SINGLE–PHASE NATURAL CIRCULATION IN SIMPLE CIRCUITS - REFLECTIONS ON ITS NUMERICAL SIMULATION -

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ABSTRACT

The numerical aspects of natural circulation simulation are reviewed considering some open literature since the pioneering work of Welander (1967). The analysis starts reviewing related bibliography, and then turns to some early calculations. Some examples of code verification results dealing with experimental and theoretical results in loops are shown. In this way, a limited survey of related bibliography is introduced. The goal in mind was getting insights for the use of macro thermal-hydraulics codes. The analysis of Welander (1967) was generalized to consider turbulent flow. Having defined a theoretical stability map for the prototype problem, an unstable flow condition is defined to check the effect of the nodalization on the appearance of oscillations. In this way, it is possible to define the limits of applicability of a coarse nodalization. These results serve to illustrate how time domain codes may be used to analyze these problems and the effect of considering different constitutive laws in the computed linear stability map. It must be emphasized that the results are quantitative.

1. INTRODUCTION

The motivation for the numerical modeling of natural circulation flows (NCFs) in hydraulic circuits is based on the important applications of this subject in the engineering sciences. References to this type of flows in the last twenty years are so numerous that should provide a trivial proof of this assertion. Then, focusing on some particular aspect of this vast subject may allow for providing useful information. This presentation will focus on the numerical aspects of 1-D calculation of NCFs in the context of nuclear safety evaluations.

To comply with this goal, the following list presents some of our motivations to deal with this subject:

a) Single-phase natural circulation has a widespread range of utilization in industry, including conventional heat transfer applications, solar energy conversion and nuclear reactor cooling.
b) In the nuclear field, relying upon passive heat transfer mechanisms during plant operation and/or after postulated accidents in innovative reactors has raised new concern about the adequacy of the existing driving forces in providing regular and reliable natural circulation modes for heat removal.
c) It is difficult to establish which are the appropriate values of system parameters, like friction losses in loop components, because the flow in pipes and flow restrictions like fittings and valves is usually non-developed.
d) Lumping volumes of complicated geometry in simple ones usually determines the validity of the computational results.
e) No matter how simple the hydraulic loop can be, its behavior is usually interesting. Depending on the ratio of forcing forces (heat sources/sinks strength) to the integrated friction along the loop, the flow may become oscillatory, showing flow reversals.
f) It is well known that numerical schemes usually used in the numerical simulation of NCFs (laminar or turbulent) introduce damping in the solution. Therefore, unstable flows may be turned stable because of this added friction.
g) Numerical schemes may affect the expected convergence of computed results, even in simple situations. These effects may originate in the numerical coupling of the discrete equations or the lumping criteria, among other causes.

It is first necessary to define what we do understand by “hydraulic circuits”. In what follows we will consider systems that may be represented by one-dimensional components like pipes, elbows fittings, valves and other components of simple geometry, amenable to one-dimensional (1-D) modeling. Scaling NCFs to get appropriate, representative experimental apparatus of real life installations is not trivial and has been the subject of many analyses up to present. Relevant information on this subject may be found in Zvirin (1981), Ishii and

Kataoka (1984), D'Auria et al. (1991), Vijayan and Austrogesilo (1994) and Wulff (1999). This is an important aspect because it defines if the 1-D model will reasonably represent a given component. Sometimes, scaling forces 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 driving force), then, if the system is scaled accordingly to the power/volume ratio, the cross 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 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. The balance between these aspects is a challenge to any NCFs modeling practitioner.

The definition of system parameters resorts to well established practices, e.g. using Idel'chik's (1966) handbook. This is the usual practice but, for non-developed or time dependent flows, there are well known limitations. The same reasoning applies to closure correlations like friction resistance laws. These aspects are reviewed in many references, e.g. Zvirin (1981). The balance between friction and driving forces determines steady state in NCFs. Then, depending on our choice for closure laws, the system may present interesting peculiarities. We will come back to this aspect later, to show quantitative results.

CNFs are non-linear in essence. The modeling of the dynamic behavior of non-linear systems is presently accomplished by different techniques, depending on the characteristics of the considered problem. We leave apart lumped parameter models despite their usefulness for studying, for example, the system behavior beyond the stability threshold. It is our interest to focus in the solution of NCFs as represented by non-linear partial differential equations (PDEs). Frequently they are the only feasible choice for adequately modeling the behavior of distributed parameter systems. Then, appropriate techniques must be applied to get a reasonable picture of both stability conditions and unstable transient behavior. Two techniques are mainly used in these cases, namely: the *nodal method*, consisting in discretizing the original PDEs with main reference to an appropriate space and/or time grid, in order to obtain either systems of first order ODEs or systems of algebraic equations to be solved by conventional techniques and the *modal method*, consisting in considering the system response as a linear combination with time dependent coefficients of prescribed spatial modes, thus obtaining more or less coupled systems of ODEs.

Discretization of PDEs by numerical schemes leading to systems of algebraic equations is almost mandatory in complex cases, e.g. when a realistic simulation of plant behavior is necessary. The large thermalhydraulic (TH) system codes adopted for safety analyses of nuclear power plants are relevant examples of this choice. However, when applied to fluid-dynamic instabilities, most of the adopted numerical methods are found to be conditioned by the effect of truncation error; this introduces unwanted dissipative and dispersive effects, globally referred to as *numerical diffusion*, which may change the predicted dynamic behavior of the system. These effects are often found to make difficult a reliable stability analysis by numerical means, see e.g. Bau and Torrance (1981), Misale and Tagliafico (1987), Vijayan et al. (1995) and Wu and Almenas (1995). Examples of accurate estimates of the effect of numerical diffusion on the predicted degree of stability or instability are not so frequent. The work by wulff et al. (1992) is a rare example of a detailed quantitative assessment of the effect of truncation error in the prediction of Lasalle-2 BWR oscillations. Basic references to the effects of the numerics on computed results are the works of Stuhmiller and Ferguson (1979), Barre et al. (1993), Mahaffy (1993), Yih Yin Hsu (1994) and Ginestar and March-Leuba (1998). In passing, it may be mentioned that the work by Stuhmiller and Ferguson (1979) was one of the most interesting reports on numerical diffusion that this author has found. It was quantitative, practical and simple, although limited to the unsteady1-D scalar-advection equation. A simple demo implementation of the methods listed by Stuhmiller and Ferguson (1979), complemented with some other schemes and different types of waveforms proved to be useful for teaching purposes. The last four points in our list deal with aspects that are closely related to the subject of this presentation. They will be developed in what follows. It would suffice here to point that these aspects are related, involving modeling criteria and numerical properties of the schemes. In the common case of an end code user facing different code options, the so-called user effects will affect the results. The latter received careful attention quite recently in the field of nuclear safety evaluations (e.g. see the papers in IAEA, 1999).

