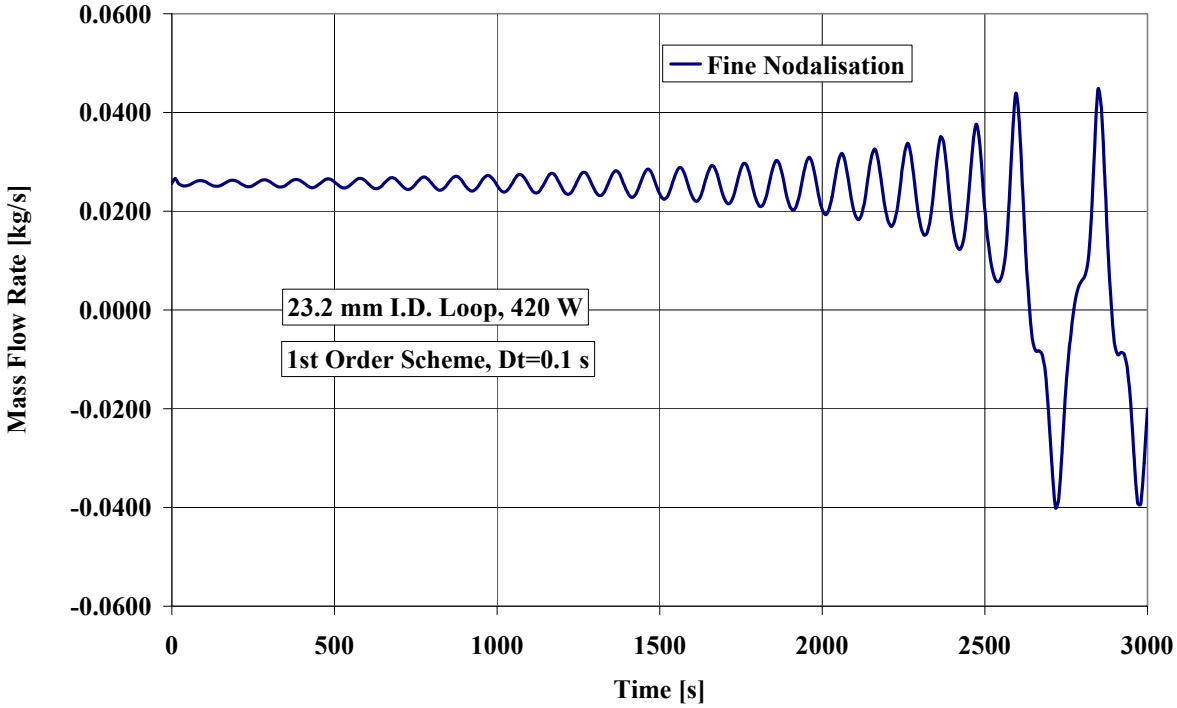


Figure 7 Results of a TRANLOOP calculation with the fine nodalization and the first order, FTUS scheme for the case with 420 W heater power, friction law as in [22]

It must be noted, nevertheless, that going from a simple 1D code to the CFD approximation implied using a three days of CPU time of CPU time in comparison with few minutes on the same PC. Figure 10 shows another evident advantage of the CFD approach: the degree of detail that can be obtained for the analysis of flow patterns. In this case, levels of flow velocity exemplify it. Relatively slow flow regions are shown in green following pipe bends.

In the case analyzed above, it is evident that the CFD code allowed recovering the physics, in the sense that instability is driven by fluid stratification in the horizontal heated pipe and it was correctly described.

Now it will be shown that this can be simulated using a 1D approximation too. In the penultimate paragraph of the introduction, it was suggested how to circumvent a situation like the one mentioned above using 1D codes. In [26], a detailed analysis of the behavior of NC loops with various heater-cooler configurations but similar in layout to the one in [20]. In this case, the different loop configurations were investigated, aimed at determining the stability behavior of the loop for different heating powers. In this case, the question of appropriate friction closure correlation was out of question. Figure 11 shows the comparison of the results from the experiment and the ones obtained using RELAP5 and TRANLOOP with converged discretizations in the particular case of 105 W of heating power. This Figure includes an insert showing the long term behavior of the solution as predicted by RELAP5, to be further discussed in what follows.

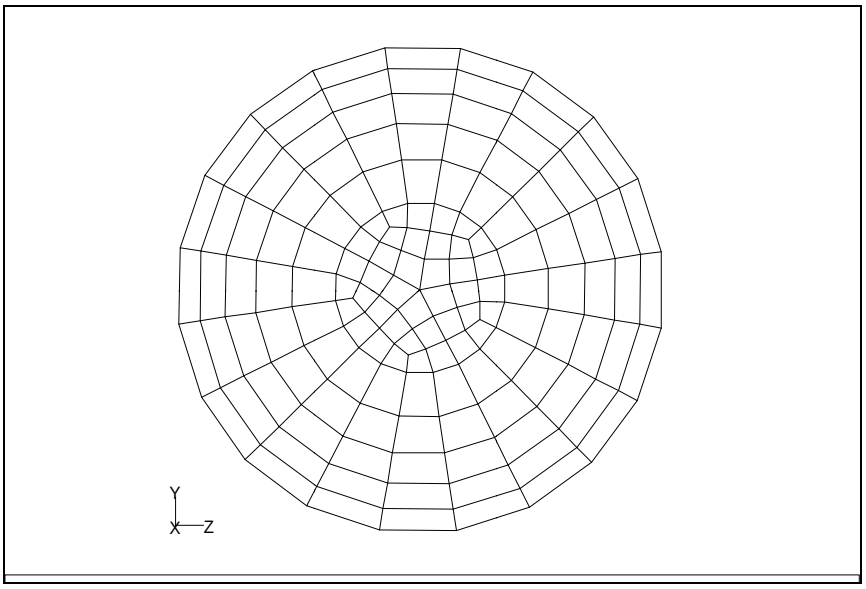


Figure 8 Sketch of the grid adopted in the FLUENT 6.0 calculations for loop cross section discretization

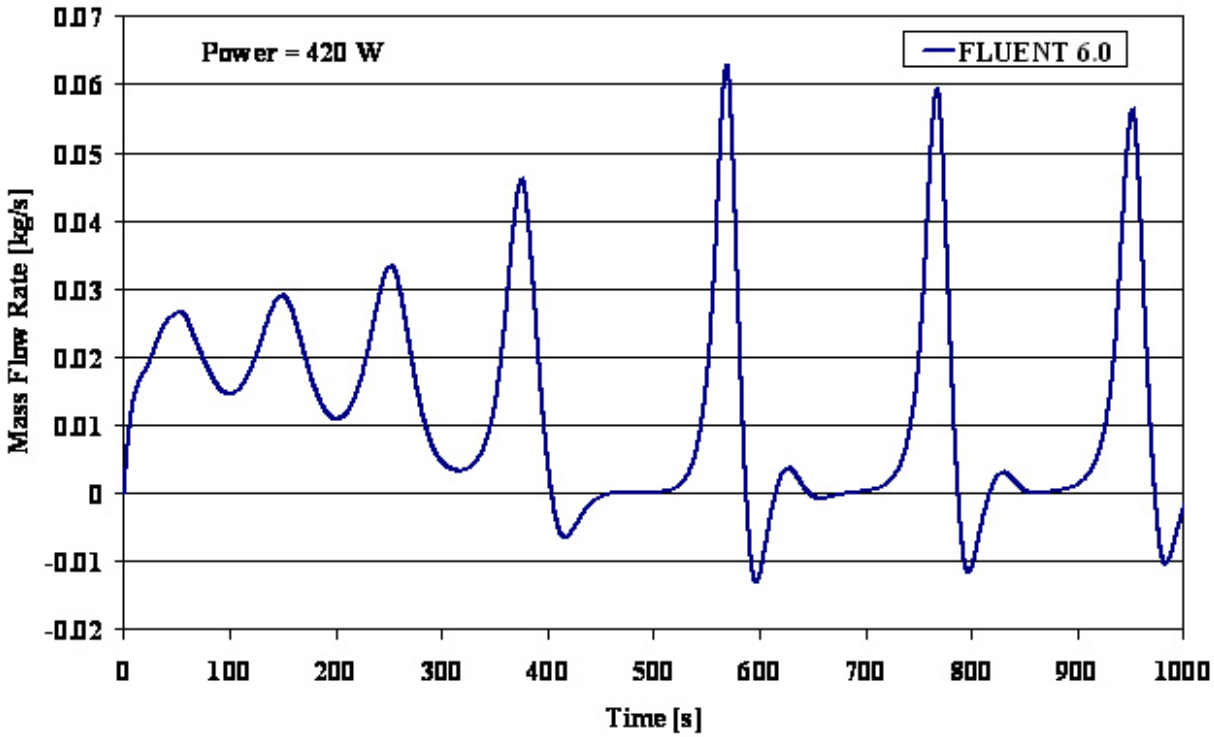


Figure 9 Transient results obtained by the FLUENT 6.0 code for the 420 W heater power case

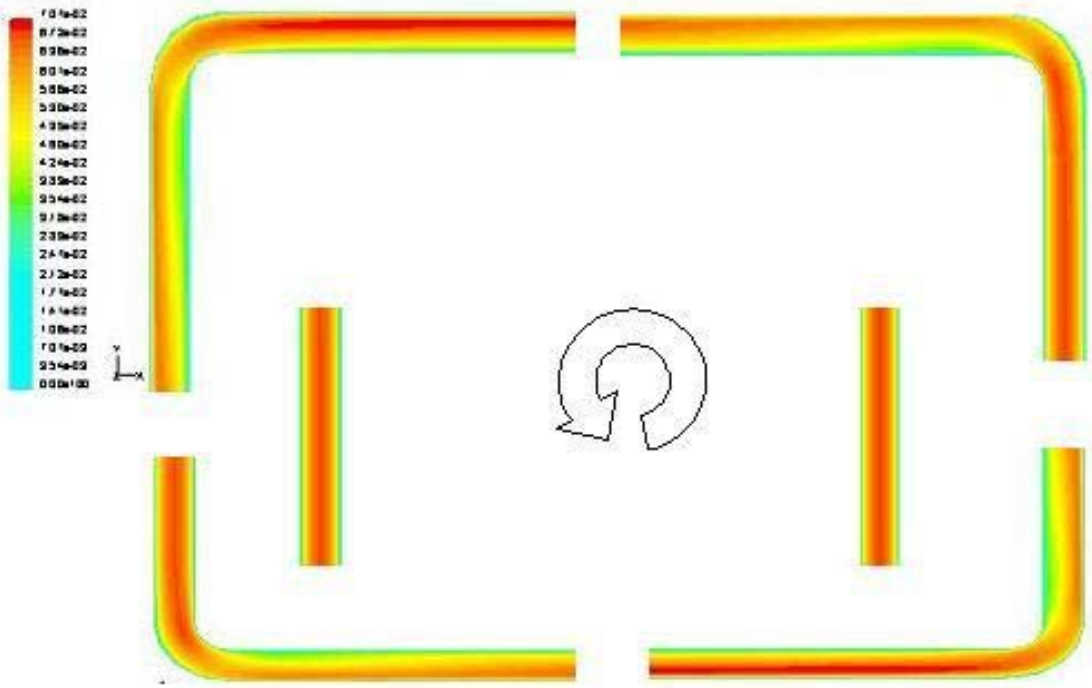


Figure 10 The distribution of steady-state velocity vectors magnitude, 420 W

As may be observed, after an initial correct trend prediction, the simulated cases lead to flow stagnation. Again, using a CFD approach, unstable behavior was recovered. In [26], this was discussed in the following terms: The phenomenon of plug formation and attraction to zero-flow condition can be identified in the predictions of both codes at low power. In fact, even if the calculations were performed starting from conditions relatively close to steady state ones in both cases, the flow stagnation sometimes observed after some of the flow reversals, due to the formation of the very hot plug of fluid when the flow vanishes, which will condition all the subsequent transient. In fact, while in TRANLOOP results, once reached the zero-flow condition, the loop circulation is not able to restart, in RELAP5 predictions subsequent flow pulses, much sharper than in the experimental data are observed. This difference was related only to the absence in TRANLOOP of any allowance for the simulation of voiding, occurring when the still fluid in the heater is heated up to the saturation temperature. It was also found that the pulses predicted by RELAP5 are due to void generation in the heater, not possible to be predicted if a Boussinesq fluid is assumed as in TRANLOOP. However, this pulsating mechanism shown by RELAP5 has nothing to do with the actually observed phenomenon; in fact, sub-cooled boiling at the heater surface was observed in this configuration at powers beyond 408 W.

The phenomenon of the attraction by the zero-flow condition occurred randomly in the one-dimensional simulations, showing that the mechanism for hot plug formation can be correctly predicted by one-dimensional codes, though the additional phenomena that restore flow conditions are not conveniently modelled. Occasionally, it was observed in some calculation cases that the flow stagnation could be avoided by fluid inertia, which maintained sufficient flow in the heater to avoid a too strong heating of the fluid plug. This was also suspected to be the reason for the incorrect prediction by TRANLOOP [20], leaving open the question of how to simulate it in a realistic way such oscillatory behaviour. Anyway, the question of attraction to fixed points in non-linear problems is complicated and out of the scope of the present discussion.

Using again a CFD approach, with detailed nodalizations of the heating zone (see Figure 12) the unstable flow condition was correctly simulated, as shown in Figure 13.

When possible, some intuitive remediation to the question of stratification and flow pattern may be considered. Figure 14 is an alternative nodalization of the heater pipe in the loop. As may be observed, the possibility of stratification and recirculation is allowed via cross-junctions between two parallel pipes

with half of the power in each one. The results obtained using RELAP5 are shown in Figure 15, where the unstable condition is recovered, even for less power. The evolution of fluid temperature shows how stratification and cross flows are correctly coupled. There is no claim here that all problems may be solved in this way, but experimental pool reactors have been also simulated in this way. It is left to the Safety Analyst to decide which level of detail is appropriate for a given specific problem. However, Engineering Judgment is mandatory in these cases and must carefully exercised. This aspect will be considered in what follows.

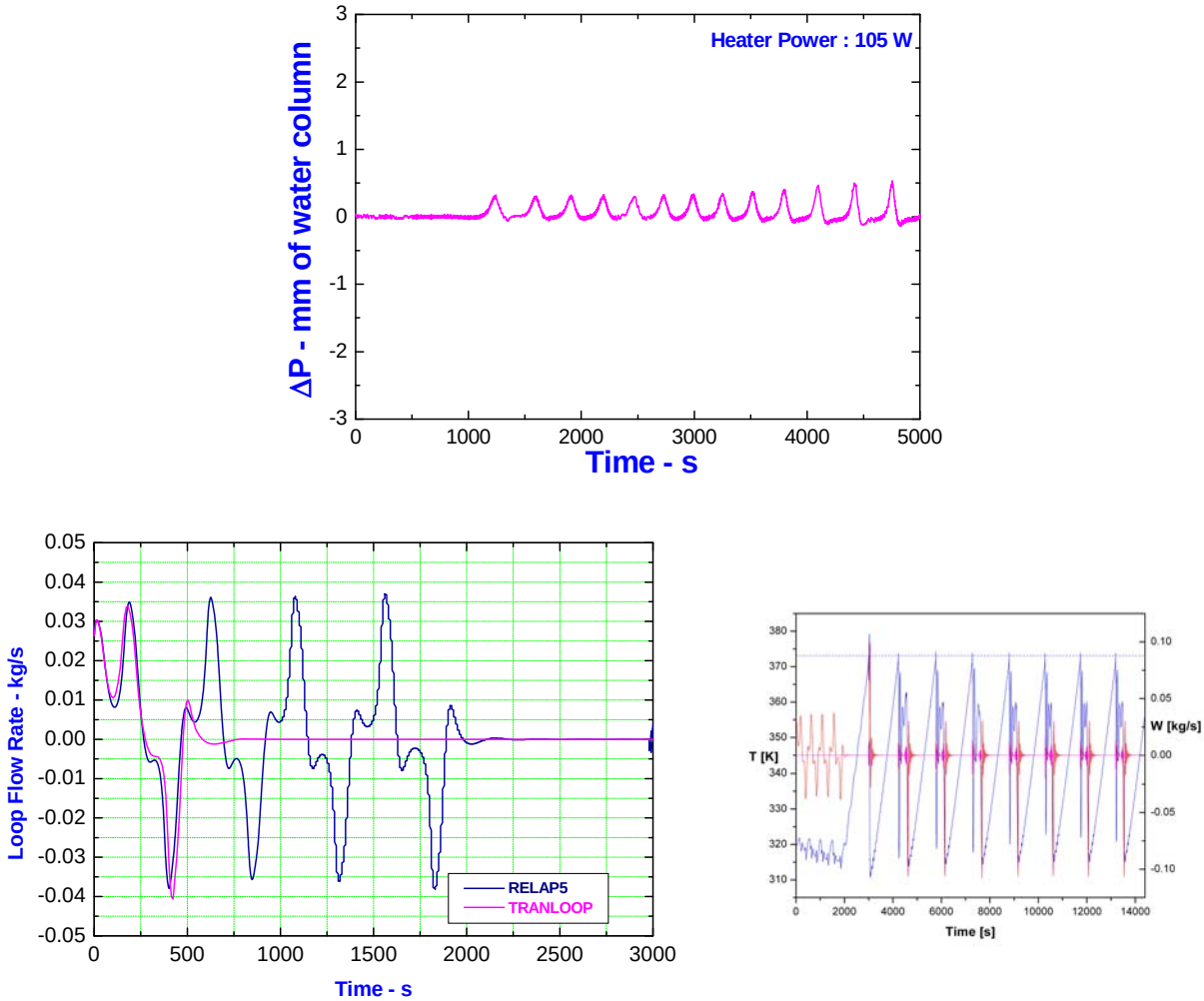


Figure 11 Comparison of experimental and simulated trends using RELAP5 and TRANLOOP [26]