2. NUMERICAL SIMULATION OF 1-D NCFs

In the papers by Ferreri and Doval (1984, 1985, 1988)) and Doval and Ferreri (1988), we started to document our experience on the numerical modeling of NCFs in nuclear safety related problems. Obviously, this subject, together with the well posedness of the governing equations in thermal-hydraulics used to be (and continues to be) a field of active work. The problem we faced was using TH system codes to compute the transition from forced circulation to NCF in a nuclear power plant. The codes used, as described in Ferreri and

Doval (1984), failed to converge toward a solution in the last stage of the simulation. This fact and the need to get results lead us to develop a 1-D, single-phase general code, including concentrated and distributed heat sources and sinks to compute NCFs. This development included the time for code verification and validation. These aspects are documented in Ferreri and Doval (1984). It is curious that Ferreri and Doval (1985) was considered too basic to be included as a companion paper to Doval and Ferreri (1988). However, it documented the damping of signals as a function of discretization in a closed loop.

In Ferreri and Doval (1984), the developed code consisted in a 1-D version of the iterative, semi-implicit SOLA algorithm. It considered an implicit finite-difference method for the energy equation in the primary loop and heat exchangers. The momentum equation was solved in two ways: a fully discrete finite-difference method using the forward-time, upwind-space (FTUS) approximation and a formulation obtained by the usual integration along the loop. The cases considered were:

1. the results in Zvirin and Greif(1979), that introduced this author to the paper by Welander (1967)
2. the validation with the results of Zvirin et al. (1981)
3. the computational simulations of toroidal loops by Mertol (1981)

It is worth introducing some remarks on these simulations. They were aimed at providing us some hints on the convergence of the numerical results to theoretical and experimental results. In Zvirin and Greif (1979), no instabilities were found, even in cases of theoretically unstable flows. These authors attributed this to the analysis technique used. The tests reported in Ferreri and Doval (1984) allowed for reproducing Welander's (1967) results and studying the effect of the friction correlation and the number of nodes (i.e. of the numerical diffusion) in the transient behavior of the loop. Consideration was given to the minimum number of cells providing enough damping to keep the results stable (in stable cases) and rapidly convergent. The economy on cell number was mandatory because of CPU time and memory restrictions by these years. Keeping in mind the final application of the code, the results in Zvirin et al. (1981) were considered. They consisted in the NCF in a "nuclear loop", formed by parallel loops and plenty of fittings. The results reported by Ferreri and Doval (1984) were compared with those in Zvirin et al. (1981). Surprisingly, our results got better approximation with respect to the experimental ones. No doubt, it was due to a fortuitous choice of better system parameters, that critical aspect we mentioned in the introduction. The theoretical results reported in Ferreri and Doval (1984) also considered the neutral oscillations in a toroidal loop as given by Mertol (1980). In this case the task was determining the minimum number of cells necessary to keep the system in neutral oscillatory state around the theoretical steady-state flow rate. We learnt a rule: one to one ratio up to one to three between length and diameter usually assured catching flow oscillations. The analysis of non-linear systems, as applied to NCFs in loops, was beginning with a theoretical analysis by Hart (1984, 1985). The conceptual explanation of flow instabilities in Welander (1967) remained valid in these analyses. Bau and Wang (1992) reviewed the literature related to this way of analysis. It kept growing up to date.

The aforementioned process of verification and partial validation of the code allowed us to simulate the situation of our interest, namely: the single-phase NCF in a simplified version of a nuclear power plant (NPP). It must be mentioned that in this NPP (Atucha-I pressurized, heavy-water NPP) the core consists in nearly 250 vertical channels immersed and packed in a moderator tank. Therefore, the 1-D approximation was a reasonable one. The first stage of the transient consisted in a pump trip without depressurization. Then, after the reactor scram, the flow diminished up to the point in which NCF was established. At this point, the system code (RELAP4/MOD5 by these days) ceased to converge. The values of the system parameters were feed to our in-house developed NCF code and, after some minor oscillations, O(10%), stabilized quite nearly to the macrocode values. After this, we simulated a transient, whose results in the long term, i.e. the steady-state flow rate for residual power, fairly agreed with the one known by design. It was a signal of the appropriate simulation of the ratio between driving forces to loop friction. These important phenomena, in the case of CANDU pressurized, heavy-water NPP was not considered at that time. However, up to recently Vijayan and Date (1990, 1992) has been the subject of active research. Then, in spite of the limited validity of the code capabilities the results were quite good. In the author's opinion, it was just a consequence of the time spent during the stage of verification and partial validation.

The use of TH system codes is essential for the safety assessment of NPPs. Doing so leads to the question of the validity of the results, in terms of the adopted simulation criteria. Discretization is the obvious subject of interest here and in what follows we will focus our interest in this important aspect of code utilization. There are many references associated with this subject, see e.g. the works by D'Auria et al. (1991, 1997, 1998) and Wulff (1992).

Based on the experience gained in the aforementioned developments, it was decided to check the applicability of the new series of TH systems codes like RELAP5/MOD3.2 (see Carlson et al., 1990) in the calculation of unstable flow problems. There was also another motivation: for sure, the same limitation should exist because the numerical approach was similar to previous versions and the nodalization practice was the

same. We also found increased interest on the subject in blind inter-comparison experiments, e.g. the final report by Ferraz Bastos (1997).] and simultaneous, work as in Wu and Almenas (1995), among many others.

The approach was taking again the results of Welander (1967), setting up an unstable problem, analyze the problem as a standard physical problem using RELAP5/MOD3.x and checking the nodalization until obtaining the expected unstable solution. At the same time, analytical results regarding the stability analysis for turbulent flow were derived and some codes with different numerical schemes were developed and tested. Finally, the results included different loop geometry. The technique was also extended to include simple models in two-phase flows. All this work was summarized in Ferreri et al. (1995), Ambrosini and Ferreri (1997a, 1997b and 1998) and Ferreri and Ambrosini (1999). What follows is a brief presentation of these results, making free use of some texts in these references.

In Ferreri et al. (1995), Welander's (1967) problem -referred as WP67 from here on- was put under analysis using the RELAP5.x series of codes. As already mentioned, these results deal with the natural circulation in a very simple situation, namely: flow driven by buoyancy in a loop constructed with parallel, adiabatic, vertical tubes. The loop has a point heat source in its bottom and a point heat sink in its top. The mode of heat transfer is such that the product of the heat transfer coefficient in the heated length by the heated length is kept constant when the heated length tends to zero. This defines the heating rate. The same concept is applied in the heat sink. In this way, the physically finite heat source (sink) becomes a point. Welander (1967) performed his analysis only for laminar flow. However, his results may be generalized to consider turbulent flow. Chen (1985), among many other authors, performed such analysis for a more general loop considering heated (cooled) horizontal tubes of finite length. In Ferreri et al. (1995) the analysis in WP67 was generalized in order to keep strictly the same hypotheses of the original derivation.

Fig. 1 shows the geometry of this simple hydraulic system, adapted from WP67. It is a schematic representation of the loop, appropriate for its discretization following the RELAP5 code specifications. The vertical legs are adiabatic, smooth, circular tubes of length L/2 and diameter D. The length of both the heat source and the heat sink is S. The cross section of the tubes is A. When S tends to zero, the heat transfer from/to the heat source/sink (shaded in the Figure) is increased to keep constant the total heat transferred.

To deduce the governing equations, the validity of the Boussinesq expansion of the fluid density in terms of temperature will be assumed. The friction will be computed from the Poiseuille law for laminar flow and from the Blasius law for turbulent flow.

Then, the governing equations are:

i) The momentum equation integrated along the loop:

$$\frac{dq}{dt}+\frac{a\cdot R}{16}\left(\frac{D}{\nu\cdot A}\right)^{1-\theta}\cdot q^{2-\theta}=\frac{\beta g A}{L}\int_0^{L/2}(T-T_0)\cdot ds$$

In this expression, the anti-symmetry of the system has been considered.

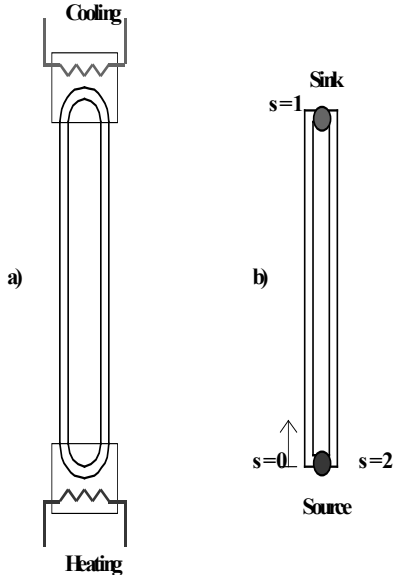

FIGURE 1a,b A schematic view of the natural circulation loop, adapted from Welander (1967)

ii) The energy equation, expressed in terms of temperature:

$$\rho C_p\left[\frac{\partial T}{\partial t}+\frac{q}{A}\frac{\partial T}{\partial s}\right]=\begin{cases}\pi DSH(T_F-T)\\0\end{cases}$$

In this equation, the first equality holds at the source/sink, and the second indicates the adiabatic walls of the tubes.

iii) The heat balance at the point heat source/sink:

$$T_S-T_{SI}=(T_F-T_{SI})\cdot\left[1-e^{-\left(\frac{\gamma HS}{q}\right)}\right],\qquad q>0$$

In the previous equations, written in dimensional form, q is the volumetric flow-rate, T is the fluid temperature, H is the heat transfer coefficient, ν is the fluid kinematical viscosity, ρ is the reference fluid density, θ is a coefficient equal to 1 for laminar flow and 1/4 for turbulent flow (the exponent in the Blasius friction law), a is the coefficient in the friction law: it equals 16 for laminar flow and 0.079 for turbulent flow, β is the volumetric expansion coefficient of the fluid and g is the acceleration of the gravity. The sub-index SI means a condition evaluated at the input of the source, sub-index S is a condition prevailing in the source and sub-index F indicates temperature evaluated at the source wall. In the momentum equation there is a derived coefficient R and, in the energy equation, it is γ. Their definitions are:

$$R=32\frac{\nu}{D^2}\qquad\text{and:}\qquad\gamma=\frac{\pi D}{\rho C_P}$$

The definition of R takes into account the total frictional force that must exist in the loop to make the results in WP67 coincident with those given considering the Poiseuille's law.

If the temperature at the heat source wall is set at ΔT degrees above the average loop temperature and considering steady state, the flow-rate may be found using the previous equations, from the following implicit equation:

$$2\delta\cdot q_{SS}^{2-\theta}=\Delta T+\delta\cdot q_{SS}^{2-\theta}\cdot\left[1-e^{-\left(\frac{\gamma}{q_{SS}}HS\right)}\right]$$

where δ is defined by:

$$\delta=\frac{2a\left(\frac{D}{A\nu}\right)^{1-\theta}\frac{\nu}{D^2}L}{\beta gAL}$$

The solution must be iterated if the flow-rate does not coincide with the postulated flow regime. In non-dimensional terms this equation specifies the relation between flow-rate and steady state temperature in the loop, namely:

$$\frac{2\cdot Q_{SS}^{2-\theta}}{\frac{\alpha}{\varepsilon_1}+Q_{SS}^{2-\theta}}=1-e^{-\frac{1}{Q_{SS}}}$$

where:

$$Q=\frac{q}{(KS)A}\ ;\quad\Theta=\frac{T}{\Delta T}\ ;\quad\alpha=\frac{\beta g\Delta TL}{2(KS)^2}\ ;\quad K=\frac{\pi DH}{\rho C_P A}\ ;\quad\varepsilon_1=\frac{a}{16}\left(\frac{DKS}{\nu}\right)^{1-\theta}\cdot\varepsilon\ \text{ and }\quad\varepsilon=\frac{RL}{2(KS)}$$

When θ=1 and a=16 the previous equations reduce to the ones in WP67. The linear analysis of the stability of the steady state equations may be performed in similar terms as in WP67. Now, ε_1 is an additional parameter measuring the influence of the Reynolds number in the system. For a given value of Q, the effect of increasing the Reynolds number consists in a shift of the neutral stability curve toward lower values of ε