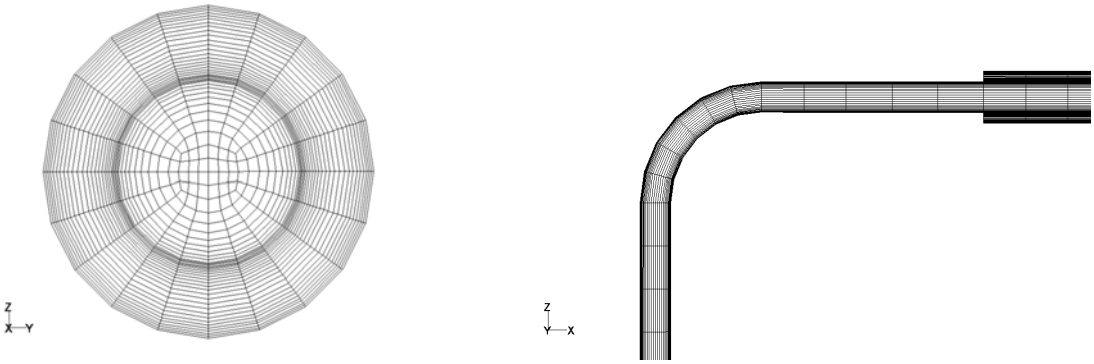


Figure 12 The nodalization adopted for the CFD simulations

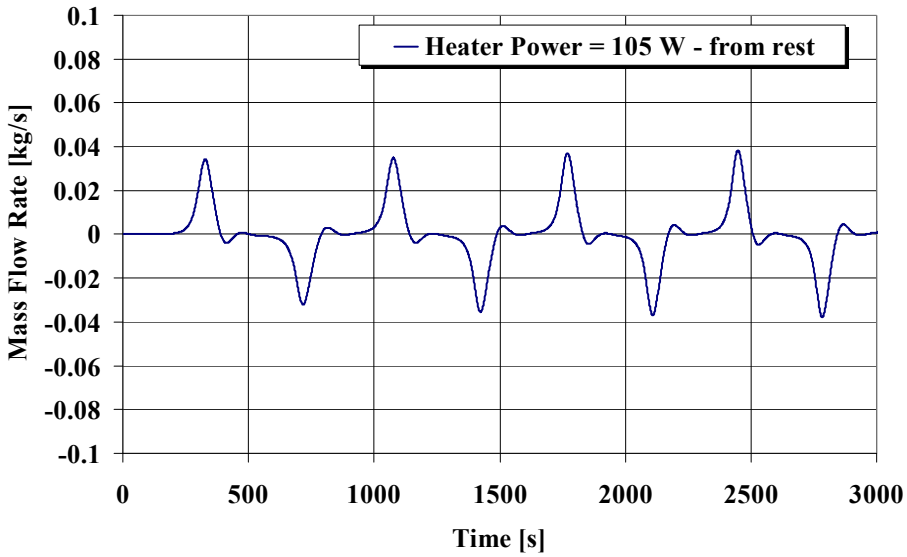


Figure 13 CFD simulation of the 105 W heating power case using FLUENT 6.0

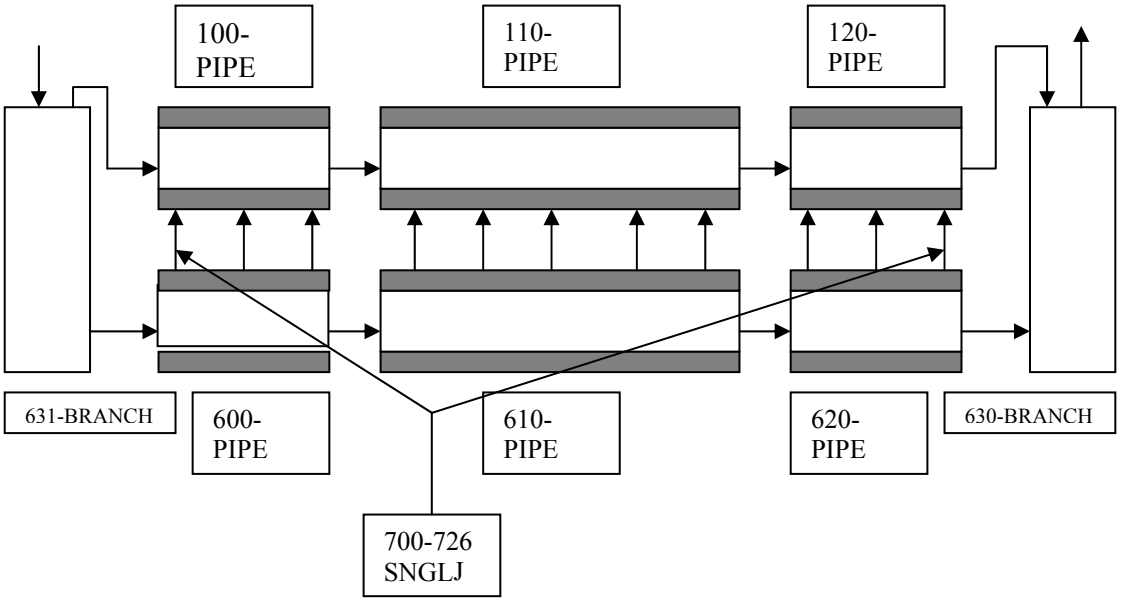


Figure 14 An alternative nodalization for the horizontal heater

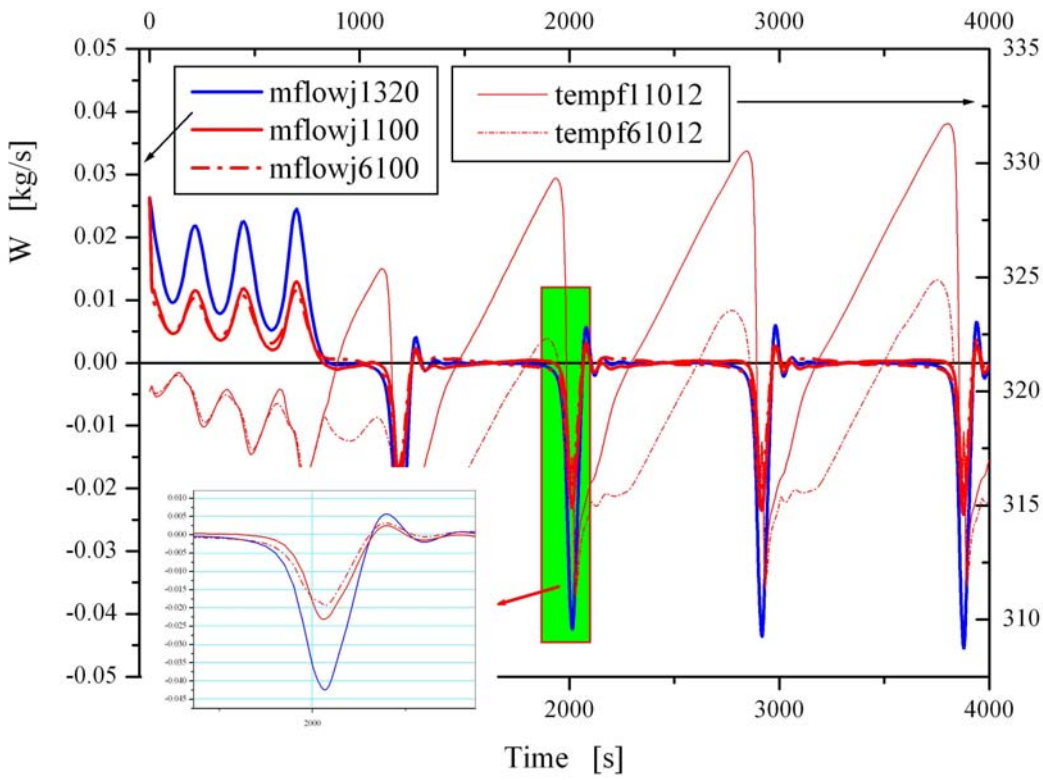


Figure 15 Time variation of mass flow-rate and temperature using the modified nodalization

Perhaps, one way of looking all the above mentioned results is in the light of the search for convergence of results. This is, perhaps, the easiest step in computational analysis of engineering problems but only conceptually. In fact, it means that grid size, as measured by some suitable norm, is compatible with the accuracy of resolution of some type of boundary layer. This may be a momentum boundary layer as in the

vicinity of a wall, the depth of heat penetration in a solid or the time history of some suitable dependent variable as a function of its time scale, among many other possible examples. What must be considered is that a given boundary layer behavior must be solved accurately enough. Searching for grid convergence is not a too costly activity in simple integration domains, like the 1D cases herein considered. In multi-dimensional domains, the use of multiple scale calculations tends to keep detail and accuracy at an appropriate level in the entire integration domain. Shape and size variation of computational cells affect the global accuracy.

In the case of natural circulation in unstable flow conditions analyzed using this type of time domain computer codes; the problem consists in using a spatial discretization fine enough as to minimize the amount of numerical diffusion. It is added in the process of solution as a consequence of the inherent properties of the discrete scheme (the advantage of its control will be evident in paragraph 7). This diffusion is usually associated with first-order spatial discretization. It may be argued that using $\boldsymbol{O}(1)$ numerical schemes should not be recommended in general. However, most engineering thermal-hydraulic systems codes use this approximation to circumvent a worse limitation: the ill-posedness of governing equations.

The interaction of flow stabilization and discretization may be exemplified resorting again to results in [9], as shown in Figure 16, where the flow rate in a toroidal loop was obtained using the FTUS scheme, 1000 spatial nodes and C_{OU}=0.8. The results are compared with the ones obtained using a modal expansion- it is free of numerical diffusion- with 500 modes and adding the numerical diffusion corresponding to the previous approximation. It may be observed that the results are nearly the same. Then, it may be concluded that the usual interaction between the numerics and physics persists in this non-linear case.

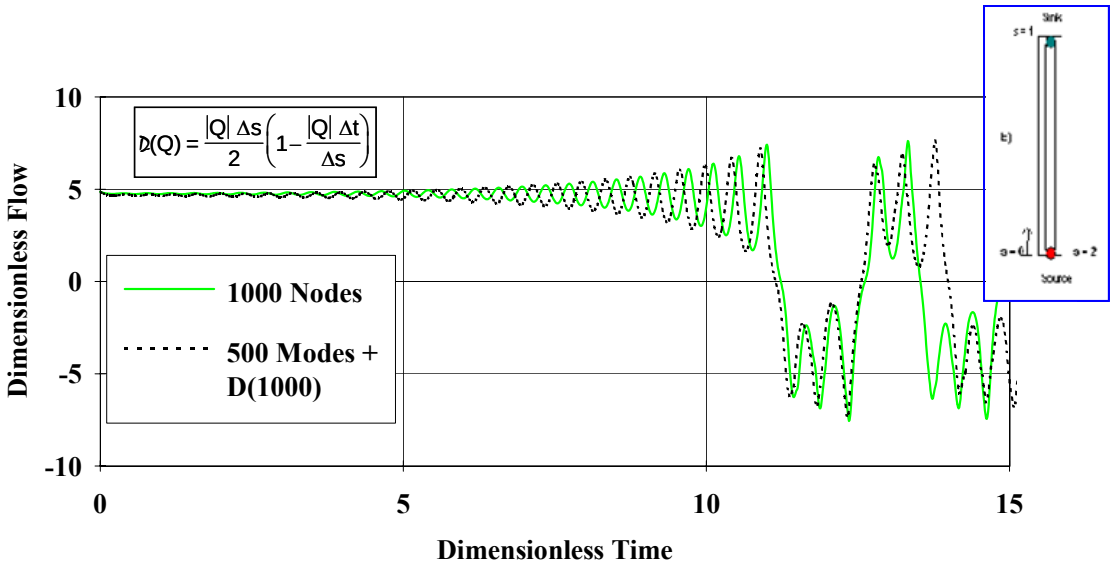


Figure 16 The flow rate for the FTUS scheme using 1000 nodes and its simulation using a modal expansion of 500 modes and adding the numerical viscosity corresponding to 1000 nodes.

7. NUMERICAL SOLUTION TECHNIQUES FOR 1D, NC FLOWS

The analysis of the stability of natural circulation (NC) based on numerical techniques will be presented in this restricted context, namely nominally 1D flows in single phase. As already mentioned, This limited context may be, at least, justified due to its own importance, the common kind of problems regarding the numerical techniques between single and two-phase phenomena (interface tracking included) and the huge experimental database associated to volume scaled, almost 1D configurations (ITFs).

7.1 A Measure for Instability in NC Flows

In previous work [27], a methodology was developed for studying the linear stability behaviour of steady-state conditions in single-phase thermosyphon loops "as predicted" by a given numerical method. This methodology involved the explicit differentiation of numerically discretized equations around the addressed steady-state condition obtaining Jacobian matrices to be used in producing a matrix, identified as **A**, embedding the linear dynamics of the system. In particular, if

$$F\left(y^{n+1}, y^{n}, p\right) = 0 \tag{16}$$

represents the numerical scheme, relating the *(2N+1)*-vector of system state variables, **y**, (*N* fluid temperatures, *N* wall temperatures and the loop flow rate) at two subsequent time levels (t^n and t^{n+1}) and **p** is a vector of physical and numerical parameters, it is:

$$\delta y^{n+1} = -\left[\left.\frac{\partial F}{\partial y^{n+1}}\right|^{s}\right]^{-1} \cdot \left[\left.\frac{\partial F}{\partial y^{n}}\right|^{s}\right]\delta y^{n} = A\left(y^{s}, p\right)\delta y^{n} \tag{17}$$

in which the superscript *s* identifies the considered steady-state conditions. Discussion of the eigenvalues of **A** allows getting information about stability. In particular, the spectral radius of the matrix, $\rho_{\mathbf{A}}$, can be used to define the following useful quantity

$$z_R = \frac{1}{\Delta t}\ln\left(\rho_{\mathbf{A}}\right) \tag{18}$$

where $\Delta t = t^{n+1} - t^{n}$ is the adopted time increment. This quantity takes negative or positive values for stable or unstable behaviour, respectively; discussion the value of Z_R for different values of the independent physical or numerical parameters allows setting up quantitative stability maps. Similarly, other useful information can be obtained, e.g., on the frequency of the fastest growing (or least damped) oscillations [27].

The approach based on the calculation of Jacobian matrices turned out useful for automatic sensitivity analyses, as reported in [28] and will be discussed in some detail in Paragraph 9. A different approach has been also utilised [31] that has the advantage to avoid the cumbersome algebra (this was not the case in [28] because of the automatic differentiation procedure implemented) involved in getting the Jacobians and is more computationally oriented. This methodology makes direct use of the transient solution algorithm, introducing small perturbations in the components of vector $\mathbf{y^n}$ to construct the matrix **A** by repeatedly advancing the transient algorithm. This procedure assures complete coherence between the results of the linear stability analysis and those of the transient non-linear calculations. As a further advantage, the same methodology could be applied to complex codes whose models are very complicated or even completely unknown. However, as mentioned also in [31], numerical differentiation has also drawbacks related to the optimum choice of perturbations in variables, whose values must be carefully selected to avoid obtaining inaccurate data.
The decay ratio or the quantity

$$\Delta\rho = \rho_A - 1 \tag{19}$$

can be used in place of z_R, if considered preferable for any reason. The stability criterion takes therefore the following equivalent forms

$$\begin{cases} z_R < 0 & \text{or} \quad \Delta\rho < 0 \ \text{ stable system} \\ z_R > 0 & \text{or} \quad \Delta\rho > 0 \ \text{ unstable system} \end{cases} \tag{20}$$

Figure 17 shows how both quantities vary in a case of theoretical interest to be considered later, i.e. the loop described by P. Welander [32], when the number of nodes changes. In this figure, α is a measure of the driving force and ε the corresponding to the friction in the loop.

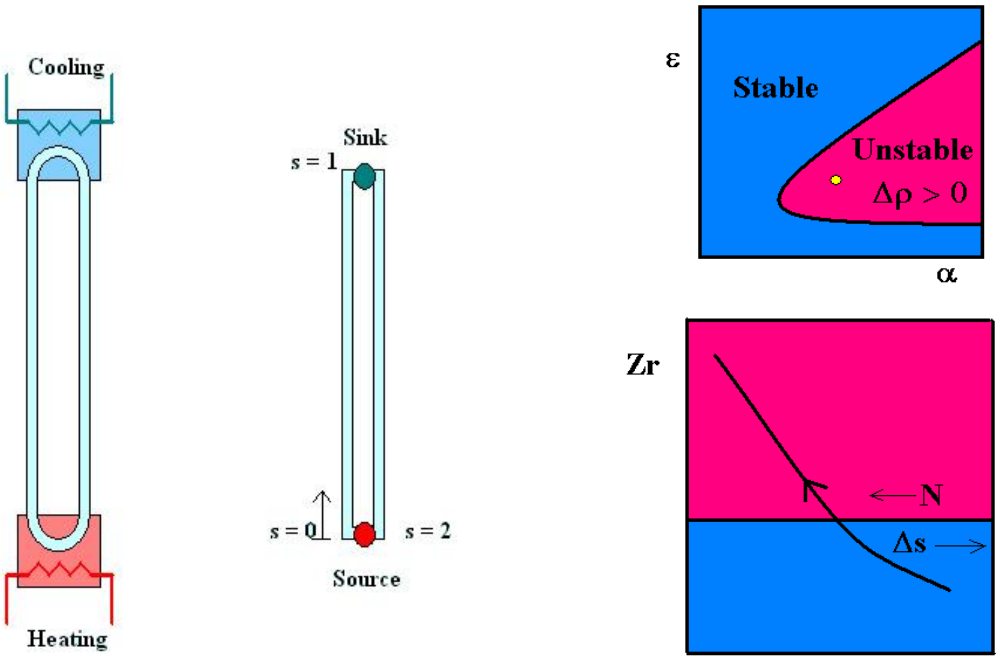


Figure 17 The trends of Z_R and ρ_A with nodes number (N) variation

7.2 Governing Equations

Having defined the variables that may measure the stability of the NC system as given by Equations (16) to (20), it seems obvious that now the goal consists in defining the governing equations and their discrete representation. Then, in what follows, the governing equations for 1D, single-phase flow for a loop will be firstly considered. Secondly, the definition and use of the discrete technique will be stated. This will be done following the analysis of [33]. Finally, the paragraph will be closed with a survey of the effects of numerical diffusion on stability boundary predictions as discussed in [27].

Let us consider a single-phase closed loop with assigned geometry. With the usual assumption of a Boussinesq fluid and considering an arbitrary distribution of heat sources and sinks, the equations governing the dynamics of the flow are:

Energy balance:

$$\rho_f C_{p,f} A_{f,i} \left.\frac{\partial T_f}{\partial t}\right|_i + C_{p,f} W \left.\frac{\partial T_f}{\partial s}\right|_i = \Pi_{w,i}^{in} \hat{h}_{w,i}^{in} \left(T_{w,i} - T_{f,i}\right) \tag{21}$$

Momentum balance:

$$\begin{aligned} &\rho_f A_{f,i} \Delta s_i \frac{dw_i}{dt} = \\ &- A_{f,i} \Delta s_i \rho_f g_i \left[1 - \beta_f \left(T_{f,i} - T_f^0\right)\right] - \left[\Pi_{f,i}^{frict} \Delta s_i f'(Re_i) + A_{f,i} K_i\right] \frac{1}{2} \rho_f |w_i| w_i \\ &- A_{f,i} \Delta p_i - A_{f,i} \Delta p_{acc,i} \end{aligned} \tag{22}$$

Where, despite of the use of spatial derivatives it has been implicitly assumed in the notation that the loop is discretized by nodes (control volumes as in Figure 18) having a uniform flow area $A_{f,i}$ and a length Δs_i, wetted and heated perimeters identified by $\Pi_{f,i}^{frict}$ and $\Pi_{w,i}^{in}$. In the above relationships, the mass flow rate is W, velocity is w_i, the reference fluid density is ρ_f (at the reference temperature T_f^0), the specific heat at constant pressure $C_{p,f}$, the isobaric expansion coefficient β_f and the local fluid

temperature $T_{f,i}$, while the temperature of the facing wall is $T_{w,i}$. The overall conductance between the middle of the heat structure thickness and the fluid is represented by $\hat{h}^{in}_{w,i}$, accounting for both heat conduction within the wall and convection at its surface. Distributed and singular pressure drops are considered by the related Fanning factor $f'(Re_i)$, function of the Reynolds number through assigned laws, and the singular pressure drop coefficients K_i. Finally, g_i is the gravity component along the node axis and $\Delta p_{i,acc}$ and Δp_i are the pressure drop due to acceleration and the total pressure drop across the node.

Making use of the definitions

$$w_i = \frac{W}{\rho_f A_{f,i}} \qquad \lambda_{wf,i} = \frac{\Pi^{in}_{w,i}\hat{h}^{in}_{w,i}}{\rho_f C_{p,f} A_{f,i}}$$

the energy balance equation takes the form

$$\left.\frac{\partial T_f}{\partial t}\right|_i + w_i \left.\frac{\partial T_f}{\partial s}\right|_i = \lambda_{wf,i}\left(T_{w,i} - T_{f,i}\right) \tag{23}$$

On the other hand, taking the summation of both sides of the momentum equation over the node index and considering that integration of the terms $\Delta p_{i,acc}$ and Δp_i along a closed loop is zero, it is found:

$$\frac{dW}{dt} = \frac{\rho_f \beta_f}{I}\sum_{i=1}^{N}\Delta s_i g_i T_{f,i} - \frac{F(W)}{I}|W|\,W \tag{24}$$

Where:

$$I = \sum_{i=1}^{N}\left(\frac{\Delta s_i}{A_{f,i}}\right) \qquad F(W) = \sum_{i=1}^{N}\left[\frac{\Pi^{frict}_{f,i}\Delta s_i}{2\rho_f A^3_{f,i}} f'(Re_i)\right] + \sum_{k=1}^{N_{sing}}\left[\frac{K_k}{2\rho_f A^2_{f,k}}\right] \tag{25}$$

As it can be seen, it is assumed that singular pressure drops are not assigned in each node but at N_{sing} specified locations, characterized only by a reference area $A_{f,k}$.

Finally, a lumped parameter approach is used for representing heat structure behaviour, leading to the following energy balance equation:

$$\frac{dT_{w,i}}{dt} = -\lambda_{w,i} T_{w,i} + Q_{w,i} \tag{26}$$

Where:

$$\lambda^{out}_{w,i} = \frac{\hat{h}^{out}_{w,i}\Pi^{out}_{w,i}}{A_{w,i}\rho_{w,i}C_{pw,i}} \qquad \lambda^{in}_{w,i} = \frac{\hat{h}^{in}_{w,i}\Pi^{in}_{w,i}}{A_{w,i}\rho_{w,i}C_{pw,i}}$$

$$\lambda_{w,i} = \lambda^{out}_{w,i} + \lambda^{in}_{w,i} \qquad Q_{w,i} = \frac{q'''_{w,i}}{\rho_{w,i}C_{pw,i}} + \lambda^{out}_{w,i}T^{out}_{f,i} + \lambda^{in}_{w,i}T_{f,i}$$

in which the temperature of the outer fluid $T^{out}_{f,i}$ and the outer structure surface conductance $\hat{h}^{out}_{w,i}$ appear together with structure density $\rho_{w,i}$, specific heat $C_{pw,i}$, cross section area $A_{w,i}$ and outer perimeter $\Pi^{out}_{w,i}$. Moreover, $q'''_{w,i}$ is the specific power per unit volume possibly generated in the structure material by electrical heating or any other means. As mentioned, the evaluation of the inner and outer surface conductances $\hat{h}^{in}_{w,i}$ and $\hat{h}^{out}_{w,i}$ involves to calculate (or impose) inner and outer fluid heat transfer coefficients and appropriate conductive resistances between the middle of the structure thickness and the two surfaces; this is made accepting conventional heat transfer correlations for forced internal flow (e.g., the Colburn correlation) and assuming cylindrical structure shells.

7.3 Discretization of Governing Equations

Only the results of [33] will be given here. The interested reader may find the details in said reference. The equations expressing energy balance in the fluid and in the structures and momentum balance in the fluid are combined to calculate the transient behavior of the system. In what follows reference will be made to Figure 18.

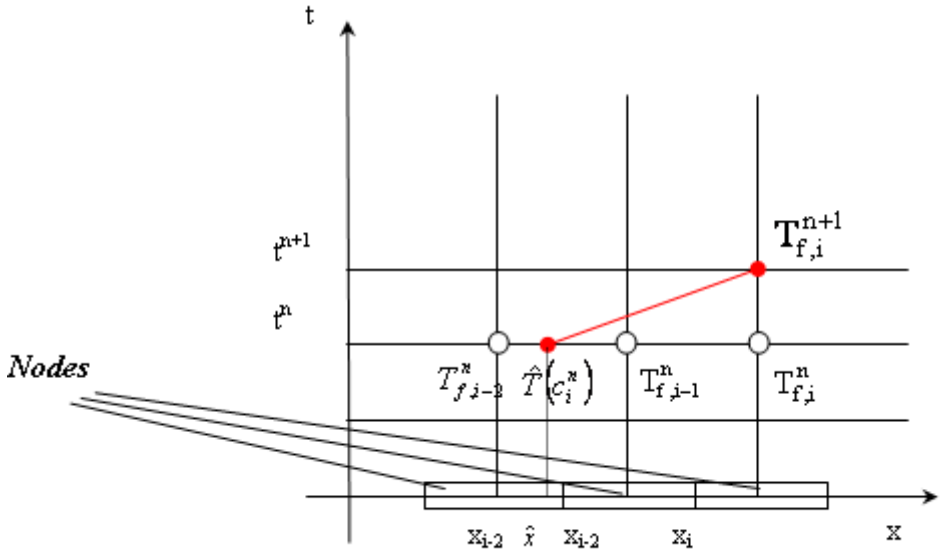


Figure 18 Definition of the discretized integration domain

Momentum equation is discretized in time giving

$$W^{n+1} = \frac{W^n + \frac{\rho_f \beta_f \Delta t}{l} \sum_{i=1}^{N} \Delta s_i g_i T_{f,i}^{n+1}}{1 + \frac{F(W^n)\Delta t}{l} |W^n|} \tag{27}$$

On the other hand, the relationship to advance in time heat structure temperature is obtained making use of the analytical solution of the related energy balance equation:

$$T_{w,i}^{n+1} = T_{w,i}^n e^{-\lambda_{w,i}^n \Delta t} + \frac{Q_{w,i}^n}{\lambda_{w,i}^n} \left[1 - e^{-\lambda_{w,i}^n \Delta t} \right] \tag{28}$$

The corresponding time-averaged heat structure temperature during the time-step is

$$\overline{T}_{w,i}^{n,n+1} = T_{w,i}^n \frac{1 - e^{-\lambda_{w,i}^n \Delta t}}{\lambda_{w,i}^n \Delta t} + \frac{Q_{w,i}^n}{\lambda_{w,i}^n} \left[1 - \frac{1 - e^{-\lambda_{w,i}^n \Delta t}}{\lambda_{w,i}^n \Delta t} \right] \tag{29}$$

The discretization of the energy equation deserves special attention, since is it the one governing the advection of perturbations which, in turn, drive the flow instabilities. The concept adopted in [33] was keeping the desirable transportive[5] properties of the upwind approximations and, at the same time, having full control of the numerical diffusion and the effects of heat sources.