Let us now consider a lumped parameter approach to model the heat transfer from the heat source toward the fluid (the anti-symmetrical situation must be considered for the sink). The steady state energy equation, evaluated at the source, gives the value of the temperature in the fluid. For this purpose the steady state energy equation and an upwind approximation are used. Then, the value for the fluid steady state temperature at the source is:

$$\Theta_{SS} = \frac{1}{1+2Q_{SS}}$$

Taking into account that Q_{SS} depends only on the quotient α/ε and on ε_1 that are non-dimensional parameters depending on the parameters of the system and on the product K.S that must be kept constant, it may be concluded that the results obtained applying the r.h.s. of the energy equation as it stands, will not change increasing the nodalization. For example: if $\alpha/\varepsilon=2$ and $\theta=1$ (laminar flow), then $Q_{SS}=0.958$ and $\Theta_{SS}=0.479$ from the theory. The value, as computed from the above given approximation is $\Theta_{SS}=0.342$. There is only one way for the obtaining of the correct steady state value of TS, it is to get the analytical solution of of the boundary condition expression, averaging over the length S. Following this procedure and using the upwind approximation for the advective term, the expression for Θ_{SS} is:

$$\Theta_{SS} = \frac{F}{2-F} \quad , \quad \text{where: } F = 1 - e^{-1/Q_{SS}}$$

The value of Θ_{SS} computed with this expression is coincident with the theoretical value. This analysis is quoted in Ferreri and Ambrosini (1999), and was documented by Grandi and Ferreri (1991).

The geometry of the loop and the working conditions are described in what follows. The loop was 10 m high (L = 20 m), formed by two parallel smooth tubes of 0.1 m of internal diameter. The heat source/sink were simulated considering heat structures of cylindrical geometry of 0.2 m internal diameter. To keep their temperature fairly constant, a wall material of high thermal conductivity (100 W/m^{2}K), with a volumetric heat capacity of 10000 J/m^{3}K) was considered. The wall was made very thin (0.0001 m). The roughness parameter was 10^{-7}. The flow parameters were as follows: The initial temperature in the fluid was 193.15 K. and after 0.1 s the temperature at the source wall was raised to 303.15 K. The flow was started imposing an arbitrary, small flow-rate of 0.001 kg/s. The imposed heat transfer coefficient at both the heat source and the heat sink was 1000 W/(m^{2}K). The time step in the integration was 0.5 s, while the spatial increment was variable and will be specified case by case in the analysis to follow. The flow started at very low flow-rate and began to grow up to the steady state value. The temperature in the loop increased up to the moment in which it reached an average value as given by its theoretical value, the latter depending on the adopted criteria for the source/sink lumping.

The effect of heated length parameter will be discussed first. For these calculations the following spatial discretization have been considered: 10 nodes in each leg (Δx = 1 m) and S = 1.0, 0.5 and 0.1 m (correspondingly, the values for H were: 1000, 2000 and 10000 W/m^{2}K). It must be pointed out that the flow was theoretically unstable with these parameters. The code was RELA5/MOD3.0. As expected, the value of the steady state temperature was almost the same, with small differences that were due to the different total friction in the loop. Then, to improve convergence toward theoretical values, an average, lumped heat source was used, as suggested previously. It leads to convergence in heat transfer rate.

Let us now consider the problem of convergence of the code results to the expected, unstable results. To do this let as suppose that we do not know that the flow is unstable and proceed like engineering judgment suggests: look for convergence of computed results. For this purpose the nodalization considering S=0.1m and 10000 W/(m^{2}K) were used. The number of nodes in each leg was varied accordingly up to the point in which the expected chaotic behavior was obtained. The latter made its first appearance when the number of nodes per leg was increased from 25 to 50. Nearly neutral oscillations in flow-rate were observed for 37 nodes per leg. More than 20 runs were made to test different cases, including laminar flow and stable situations Ferreri and Ambrosini, (1999).

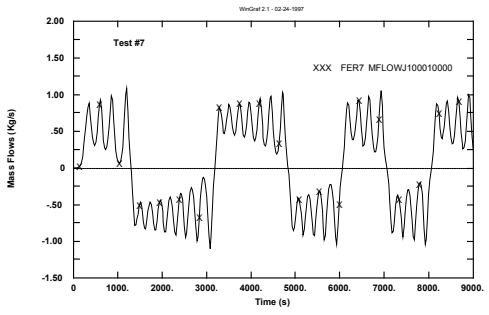

Figure 2 Time variation of flow-rate. Number of nodes per leg: 90, S=0.1m, α = 339, ε=2.3

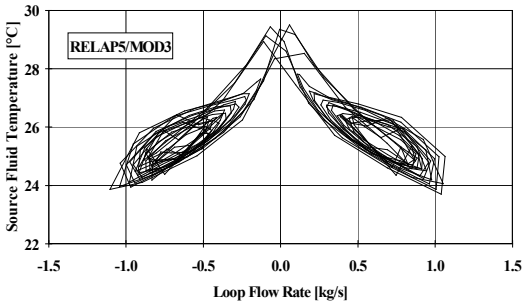

Figure 3 Projection of the attractor in the phase space as calculated by RELAP5/MOD3 using 90 nodes per leg, α = 339, ε =2.3

Fig. 2 shows the time variation of flow-rate using 90 nodes per leg and 0.001 Kg/s of starting flow-rate. As may be observed the flow is oscillatory, switching from positive to negative values after some cycles of oscillation. Fluid temperature varies correspondingly. The system behavior may be observed more clearly when the temperature in the source is plotted versus flow-rate in the loop. Fig. 3 is a clear indication of the chaotic behavior of the system. This behavior is not surprising. What is interesting is that it was obtained using the RELAP5 code. The same considerations would apply to any other systems code.

In what follows, a more detailed numerical analysis will be outlined, making reference to the FTUS approximation. This numerical scheme is quite similar to the one used in RELAP5. Then the algebraic equations expressing the energy balance for q>0 are the following:

$$\Theta_i^{n+1} = (1 - C)\,\Theta_i^n + C\,\Theta_{i-1}^n \qquad (i=2, \ldots, N-1)$$

$$\Theta_N^{n+1} = \left(1 - C - \frac{\Delta t}{\Delta s} F_{nod}(Q^n)\right)\Theta_N^n + C\Theta_{N-1}^n - \frac{\Delta t}{\Delta s} F_{nod}(Q^n)$$

$$\Theta_1^{n+1} = -\Theta_N^{n+1}$$

with similar expressions for q<0. C is the cell Courant number: $C = \frac{Q^n \cdot \Delta t}{\Delta s}$ and $\Delta s = \frac{1}{N-1}$ is the space interval, with N being the number of nodes. The function $F_{nod}(Q)$ is a source-sink heat transfer multiplier, similar to the one adopted for the nodal expansion, introduced in order to calculate the steady-state conditions in coincidence with the exact solution.

The momentum equation is discretized in time as follows:

$$Q^{n+1} = Q^n + \left(\alpha \Delta s \sum_{i=1}^{N-1} \frac{\Theta_i^n + \Theta_{i+1}^n}{2} - \varepsilon (Q^n)^{2-\theta}\right)\Delta t$$

The assessment of the effects of nodalization on the onset of instabilities will be performed using the previous expressions. However, as will be mentioned later, some other methodologies have been also considered. This approach can be considered the numerical analogue of the classical linear stability analysis of PDEs. The main reasoning behind the methodology is shortly summarized in what follows. A finite-difference numerical method for a time-marching problem can be written as an algebraic N-vector equation relating the N values of the unknown function at the n-Th. and (n+1)-Th. time level ($\underline{y}^n$ and $\underline{y}^{n+1}$), grid parameters (in the present case, Δs and Δt) and physical parameters (α, ε). This algebraic equation represents the discretized form of the original PDEs together with the related boundary conditions. In our specific case for the above-described numerical methods it is:

$$\underline{F}(\underline{y}^n, \underline{y}^{n+1}, \Delta t, \Delta s, \alpha, \varepsilon) = 0 \qquad (1)$$

It will be now shown that studying stability of steady-state solutions of a mathematical problem is capable of clearly pointing out the effect of truncation error brought about by the nodalization and that care must be taken in avoiding numerical instabilities or in recognizing them in the obtained stability maps.

The vector function $\underline{F}$ is generally non-linear. Therefore, determining the steady state conditions (i.e., the fixed points) may require the iterative solution of the equation:

$$\underline{F}(\underline{y}^n = \underline{y}_{SS}, \underline{y}^{n+1} = \underline{y}_{SS}, \Delta t, \Delta s, \alpha, \varepsilon) = 0 \qquad (2)$$

Once the fixed points have been determined, their stability can be studied through linearization by perturbation. Then, considering small deviations from the selected fixed point:

$$\underline{y}^n = \underline{y}^S + (\delta \underline{y})^n \qquad \underline{y}^{n+1} = \underline{y}^S + (\delta \underline{y})^{n+1}$$

Substituting into Eq. (1), second order terms can be neglected and Eq. (2) can be used to reach the following relationship between perturbations at the n-Th. and at the (n+1)-Th. time levels:

$$(\delta \underline{y})^{n+1} = -(\underline{\underline{J}}_S^{n+1})^{-1} \cdot \underline{\underline{J}}_S^n \cdot (\delta \underline{y})^n$$

where $\underline{\underline{J}}_S^n$ and $\underline{\underline{J}}_S^{n+1}$ denote the Jacobean matrices of $\underline{F}$ with respect to $\underline{y}^n$ and $\underline{y}^{n+1}$ respectively, calculated at the selected fixed point. It is then argued that stability can be discussed considering the eigenvalues of the matrix:

$$\underline{\underline{A}} = -(\underline{\underline{J}}_S^{n+1})^{-1} \cdot \underline{\underline{J}}_S^n$$

as results assuming exponential growth or decay of perturbation vectors. In particular, given the spectral radius of the matrix, $\rho(\underline{\underline{A}})$, it is useful to consider the quantity:

$$\Delta\rho = \rho(\underline{\underline{A}}) - 1$$

quantifying the *margin in excess to neutral stability*. It takes negative values for stable conditions and positive values for unstable ones. This quantity can be therefore used to find neutral stability conditions and to set up stability maps. Then, it is here preferred to calculate $\Delta\rho$ throughout a selected α,ε rectangular domain, thus identifying with the aid of contour plots regions with a different degree of stability. This method is easier to implement in computer programs and has the advantage to provide a greater deal of information, at the price of a reasonable increase in computing effort. Fig. 4 shows the results obtained for the FTUS method with 30, 40, 50 and 100 nodes and $\Delta t=10^{-4}$.

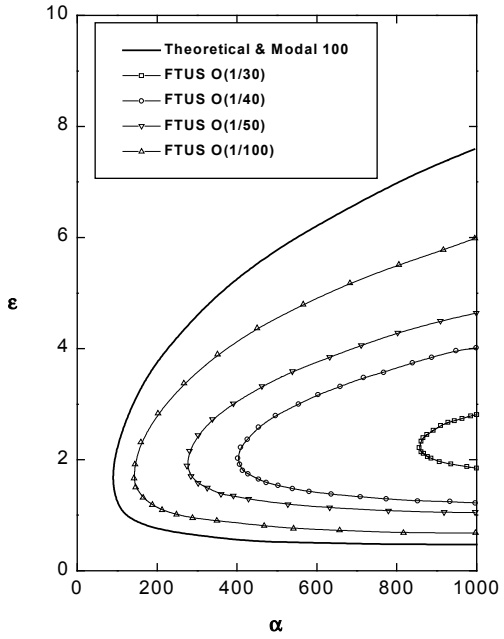

Figure 4 The effect of the number of nodes on the neutral stability curve using FTUS

It is interesting to compare the results obtained using the explicit upwind method with the results of a modal solution with a second order term simulating numerical diffusion. With this aim, the diffusion coefficient is defined as:

$$D(Q) = \frac{|Q|\,\Delta s}{2}\left(1 - \frac{|Q|\,\Delta t}{\Delta s}\right)$$

as resulting from the analysis of truncation error for the FTUS method. Fig. 5 shows the predicted flow rate variation with time. The diffusion coefficient was the one corresponding to 1000 nodes under the FTUS approximation. The number of modes considered in the modal expansion was 500. As may be observed, both approximations behave similarly. Exact coincidence is precluded by the non-linearity of the system. It may be shown that the predicted stability conditions are very similar for the nodal and the modal solution with equivalent dissipative effects and the agreement is improved by increasing the number of nodes. This confirms the overwhelming importance of the second order term alone in determining the overall truncation error effect on stability predictions.