[5] The transportive property of a numerical scheme consists in its ability for propagating information only in the domain of dependence of the (hyperbolic) partial differential equation.

The corresponding relationships, extended to the case of non-uniform space discretization and duct flow area also are a function of flow direction. In such a case, considering the occurrence of forward or reverse flow and the periodic flow boundary conditions, it is:

$$W^n \geq 0$$

$$\Rightarrow \quad \dot{T}^n_{f,1} = \left[1-\xi_{w,1}\right]T^n_{f,1} + \xi_{w,1}\, T^n_{f,N}$$

$$+\left[1-\alpha^n_1 + \xi_{w,1}\,\alpha^n_1\right]\frac{\Delta s_1}{w^n_1}S^n_1 + \left[1-\alpha^n_N\right]\xi_{w,1}\,\frac{\Delta s_N}{w^n_N}S^n_N$$

$$\dot{T}^n_{f,i} = \left[1-\xi_{w,i}\right]T^n_{f,i} + \xi_{w,i}\, T^n_{f,i-1}$$
$$+\left[1-\alpha^n_i + \xi_{w,i}\,\alpha^n_i\right]\frac{\Delta s_i}{w^n_i}S^n_i + \left[1-\alpha^n_{i-1}\right]\xi_{w,i}\,\frac{\Delta s_{i-1}}{w^n_{i-1}}S^n_{i-1} \qquad (i=2,\ldots,N)$$

where

$$\xi_{w,1} = \xi_{w,1}\left(W^n\right) = \frac{W^n\Delta t - \rho_f A_{f,1}\Delta s_1}{\rho_f A_{f,N}\Delta s_N + \rho_f A_{f,1}\Delta s_1}$$

$$\xi_{w,i} = \xi_{w,i}\left(W^n\right) = \frac{W^n\Delta t - \rho_f A_{f,i}\Delta s_i}{\rho_f A_{f,i-1}\Delta s_{i-1} + \rho_f A_{f,i}\Delta s_i} \qquad (i=2,\ldots,N)$$

and

$$\alpha^n_i = \alpha\left(\frac{w^n_i}{\lambda^n_{wf,i}\Delta s_i}\right) = \frac{w^n_i}{\lambda^n_{wf,i}\Delta s_i}\left[\frac{\dfrac{\lambda^n_{wf,i}\Delta s_i}{w^n_i}}{1-e^{-\frac{\lambda^n_{wf,i}}{w^n_i}\Delta s_i}} - 1\right] \qquad (i=1,\ldots,N)$$

$$W^n < 0$$

$$\Rightarrow \quad \dot{T}^n_{f,i} = \left[1-\xi_{w,i}\left(W^n\right)\right]T^n_{f,i+1} + \xi_{w,i}\left(W^n\right)T^n_{f,i+2}$$

$$+\left[1-\alpha^n_{i+1} + \xi_{w,i}\,\alpha^n_{i+1}\right]\frac{\Delta s_{i+1}}{\left|w^n_{i+1}\right|}S^n_{i+1} + \left[1-\alpha^n_{i+2}\right]\xi_{w,i}\,\frac{\Delta s_{i+2}}{\left|w^n_{i+2}\right|}S^n_{i+2} \quad (i=1,\ldots,N-2)$$

$$\dot{T}^n_{f,N-1} = \left[1-\xi_{w,N-1}\right]T^n_{f,N} + \xi_{w,N-1}\, T^n_{f,1}$$
$$+\left[1-\alpha^n_N + \xi_{w,N-1}\,\alpha^n_N\right]\frac{\Delta s_N}{\left|w^n_N\right|}S^n_N + \left[1-\alpha^n_1\right]\xi_{w,N-1}\,\frac{\Delta s_1}{\left|w^n_1\right|}S^n_1$$

$$\dot{T}^n_{f,N} = \left[1-\xi_{w,N}\right]T^n_{f,1} + \xi_{w,N}\, T^n_{f,2}$$
$$+\left[1-\alpha^n_1 + \xi_{w,N}\,\alpha^n_1\right]\frac{\Delta s_1}{\left|w^n_1\right|}S^n_1 + \left[1-\alpha^n_2\right]\xi_{w,N}\,\frac{\Delta s_2}{\left|w^n_2\right|}S^n_2$$

where

$$\xi_{w,i} = \xi_{w,i}\left(W^n\right) = \frac{\left|W^n\right|\Delta t - \rho_f A_{f,i+1}\Delta s_{i+1}}{\rho_f A_{f,i+2}\Delta s_{i+2} + \rho_f A_{f,i+1}\Delta s_{i+1}}$$

$$\xi_{w,N-1} = \xi_{w,N-1}\left(W^n\right) = \frac{\left|W^n\right|\Delta t - \rho_f A_{f,N}\Delta s_N}{\rho_f A_{f,1}\Delta s_1 + \rho_f A_{f,N}\Delta s_N}$$

$$\xi_{w,N} = \xi_{w,N}\left(W^n\right) = \frac{\left|W^n\right|\Delta t - \rho_f A_{f,1}\Delta s_1}{\rho_f A_{f,2}\Delta s_2 + \rho_f A_{f,1}\Delta s_1}$$

$$\alpha_i^n = \alpha\left(\frac{w_i^n}{\lambda_{wf,i}^n \Delta s_i}\right) = \frac{\left|w_i^n\right|}{\lambda_{wf,i}^n \Delta s_i}\left[\frac{\dfrac{\lambda_{wf,i}^n \Delta s_i}{\left|w_i^n\right|}}{1 - e^{-\frac{\lambda_{wf,i}^n}{\left|w_i^n\right|}\Delta s_i}} - 1\right] \qquad (i = 1, \ldots, N)$$

It is interesting to note that, putting $\xi_{w,i} = 0$ and $\alpha_i^n = 1$ in each node, i.e. letting zero the weighting coefficients for upwinding of advection and the balancing of heat sources effects on the computing cell, the low diffusion scheme reverts to the classical first order upwind scheme with pointwise evaluation of the source. On the other hand, putting $\xi_{w,i} = 0$ and assuming α_i^n as given above allows obtaining a first order method having a similar advantage in evaluating steady-state conditions as obtained by appropriate correction factors in [27].

7.3 Some Selected Results from [33]

The results to be shown are selected purposely to exemplify why it is worth considering schemes with controlled numerical diffusion. The loop of [22] will be considered again. Three discretizations have been chosen, namely: “very coarse - 10 nodes per vertical leg”, “coarse - 21 nodes” and “fine - 90 nodes”. The very coarse nodalization implies roughly a 20:1 grid aspect ratio. In all cases the horizontal pipes have been discretized using 12 nodes.

Figure 19 shows the results obtained using the conventional FTUS method and the one herein reviewed. Remarkably, the physically unstable behavior of the loop is well represented in the second case for all the nodalizations. This is not the case with the conventional FTUS method. Many other calculations have been performed in relation with the results in [32], constructing stability maps almost free from numerical diffusion effects.

The above advantages clearly appeared in the application to one-dimensional single-phase flow; a further study is needed for assessing the feasibility of the application of a similar scheme in two-phase flow problems. A major difficulty in this respect is that some two-fluid codes are based on a differential problem having an ill-posed mathematical character, which discourages any attempt to increase the level of accuracy of the numerical method, possibly leading to the prediction of unexpected unstable behaviour. However, when single-phase stability problems are addressed the low diffusion scheme showed to be capable of very good performances. This suggests that the method could be considered in codes as an option to be activated at least when dealing with single-phase flow to get dissipation-free results, strongly improving the reliability of their stability predictions.

7.4 Systematic Application to Stability Analysis [20], [27], [33]

The above methodology and some conventional methods [27] have been applied systematically to investigate the stability of 1D, NC flows. These applications lead also to emphasize the effect of closure correlations in stability maps. The results of [20], may be summarized considering Figure 20. The calculations correspond to the friction law given by the continuous, experimental one. The results of [27] are related to the application of discrete schemes of different truncation errors to the Welander´s loop. In this way, the Authors analyzed said case and determined quantitatively how the stability map are influenced by numerical diffusion. As shown above, for the discrete schemes herein considered, numerical diffusion can be directly related to the space increment. Then, the number of nodes per leg

determines the degree of damping. Figure 21 [27] is an example of how, for the loop illustrated in Figure 17, the neutral stability curve is affected by discretization, in this case usng the FTUS method considering turbulent flow.. The working point selected is unstable and damping the solution leads, again, to non-conservative results. Using second order methods, leads to much less affected results, even for a very small (10) number of nodes. This is illustrated in Figure 22. The need for controlled diffusion lead to the developments of [33].

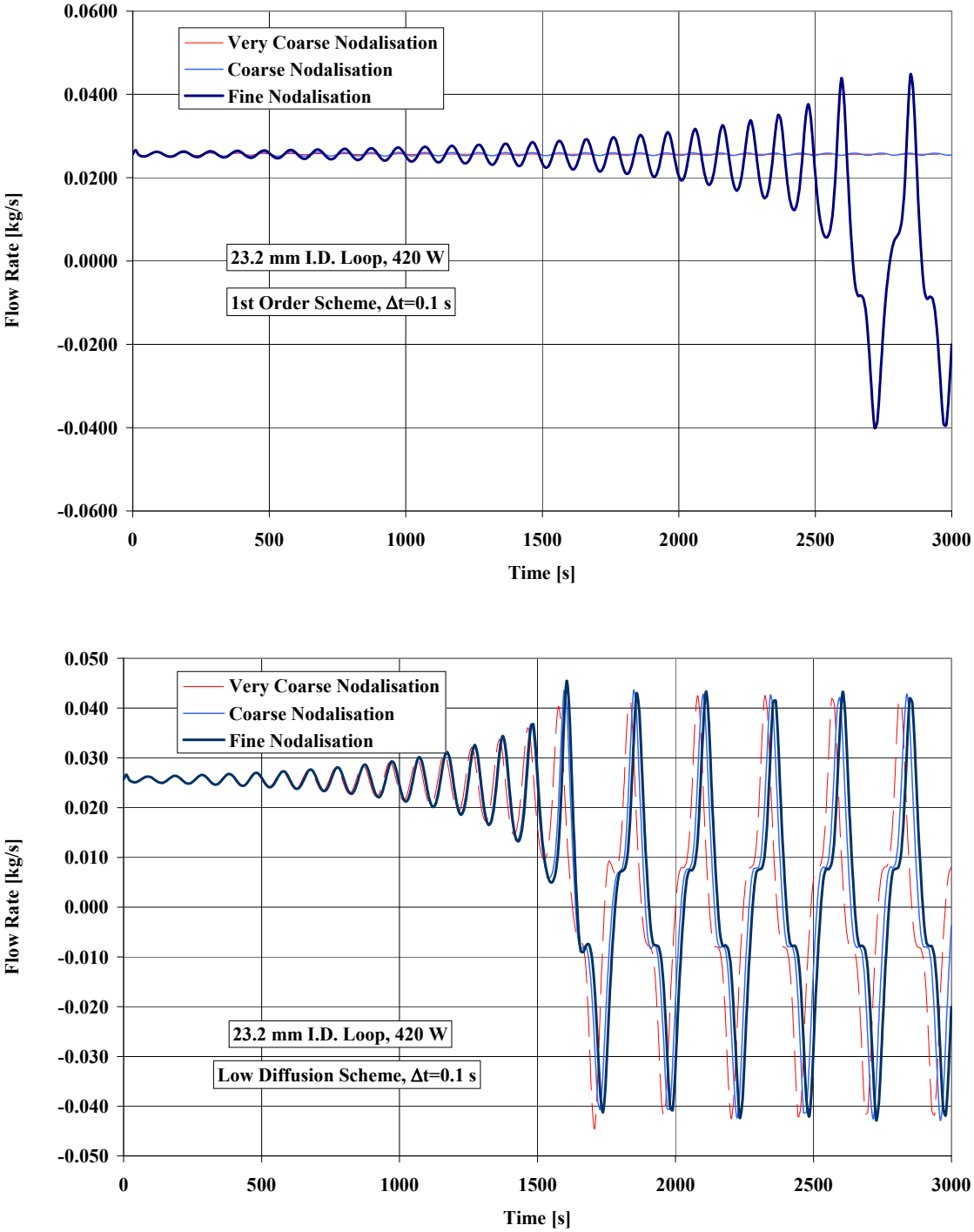


Figure 19 Comparison of unstable NC flow prediction using the FTUS method and the low diffusion method of [33]. Flow corresponds to the simulation of one experiment from [22].

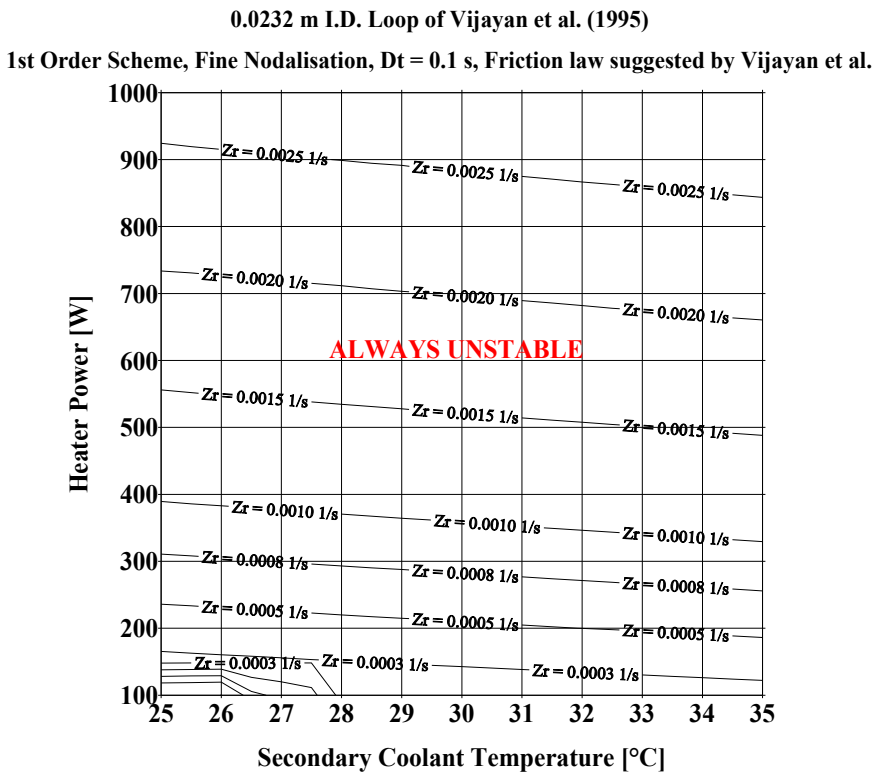


Figure 20 Linear stability map obtained by LINELOOP using the friction law suggested in [22] with the fine nodalization and the first order scheme

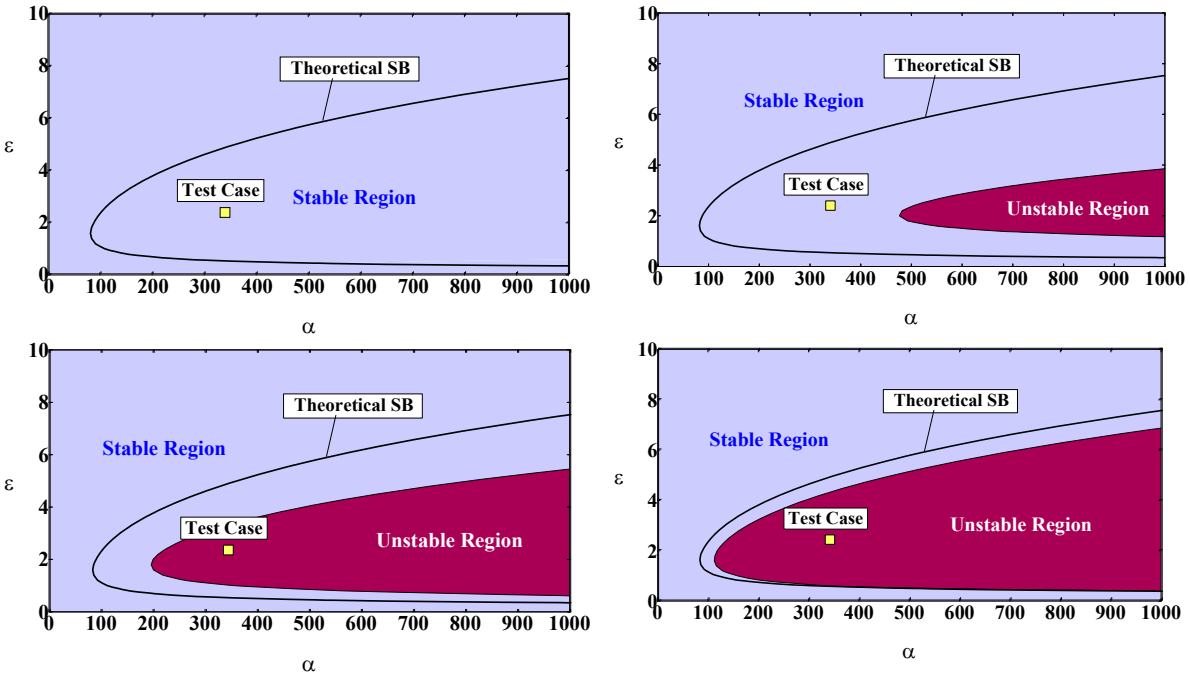
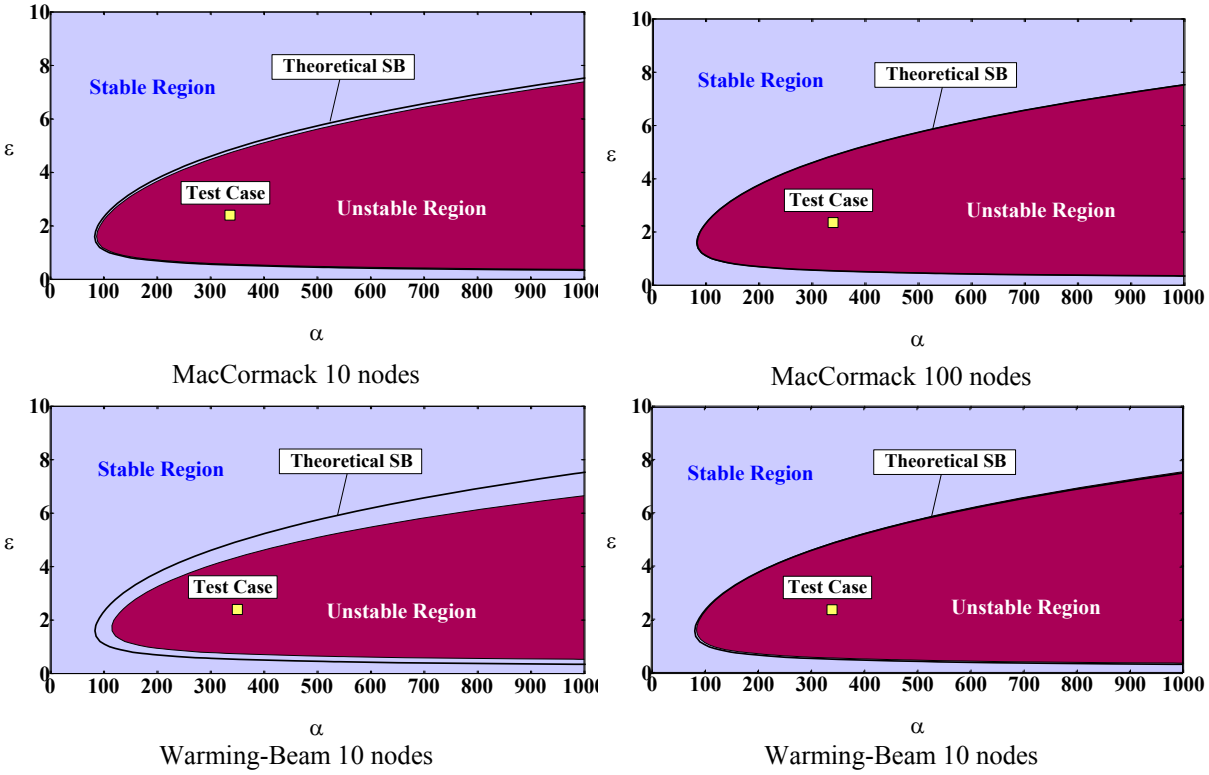


Figure 21 Linear stability maps for the upwind explicit scheme with various numbers of nodes



MacCormack 10 nodes

MacCormack 100 nodes

Warming-Beam 10 nodes

Warming-Beam 10 nodes

Figure 22 Linear stability maps for the MacCormack and the Warming-Beam explicit schemes

9. INTRODUCING SENSITIVITY ANALYSIS [28]

In previous paragraphs, it was shown how a methodology of analysis based on the numerical discretization of partial differential equations governing fluid-dynamic problems is key to get information on the capabilities of numerical methods in accurately predicting stability. An essential point of this methodology is the evaluation of the derivatives of the Jacobean matrices of the algebraic relationships that define the numerical method and the related boundary conditions. It is in this perspective that the use of automatic code differentiation tools may play an interesting role.