The analysis of the stability maps obtained with the FTUS method and C=0.8 or with second order methods and $\Delta t = 10^{-3}$, pointed out the appearance of regions of instability larger than those predicted by the reference modal solution. The possible reasons for this behavior were mainly two, namely: a) an effect of truncation error at large time steps on the velocity of propagation of perturbations along the legs, related to the dispersive effects brought about by odd-order derivatives; b) the effect of the use of a large time step in momentum equation, giving rise to a general tendency to instability due to delayed feedback

In what follows it will be shown that, although the first effect cannot be excluded, the second is the leading one, being responsible for the observed over-prediction in the extent of the unstable region.

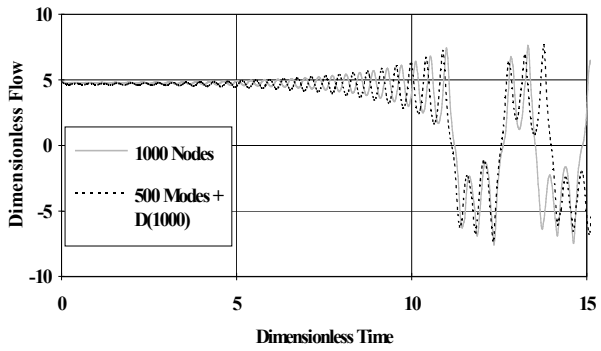

Figure 5 The flow rate for the FTUS scheme using 1000 nodes
and a modal expansion with 500 modes and the FTUS O(1000) truncation error

In all the cases considered (FTUS and second order methods), the adopted discretization for the momentum equation implied that both the temperature integral along the loop and the friction term have been evaluated making use of old-time-level quantities. The results obtained making use of this form are shown in Figs. 6 and 7, both for the FTUS method. It can be noted that in the case of FTUS with C=0.8, the over-prediction of the extent of the stability region is remarkable. In the case of the MacCormack method with $\Delta t = 10^{-3}$, a slight discrepancy with the modal solution was also found.

The following approach was used to discriminate among the possible causes of this convergence "coming from outside" to the neutral curve: a) considering a fully implicit linearized approximation of the friction term in the momentum equation: this approach did not lead to any improvement in the results. On the contrary, the degree of over-prediction was larger, showing a more pronounced dependence on C. b)Evaluating the friction term and the temperature integral term based on (n+1)-Th time level values (It did not increase too much the computational effort):

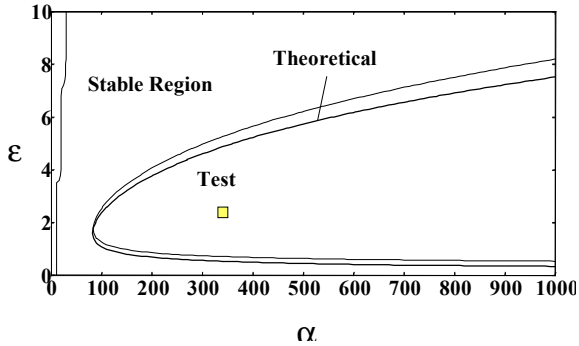

Figure 6 - FTUS scheme with C=0.8 and explicit momentum equation (30 nodes)

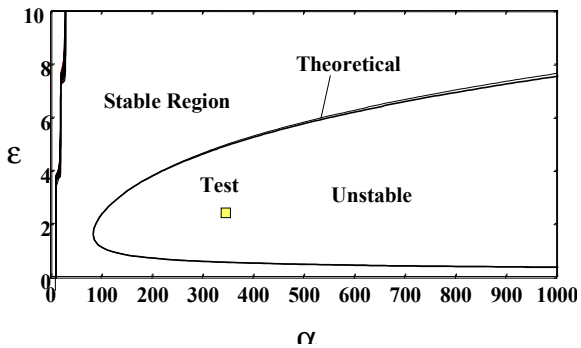

Figure 7 - FTUS scheme with C=0.8 and explicit coupling (100 nodes)

Therefore, the following form of momentum equation results:

$$Q^{n+1} = Q^n + \left(\frac{\alpha}{N-1} \sum_{i=1}^{N-1} \frac{\Theta_i^{n+1} + \Theta_{i+1}^{n+1}}{2} - \varepsilon \, (Q^n)^{1-\theta} \, Q^{n+1} \right) \Delta t$$

Using this momentum equation in the FTUS scheme, the stability maps reported in Fig. 8 were obtained. It can be noted that no over-estimate of the unstable region was found, showing the usual diffusive behavior.

The analysis above clearly demonstrates that of the two above envisaged reasons for overestimating instability, that related to the time discretization of the momentum equation is certainly dominant.

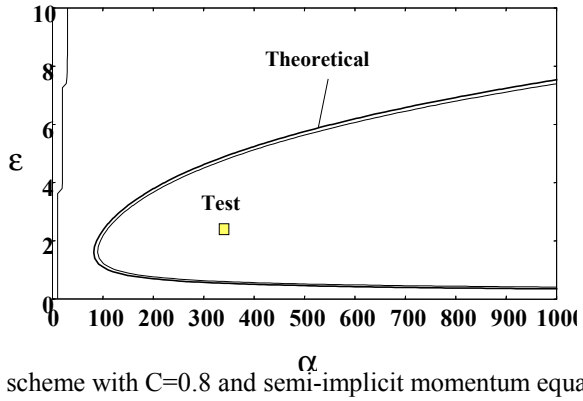

Figure 8 FTUS scheme with C=0.8 and semi-implicit momentum equation (100 nodes)

In previous paragraphs, the effect of closure relations was mentioned. In the following, we turn to this aspect in a quantitative way. The analysis of NCFs in toroidal loops with imposed heat flux is quite appropriate for this task. This problem has been studied, both theoretically and experimentally, by several authors considering different kinds of boundary conditions, see e.g. Hart (1984a,b) and Sen et al. (1985). Ambrosini and Ferreri (1997) considered the specific boundary conditions addressed by Sen (1985).

A typical case of closure law selection is related to the choice of the wall friction law. In the available literature dealing with stability of natural circulation in single-phase loops, a choice is always made about the form of the wall friction law to be used in analytical developments and about the coefficients to be adopted. This limit the analysis to either laminar flow or turbulent flow conditions, without any possibility to account for transition between them, since the Reynolds number is not used as an independent flow variable.