The sensitivity of stability results to physical and discretization parameters will be analyzed using a tool for the automatic differentiation of FORTRAN codes. This is due because FORTRAN is the programming language usually used for programming thermal-hydraulic system codes. ADIFOR (meaning Automatic DIfferentiation of FORtran) [29] is the adopted tool that allows for evaluating the derivatives of model variables with respect to model parameters.

It will only be mentioned here that ADIFOR is a pre-processor code which, given a FORTRAN 77 code that computes a function, automatically generates another, augmented, FORTRAN 77 code. It must be considered that any code may be put in the form of a function, simply by introducing a call to a main routine after setting parameter values. The latter computes the function and the derivatives with respect to a list of variables. The user must specify the list of dependent and independent variables. After generating the augmented code that calculates the specified derivatives via ADIFOR, the user must provide a new driving FORTRAN 77 code that takes into account the new set of variables. Some hints to help on the very first use of ADIFOR may be readily found in the original documentation. Many references document the accuracy of the derivatives calculated in this way. This is neither the only way to apply ADIFOR, nor ADIFOR is the only tool: the reader is referred to the available literature.

The results reported in this section deal again with the Welander's loop, because the stability properties of this prototypical problem have been the subject of the previous analysis.

Then the analysis will be applied in a limited context, namely: natural circulation in a simple system, amenable of analytical steady-state treatment. Results have been obtained using implicit coupling of the momentum and energy equations and the forward time, upwind-space finite-difference method (FTUS) for the energy equation. Numerical analysis shows that the consequences of using this approximation on the results are well known, i.e. an $O(1,1)$ solution in the space and time increments. However, the combined effects of these errors and those of the variables coupling and their quantification are not simple, at least in the field of the stability limits of natural circulation systems.

9.1 Algorithm

This paragraph presents an alternative procedure to the one developed in [9] for the calculation of the margin to neutral stability ($\Delta\rho$) sensitivity to system parameters, as will be explained later. In what follows the analysis leading to its definition will be sketched.

As told before, $\Delta\rho$ is used as a measure of the margin in excess to neutral stability and to quantify the degree of damping or amplification. It takes negative values for stable conditions and positive ones for unstable conditions. In [9], the sensitivity of $\Delta\rho$ was simply obtained by calculating its derivative with respect to $\mathbf{p}$ using the original code that allowed the calculation of $\Delta\rho$ itself. This implied obtaining the derivatives of the classical EISPACK path for the eigenvalues and eigenvectors of a general matrix. It, in turn, imposed a non-trivial computational effort when N was several hundreds.

Here, the calculation of the sensitivity of $\Delta\rho$ to parameters is based on the following algorithm:

- *Define* A *and* A^T*, respectively as the matrix relating perturbations at time steps n and n+1 and its transpose. This matrix may also be specified using* ***ADIFOR****. However, second order derivation to get derivatives of* A *with respect to* p_i *is beyond the objective of this paper, but may done by calculating Hessians with ADIFOR3, from the same software originators. Consequently,* A *will be specified analytically.*
- *Use of* ***ADIFOR*** *to automatically calculate the derivative of A with respect to system parameters*

- *Calculation of the eigenvalues of* A *and its eigenvectors,* λ_i, x.
- *Calculation of the eigenvectors of* A^T, v.
- *Determination of* i, *the index of the eigenvalue that corresponds to the spectral radius of* A *and the corresponding eigenvectors of* A *and* A^T.
- *Calculation of the sensitivity of* λ_i *with respect to system parameters.*
- *Calculation of the spectral radius sensitivity with respect to system parameters.*

In what follows, the above-mentioned steps will be expanded, specifying some details of the different procedures.

9.1.a Calculation of A and its transpose

The algebraic expressions leading to A come from the standard Finite-difference method, as defined by (1-2). It must be emphasized that the previous algorithm is general. No particular assumptions are made with respect to A, except being real, that is always the case in finite-differences models in Fluid Dynamics. Parameters are considered to be independent of time in this analysis; however, this condition may be released at the price of feasible, more laborious analysis. Given A, its transpose is also determined.

9.1.b Use of ADIFOR to automatically calculate the derivatives of A

ADIFOR 2.0D has been used to generate the augmented FORTRAN code to calculate the derivatives of A with respect to system parameters. In a general system, there are several parameters p_k. In this paper, only two scalar parameters, namely $C_{OU} = 0.8$ and $\xi = 1.75$ ($\equiv 2-\theta$, where θ is the exponent in the friction law), will be considered. A is a real matrix, non-symmetrical and almost sparse. However, the momentum equation is a full row, relating node temperatures, flow-rate and heat transfer boundary conditions.

9.1.c Calculation of the eigenvalues of A and its eigenvectors, λ_i, x

The vector of complex eigenvalues of A has been obtained using the classical EISPACK routines in their complex variable version. It may be argued that A is real but, to avoid problems of de-packing complex eigenvalues, the complex version was the adopted package. Simultaneously, the complete set of eigenvectors, x, was calculated.

9.1.d Calculation of the eigenvectors of A^T, v

In order to calculate the eigenvectors of A^T, it was necessary to perform once again the complete calculation of eigenvalues + eigenvectors, since no path in EISPACK (and LAPACK also) is available -to authors' knowledge- to perform the simultaneous calculation for a matrix and its transpose. It did not pose problems in practice, because convergence of calculations was quite fast.

9.1.e Determination of the eigenvalue corresponding to the spectral radius of A, λ_i, and the corresponding eigenvectors of A and A^T

The calculation of the spectral radius of A is quite obvious: it was a simple search for the maximum modulus of the eigenvalues vector. The interest of this search is also finding the index of the eigenvalue, denoted by i. The corresponding eigenvector, x_i, was found by simple correspondence of index. The corresponding eigenvector of A^T was found by an *ad hoc* routine performing the scalar product of the eigenvectors of A and those of A^T. It used the well-known property of their eigenvectors, namely:

$$x_i \cdot v_j = 0 \quad \text{if} \quad \lambda_i \neq \lambda_j$$

This procedure was needed because the eigenvalues of A^T are not necessarily calculated in the same order as those of A. In this way, computing the scalar products and letting the zero to almost machine precision, the corresponding eigenvector of A^T has been found without any trouble.

9.1.f Calculation of the sensitivity of λ_i with respect to system parameters

This sensitivity is measured by the derivative of λ_i with respect to system parameters. It may be obtained from the following expression [30]:

$$\frac{\partial \lambda_i}{\partial p_k} = \frac{\partial \Re(\lambda_i)}{\partial p_k} + i\frac{\partial \Im(\lambda_i)}{\partial p_k} = \Re_{\partial_k} + i \cdot \Im_{\partial_k} = \frac{\left(\frac{\partial \mathbf{A}}{\partial p_k}\mathbf{x}_i, \mathbf{v}_i\right)}{(\mathbf{x}_i, \mathbf{v}_i)}$$

where $\Re(\lambda_i)$ and $\Im(\lambda_i)$ are the real and imaginary part of the eigenvalue corresponding to the spectral radius, $\Re_{\partial_k}$ and $\Im_{\partial_k}$ are the real and imaginary part of the derivative of λ_i with respect to the k-th parameter and *(a, b)* indicates the scalar product between complex vectors. This formula may be deduced by application of the chain rule of derivation to the definition of the eigenvalue problem and a suitable permutation coming from the definition of the left eigenvalue problem. It constitutes a faster alternative to the direct calculation of $\Re_{\partial_k}$ and $\Im_{\partial_k}$ by automatic differentiation of the program calculating the eigenvalue. The latter was the approach adopted by the Authors in previous work [9].

9.1.g Calculation of the sensitivity of the spectral radius with respect to system parameters

The sensitivity of the spectral radius of A (coincident with the sensitivity of the margin to instability) is calculated from:

$$\frac{\partial \Delta\rho}{\partial p_k} \equiv \frac{\partial \rho(A)}{\partial p_k} = \frac{\Re(\lambda_i)\cdot\Re_{\partial_k} + \Im(\lambda_i)\cdot\Im_{\partial_k}}{\sqrt{\Re^2(\lambda_i) + \Im^2(\lambda_i)}}$$

This expression comes from the definition of the spectral radius and considering that the eigenvalues of A are generally complex.

9.2 RESULTS AND DISCUSSION

Figure 23 shows the stability map in the plane of α and ε, the system physical parameters. They measure, as told before, respectively the buoyancy and friction resistance in the loop. This map has been obtained using 31 nodes (dimensionless space increment $\Delta s = 1/30$), Courant number $C_{OU} = 0.8$ and the exponent of flow rate in the friction term of momentum equation given by $\xi = 1.75$. The selection of these values for C_{OU} and ξ was not arbitrary: despite the low number of nodes, they ensure low numerical diffusivity while keeping the calculations stable, on one hand, and impose turbulent flow friction, on the other. The theoretical neutral stability boundary corresponds to Welander's analysis and is shown as a reference.

The interest in the analysis to follow is showing how the solution depends on the cell Courant number (C_{OU}) and ξ ($\equiv$2-b), where b is the exponent in the friction law). This has been quantified by calculating the following derivatives: $\partial\Delta\rho/\partial C_{OU}$ and $\partial\Delta\rho/\partial\xi$. One of the maps, giving the variation of $\partial\Delta\rho/\partial C_{OU}$ is shown in Figure 24.

The results obtained were coincident with the ones in [9]. However, the computational cost was one-third the original one, confirming that the present algorithm leads to a much faster code than using ADIFOR to get the derivative of $\Delta\rho$ by direct derivation of the original code. This conclusion depends on the relative cost of calculating twice the eigenvectors vs. the cost of applying the chain rule to the whole EISPACK set.

To conclude this introduction to sensitivity analysis, it may be stated that this new algorithm was developed to permit the calculation of the sensitivity of the margin to instability ($\Delta\rho$) to system parameters. It is based on the use of ADIFOR to evaluate the derivatives of the matrix of perturbations (A) and a formula relating this derivative and the eigenvalues and eigenvectors of this matrix and its transpose. The results so obtained are coincident with the ones previously reported by the authors [9]

obtained with a more massive and, then, time-consuming use of ADIFOR. The procedure is now much faster and general. It may be stated that it may be applied to linear stability analysis based on the behavior of $\Delta\rho$ in a general case.