Trying to compensate for the above discussed deficiencies in available models, a step towards a greater realism in the analytical description of natural circulation loops was considered by Ambrosini and Ferreri (1997), namely selecting the Reynolds number as main flow variable in the dimensionless equations for the toroidal loop. The resulting equations are:

Momentum balance equation

$$\frac{d\,R_e}{d\tau} = \frac{G_r}{2}\int_0^2 g^*(s)\,\theta(s)\,ds - \frac{L}{D} f(R_e)\;R_e\,|R_e|$$

Energy balance equation

$$\frac{\partial\theta}{\partial\tau} + R_e\,\frac{\partial\theta}{\partial s} = q'''(s) + F_o\,\frac{\partial^2\theta}{\partial s^2}$$

where

$$G_r = \frac{\rho^2\, g_o\, \beta\, \Delta T\, D^2\, L}{2\,\mu^2}\;,\; R_e = \frac{\rho\, w\, D}{\mu} \quad \text{and} \quad s = \frac{2S}{L}\;,\; \theta(s) = \frac{T(s) - T_o}{\Delta T}\;,\; \Delta T = \frac{2\, L\, q_o''}{C_p\,\mu}$$

$$g^*(s) = \frac{g(s)}{g_o} \qquad q^* = \frac{q''(s)}{q_o''} \qquad \tau = \frac{t}{T} \qquad T = \frac{\rho\, D\, L}{2\mu} \qquad F_o = \frac{\alpha T}{[L/2]^2}$$

Concerning the boundary conditions it is assumed that the heat flux is uniform and constant in both the heating and the cooling sections. With these conditions, the problem has two steady-state solutions, one for positive and the other for negative flow, in a limited range of γ, which is the angle of asymmetry in heating.

As is well known, the problem is amenable to a very simple modal solution, in which only three equations are found to fully govern the dynamics of the loop, see e.g. Hart (1984a,b). With the present notation, assuming the following expression for dimensionless heat flux (corresponding to uniform heating and cooling in the two halves of the loop):

$$q^*(s) = \sum_{k=0}^{\infty} \frac{4(-1)^k}{(2k+1)\pi}\cos[(2k+1)\pi(s - \frac{\gamma}{\pi})]\;,$$

the three modal ODEs are obtained by expanding the temperature distribution in series of trigonometric functions and applying the usual weighting technique, namely:

$$\frac{d\,R_e}{d\tau} = G_r\,\frac{\Psi_1}{2} - \frac{L}{D} f^*(R_e)\,R_e\,|R_e|$$

$$\frac{d\,\Psi_1}{d\tau} = \pi\,R_e\,\Omega_1 - \pi^2 F_o \Psi_1 + \frac{4}{\pi}\sin\gamma$$

$$\frac{d\,\Omega_1}{d\tau} = -\pi\,R_e\,\Psi_1 - \pi^2 F_o \Omega_1 + \frac{4}{\pi}\cos\gamma$$

Were Ψ_1 and Ω_1 are the coefficients of the sinus and cosines of the first mode. In particular, the case with Fo=0 is considered in this paper.

To check the effect of the choice of flow regime transition criteria on the stability boundary, three different laws for the Fanning factor have been used. In particular, the laws adopted are:

a) the Blasius law

$$f(R_e) = \frac{0.079}{R_e^{0.25}}$$

b) a law with smooth transition between laminar and turbulent flow

$$f(R_e) = \sqrt{f_{lam}^2 + f_{turb}^2}$$

with

$$f_{lam} = \frac{16}{R_e} \qquad f_{turb} = \frac{0.079}{R_e^{0.25}}$$

c) the formulation by Churchill, with an σ/D ratio of 0.0001.

Plots of these relationships are shown in Fig. 9. The linear stability analysis of the equations system for the positive flow, steady-state conditions can be easily performed by the usual linearization techniques. In this work, stability maps have been obtained mapping the real part of the eigenvalue of the linearized ODE system having maximum norm, z_r. This quantity also measures the degree of amplification or damping of perturbations and is used to define the conditions for neutral stability ($z_r = 0$) and the regions of stability ($z_r < 0$) or instability ($z_r > 0$).

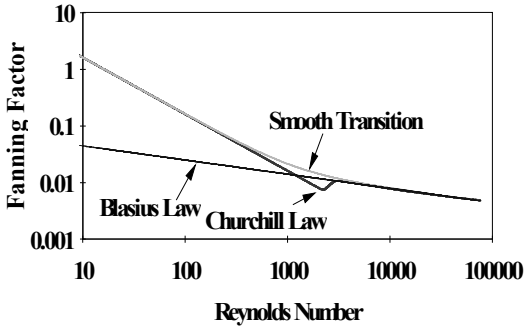

Figure 9 Different friction laws adopted for the toroidal loop

The maps in Figs. 10 to 12 clearly show the impact of the choice of the friction law on the linear stability boundary. In this connection it must be remarked that the use of a simple power law for the Fanning factor, which is the usual choice in literature on thermosyphon loops, gives a very poor representation of the situation occurring when a realistic law is used and the regime transition falls in the parameter domain of dependence.

In order to show that the previous behavior is not an artifact of numerical computation, the same map of Fig. 12 have been computed using the FTUS scheme. Fig. 13 shows almost converged results when the number of nodes increases. It is a direct poof of the dramatic influence of the closure relations, no matter what is the numerical scheme used. It may be argued that it is an obvious consequence of the modeling criteria. However, to the author's knowledge, it is no so usual to find a quantitative determination of said effects. Ambrosini and Ferreri (1997) also analyzed the results of Vijayan and Date (1990).

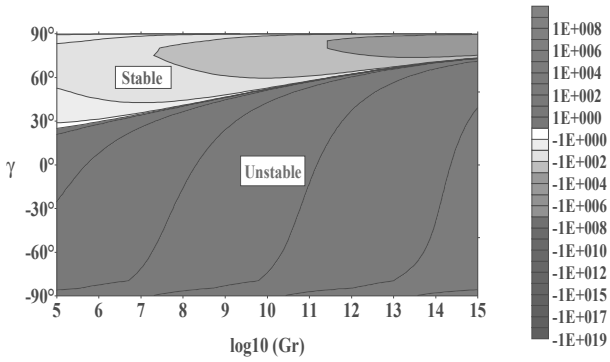

Figure 10 Modal stability map for the toroidal loop (Blasius law, L/D = 100)

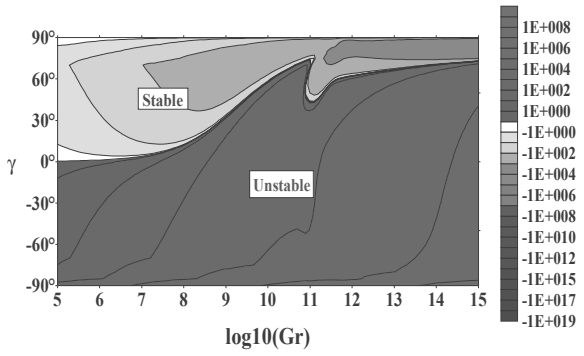

Figure 11 Modal stability map, toroidal loop (Churchill formula, $\sigma/D = 0.0001$, L/D = 100)

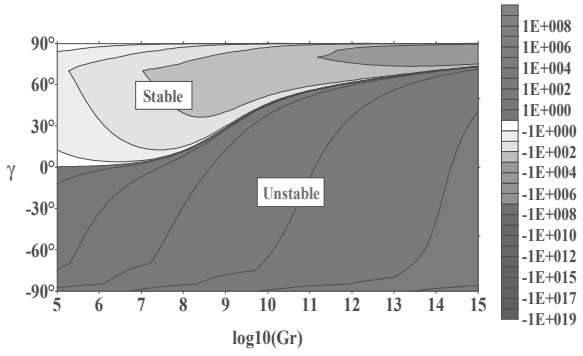

Figure 12 Modal stability map for the toroidal loop (smooth transition, L/D = 100)

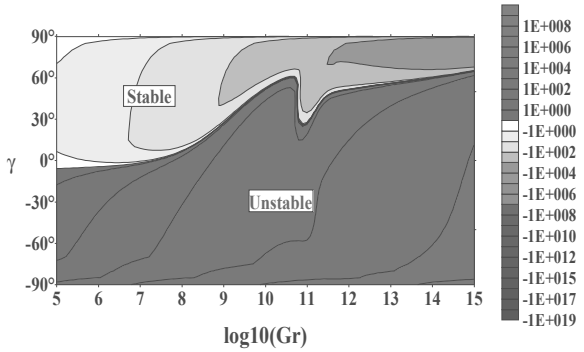

Figure 13 - Toroidal loop: quantitative stability map obtained with FTUS method using 100 nodes (Churchill friction law, $\sigma/D=0.0001$, L/D = 100, $\Delta\tau = 10^{-7}$)

CONCLUSIONS

Conclusions will be drawn from the results presented. The analysis began discussing the general aspects of NCFs in 1-D systems; following this we focused on some early results, showing the philosophy adopted for these simulations. This is the typical one: gaining experience from the use of in-house developed codes, adapted to simple situations. Here the first reflection becomes known: *the time necessary for this work to be completed may be (and usually is) conflicting with the time allowed by managers to get meaningful results.* Allowing for a reasonable balance between both times usually proves to be rewarding.

System codes must be "robust", in the usual nomenclature. Unfortunately, it means that they should produce good results (or simply results) in most cases. Experience gained shows that old problems tend to persist; no matter how recent a code may be. Avoiding numerical difficulties usually imply the use of numerical damping, the basic tenet being the use of full upwinding. Due to the intrinsic no-linearity of NCFs, coupled problems of heat and fluid flow use linearizations and/or averaging that imply changing the time constant of the computed results, adding damping. Then, the use of sensitivity analysis techniques or looking for convergence of results in a *brute force* way is again rewarding. A second reflection may be stated as: *it is fortunate that thermal-hydraulics is non-forgiving, because this forces the search for physically sound results.* It, in turn, forces the use of adequate techniques.

Time domain codes may be used to analyze unstable flows, if an adequate nodalization is used. This is not a new conclusion, but it is sometimes granted that frequency domain codes should be used. Then, the third reflection is: *as is well known, no recipe is valid for every situation.*

A TH model is defined not only by conservation equations. The simplest module in a code restricts the results. This is particularly simple to visualize in simple codes, resorting to changes of variables. This is not possible in system TH codes. The case of friction laws was exemplified, showing these effects. Then a fourth reflection may be *searching how a TH code deals with closure relations may uncover the reasons for unexpected results*.

Most of the observed qualitative trends were fully expected based on previous knowledge about the characteristics of the considered numerical schemes. The quantitative information presented provides a clear picture of the changes that truncation error may induce in predictive capabilities about stability.

In particular:
a) as well known, among first order numerical methods, explicit schemes must be preferred for stability analyses; anyway, even with explicit methods, in order to achieve acceptable performances it is necessary either to adopt Courant numbers close to the stability limit or to increase spatial detail, which may be not very convenient and feasible choices in some applications;
b) on the other hand, first order implicit numerical methods confirm to be inadequate when dealing with stability problems and should be avoided unless a very high detail is adopted in spatial discretization;
c) though the observed behavior of the considered numerical methods has mainly a diffusive character, it was found that an explicit treatment in momentum equation discretization may lead to an over-prediction of instability;
d) it is remarkable that second order explicit numerical methods could obtain with only 10 nodes a greater accuracy in predicting the stability threshold than first order ones with 100 nodes;

These considerations support the use of higher order numerical schemes in all the cases in which stability prediction is the relevant objective. However, feasibility of this choice should be demonstrated considering that:
a) a certain degree of diffusion is generally considered desirable in code applications since it helps increasing "robustness": a reasonable compromise must be reached between robustness and capability to predict the dynamic behavior in fluid-dynamic systems;
b) on the other hand, the use of higher order numerical methods can be considered advisable only when dealing with well-posed time-marching PDE problems, which is not the case for some of the present TH system codes.

ACKNOWLEDGEMENTS

The work summarized here was possible due to the support and collaboration of many colleagues. However, I must specially mention my early work with Ing. Alicia S. Doval at the CNEA, Argentina. More recently, the joint work with Dr.Walter Ambrosini, University of Pisa, proved to be fruitful. His skill and dedication allowed for obtaining many of the results herein shown. I gratefully acknowledge his collaboration. The author is also deeply grateful by the warm and generous friendship of the staff of the DCMNP, University of Pisa, along all these years of collaboration.

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