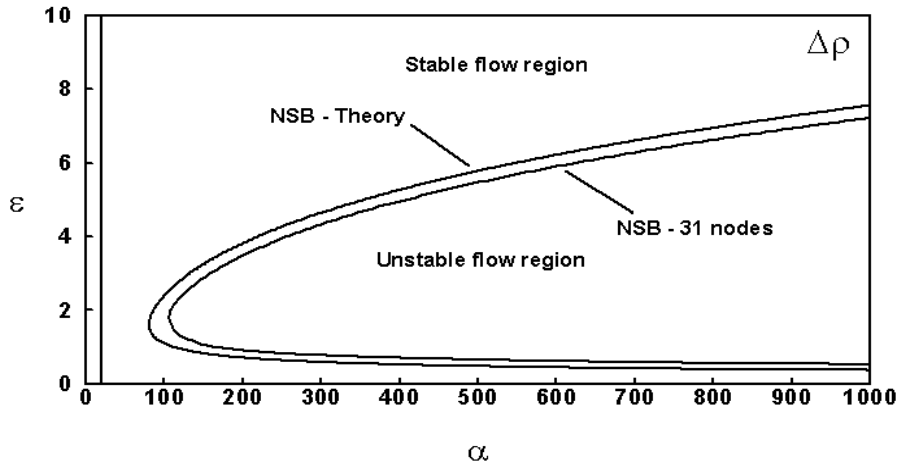


Figure 23 Map of $\Delta\rho$ for the first-order, explicit momentum, implicit temperature coupling, C_{OU}=0.8 and ξ=1.75, Δs = 1/30

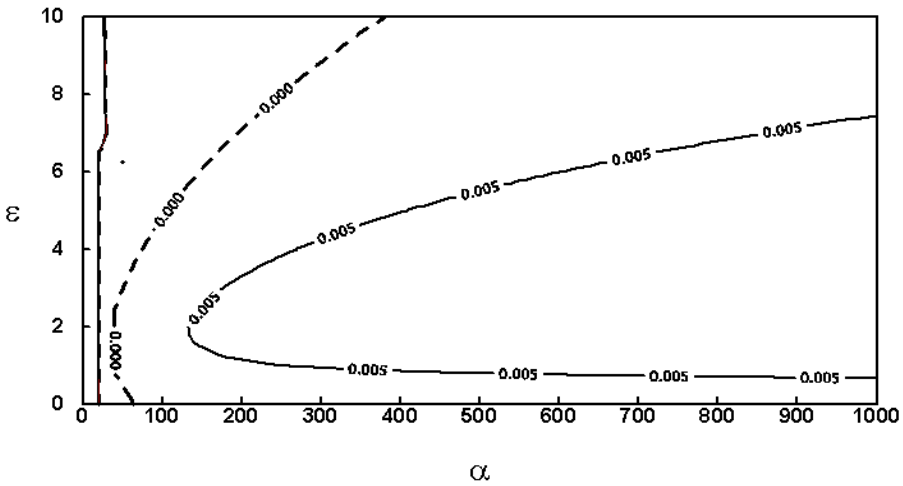


Figure 24 Sensitivity map of $\Delta\rho$ to cell Courant number ($\partial\Delta\rho/\partial C_{OU}$) for the first-order, explicit momentum and implicit temperature coupling. [C_{OU}=0.8, ξ=1.75 and Δs=1/30]

10. CFD ISSUES RELATED TO NUMERICAL PREDICTIONS OF NC AND NUCLEAR REACTOR SAFETY RELATED FLOWS

Given the level of advancement of CFD in the Computational Mechanics arena, it seems evident that the re-emerging of Nuclear Energy generation activities and constrains imposed by international Nuclear Safety guidelines and standards and improved physical models, will imply an increment of CFD activities in the field. The time to come will surely show an avalanche of works dealing with separate effects and multi-field, multiple domain computational methods that might provide a fertile ground for integral analysis.

Some collaborative efforts to elucidate the needs on CFD in relation to Nuclear Safety evaluations have been established, notably the "Evaluation of CFD methods for reactor safety analysis - ECORA" project, that involved twelve partner institutions, see [34]. The project outcome was aimed to show to end-users, utilities and regulators to which extent CFD can enhance the accuracy of safety analysis, that it implies "addressing the lack of certainty on CFD results and defining related Best Practice Guidelines (BPGs) to evaluate these results".

The objectives reached, according to authors, have been:
a) The establishment of BPGs for ensuring high-quality results and for the formalized judgment of CFD calculations and experimental data.
b) The assessment of the potential and of current limitations of CFD methods for flows in the primary system and in LWR containments, with special emphasis on pressurized thermal shocks
c) The definition of experimental requirements for the verification and validation of CFD software for flows in the primary system and in LWR containments
d) The identification of improvements and extensions to the current CFD packages needed for primary loop and containment flow analysis.
e) The implementation and validation of improved turbulence and two-phase flow models for the simulation of PTS phenomena in PWR primary systems.

The BPGs are a valuable contribution for any CFD practitioner and are closely related to many aspects considered in this paper. They are documented in [35].
This report contains detailed information on:
a) The formalized judgment of results obtained with different CFD software packages. This includes the definition and quantification of round-off, iteration and discretization errors, and the assessment of modeling errors.
b) The consistent use of CFD methods for reactor safety problems. These guidelines relate to geometry and grid generation, boundary and initial condition specification, selection of suitable physical models, and handling of solution algorithms.
c) The judgment of experiments regarding their use for verification and validation of CFD methods.

The guidelines include criteria for checking global mass, momentum, and energy balances, consistency checks for field data, and plausibility checks. Experiments are grouped in a hierarchy ranging from laboratory studies to industrial field tests. The BPGs report is intended to be a living document.

Evaluation of results validity beyond the known experimental data base range has always been one objective and an obvious difficulty of safety evaluations. Perhaps, whenever possible, designing separate effects tests to allow interpolation between extreme conditions should be a major goal to achieve from the validation point of view. The interested reader may also consult the experience reported in [36]. It may also be argued that written best practice guides are not enough. Personal exercise of them through hard working is needed. This implies the issue of user qualification, which deserved detailed discussion at these lectures. Perhaps emphasizing on the need of a discipline of analysis in depth and to promote pursuing well-founded Engineering Judgment at the Academia should be enough. Anyway, BPGs constitute a valid way to consolidate Engineering Judgment traditions.

More recently, BPGs have been updated and given a more general scope in the OECD document NEA/CSNI/R(2007)5, under the authorship of 17 specialists leaded by John Mahaffy (PSU) and an additional group of experts, whose opinions have been considered, either verbally or by e-mail.

The guidelines include (in 164 pages)

- A historical introduction, based on institutional and country contributions (most activities are reported starting in the 80's)
- Gives an account of all the aspects to be considered in setting up and applying criteria CFD methods to Nuclear Reactor Safety, including problem definitions, ranking of phenomena, gridding, verification and validation of codes. Opinions are stated in many cases and practical advises are given.
- Appropriate consideration is given to the fact that "computer simulation is much more than generating an input and observing results"
- A "check list for a calculation" is also included

Verification and validation (V&V) of CFD codes is perhaps the major present challenge for their application in NRS. A special number appeared in NED (vol. 238, 2008), edited by Prof. Y. Hassan and B. Smith, showing outcomes from "Benchmarking of CFD Codes for Application to Nuclear Safety (CFD4NRS)", 5–7 September 2006, Garching, Munich, Germany

Conclusions emerging from the meeting were:

- Best Practice Guidelines should be followed as far as practical to ensure that CFD simulation results are free of numerical errors, and that the physical models employed are well validated against data appropriate to the flow regimes and physical phenomena being investigated.
- Experimental data used for code validation should include estimates of measurement uncertainties, and should include detailed information concerning initial and boundary conditions.
- Experimenters involved in producing data for validating CFD models and/or applications should collaborate actively with CFD practitioners in advance of setting up their instrumentation. This interface is vital in ensuring that the information needed to set up the CFD simulation will actually be available, the selection of "target variables" (i.e. the most significant measurements against which to compare code predictions) is optimal, and the frequency of data acquisition is appropriate to the time-scale(s) of significant fluid-dynamic/heat-transfer/phase-exchange events.

Advanced computational tools are needed (see also [37], [38]) for, at least:

a) To implement further developments of existing physical models of two-phase flows, and the advanced, new ones proposed by the school of Ishii at Purdue and Lahey-Drew at RPI to deal with the smooth transitions in two-phase regimes, as opposed to fluid flow regime maps

b) To further develop and implement 3D, two-phase modules in commercial CFD software packages using friendly graphical user interfaces for the generation of grids and the visualization of results.

c) To develop multiple-field, multiple-scale, multi-dimensional analysis tools

d) To verify and validate all the previously mentioned theories and implementations.

In relation with d) above, it took more that thirty years to design, support, develop, consolidate and assimilate as working experience the huge mass of results associated with ITFs. Now these results are ready to be transmitted to the young generation of researchers and safety analysts. Arriving to this status by use of CFD is a present and hard future challenge to people belonging to the Nuclear Engineering community.

Another huge effort is the NEPTUNE Project, launched at the end of 2001 by EDF and CEA, considering *interalia* that

a) The major underlying stakes for the nuclear industry partners are the competitiveness of the reactors and the safety of Nuclear Power Plants.

b) The industrial situations which were identified as priority needs are all closely connected to these two major items

They consider as examples of these items:

a) The improved prediction of Departure from Nucleate Boiling (DNB) ranks among the high priority needs since it is directly linked to fuel performance;

b) the estimation of the fluid temperature field on the Reactor Pressure Vessel (RPV) in case of a Pressurized Thermal Shock (PTS) for controlling the lifespan of critical components and,
c) The prediction of the maximum cladding temperature during a Large-Break LOCA.

It seems now assured that the next generation of flow solvers will be based on different scales of solution:
a) "System" scale: dedicated to the overall description of the circuits of the reactor
b) "Component" scale, often referred to as sub channel analysis or CFD in porous media
c) "CFD or CMFD (Computational Multi-Fluid Dynamics)" where the average scale is the millimeter or less and
d) "DNS" (Direct Numerical Simulation), where the characteristic length is less than the micrometer

The needs on numerical methods (models) development include: FEM and Finite Volume methods with unstructured meshes, interface calculation and tracking, domain decomposition to deal with computation of large scale simulations, systematic application of discrete techniques in multiple thermodynamic conditions, proper treatment of interphase exchange and smooth transitions for different two-phase flow conditions and enhanced two-fluid models

Some aspects on the needs of computing resources may be summarized as follows: nowadays PCs clusters allow considering very detailed nodalizations (up to 300 10^6 FEM 3D elements grids are a feasible but a still not too common practice with 200 PCs clusters) in the Computational Fluid Mechanics arena. This allows computing the fluid flow distribution around a car in single-phase flow in a night or less starting from drawings. For a NPP, in a two loop geometry, 100 m^3 discretized at 1 cm^3 scale implies considering 10^8 elements. Then, steady state in single phase seems reachable within today computing possibilities if a multiple-scale method is used. However, it must be recalled that this implies having verified and validated parallelized algorithms as well as models amenable to this treatment.

11. CONCLUSIONS

It has been shown that CFD is not a new activity in relation to unstable flow NC computations and in Nuclear Safety. A brief historical account and some background material have been presented as an introduction to the development and use of industrial and in-house codes. It was intended to take into account the experience gained by the Authors in the simulation of experiments in rather simple 1D geometrical configurations, in single-phase flows. Comparison with experiments has been considered whenever possible and some examples of potential problems arising from closure correlations have been exemplified. In an attempt to summarize the present emphasis on the needs of an ordered transition from the use of systems codes to CFD approaches in Nuclear Safety, it may be stated that the experience gained in thirty years of using almost 1D system codes must be carefully considered. Experimentation seems considered at present to specify needs in physical and numerical models. Collaborative efforts are under way for the benefit of the whole community. Finally, it was also mentioned why a discipline of analysis in depth and to promote well-founded Engineering Judgment at the Academia would be worthwhile.

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