SENSITIVITY TO PARAMETERS IN SINGLE–PHASE NATURAL CIRCULATION VIA AUTOMATIC DIFFERENTIATION OF FORTRAN CODES

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ABSTRACT

In previous work, the authors have analyzed the influence of discretization parameters on system stability predictions using system analysis codes. The problems analyzed dealt with single and two-phase natural circulation flows in simple circuits. By a suitable selection of the ratio of the total buoyancy force in the loop to the friction resistance, the flow may show instabilities. The solution was useful to test the basic numerical properties of the RELAP5 code, such as the effect of nodalization to numerically damp the instabilities. A systematic approach was developed and fully documented. In this paper, the sensitivity of stability results to physical and discretization parameters is analyzed using a tool for the automatic differentiation of FORTRAN codes. ADIFOR, version 2.0D is the adopted tool, that allows for the derivatives of model variables with respect to model parameters. In this way, the results of previous work, which used simple, ad hoc codes are confirmed. The extension of this technique to system analysis codes seems difficult.

1 INTRODUCTION

We are interested in detecting the effects of nodalization and parameters in the calculation of stability boundaries in natural circulation flows. It may be argued that the effects of discretization are known a priori for a given numerical model. However, this knowledge may not be simply achievable in quantitative terms. Examples of these situations, as analyzed by the present authors, may be found in Ambrosini and Ferreri (1998), Ferreri and Ambrosini (1999), Ambrosini and Ferreri (1997a), Ambrosini and Ferreri (1997b) and Ferreri et al. (1995). In the frame of such studies the use of automatic differentiation of FORTRAN codes may be especially useful. Many of the authors' results dealt with the pioneering work of Welander (1967), because its stability properties was amenable to theoretical analysis.

To accomplish the task, a specific tool named ADIFOR (meaning Automatic DIfferentiation of FORtran) has been developed by C. Bischof from the ANL, USA and A. Carle from Rice Univ. USA (Bischoff et al., 1994). Its use is becoming widespread to calculate derivatives of dependent variables with respect to parameters. Why it is important to know the derivatives of dependent variables is closely associated with the construction of response surfaces to determine the uncertainties of computed results, as has been clearly stated by Isukapally (1999). Design optimization and sensitivity analysis to parameters need, in general, this knowledge. In what follows, the use of ADIFOR to help on the quantification of parameter influence on stability maps is introduced. An introductory problem is analyzed first to illustrate and validate the use of this technique. This is made in the context of the classical “tough” problem of one-dimensional, steady-state, advection-diffusion equation. It is well known that this problem has been the test problem for any type of numerical scheme and it was considered useful for the objective of the present work. Following this, the technique was applied to calculate the sensitivity of the margin to instability in single-phase natural circulation in a simple loop. Finally, the results are discussed and the conclusions are given.

2 AN INTRODUCTORY PROBLEM

2.1 Problem specification

In this paragraph, an elementary but important case is considered. It is included because it is amenable of theoretical analysis in the discrete case. Then, let us consider the classical problem of one-dimensional, unsteady, scalar advection-diffusion, as given by equation (1):

$$\frac{\partial T}{\partial t} + U\,\frac{\partial T}{\partial s} = \nu\,\frac{\partial^2 T}{\partial s^2}\quad , \qquad 0< s < L, \quad U, \nu > 0 \tag{1}$$

and boundary conditions:

$$T(t, 0) = 0,\ T(t, L) = 1,\ T(0, s) \equiv 0 \tag{2}$$

In equation (1), U is the advection velocity and ν is the diffusion coefficient, which are considered as constants for the sake of simplicity. L (≡1) is the domain length.

The steady state solution of problem (1-2) is given by:

$$T^{SS} = \frac{1 - e^{P\cdot\frac{x}{L}}}{1 - e^{P}} \tag{3}$$

where P is the Peclet number of the problem, defined as:

$$P = \frac{U \cdot L}{\nu} \tag{4}$$

2.2 Algebraic analysis

A forward time, upwind-space, finite-differences approximation for the computation of the solution of (1-2) is:

$$T_i^{n+1} = T_i^n - \frac{\Delta t \cdot U}{\Delta x}\cdot\left(T_i^n - T_{i-1}^n\right) + \frac{\Delta t \cdot \nu}{\Delta x^2}\cdot\left(T_{i-1}^n - 2T_i^n + T_{i-1}^n\right) \tag{5}$$

where i [1, M] are the grid points where the solution is calculated, M is the total number of discretization points, Δs is the space interval defined as Δs = L/(M-1) and Δt is the time step.

Provided the calculations are stable, the solution converges to:

$$T_i^{SS} = \frac{1 - (1 + P_G)^{i-1}}{1 - (1 + P_G)^{M-1}} \tag{6}$$

where P_G is the Peclet number based on the space interval, namely:

$$P_G = \frac{U \cdot \Delta s}{\nu} \tag{7}$$

The solution given by equation (6) is to be compared with the exact solution given by (3) that, at grid points, takes the form:

$$T_{e,i}^{SS} = \frac{1 - e^{\frac{i-1}{M-1}\cdot P}}{1 - e^{P}}, \tag{8}$$

Then, it is possible to obtain the sensitivity of the solution to the parameters of interest, namely: U, ν and Δs by derivation of equations (6) and (8). The difference between the values given by (6) and (8) is directly attributable to truncation error. This difference must tend to zero with Δs. The rate of convergence is, of course, *O*(1). The derivatives: $\frac{\partial T_i}{\partial \Delta s}$, $\frac{\partial T_i}{\partial U}$ and $\frac{\partial T_i}{\partial \nu}$ give the sensitivity of the computed solution at the grid points. As P increases, the sensitivity must increase, not surprisingly, toward the "knee" of the solution. The derivatives may be obtained quite easily in the case of equations (6) and (8). Their expressions may be computed as a function of s for given values of U, ν and Δs. The solution and its derivatives have been checked with the theoretical algebraic solution. They are given in Appendix A, together with other results to be discussed in what follows.

3 THE USE OF ADIFOR

The differentiation of FORTRAN codes may be accomplished using a pre-processor named ADIFOR, version 2.0D. Bischoff et al., (1994) give a detailed description of its use. Related bibliography may be found at the ADIFOR WWW site (ANL, 1999). Some introductory examples may also be found in the WWW, see for example ANL (1999), Goenka (1999) and Rightley (1999). This is not the only tool available to automatically calculate derivatives and a comparison between two of them may be found Rightley (1999).

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 only 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. Even when the codes must comply with FORTRAN 77 standards, ADIFOR accepts some common language extensions.

Some simple hints to help on the very first use of ADIFOR may be readily found in Rightley (1999). Many references document the accuracy of the derivatives calculated in this way. This is not the only way to apply ADIFOR; the reader is referred to the aforementioned literature. The use of ADIFOR is straightforward. However, the original code must be sometimes "prepared" to get the appropriate functional dependence between the independent parameters and the dependent ones. This fact turns essential to take some time to verify the automatically computed derivatives. One important feature of ADIFOR is the careful treatment of derivative exceptions when handling intrinsic functions. Its reporting capability is also of great importance.

In the present application, the original code for the computation of the solution of equation (5) was modified to consider only a simple driving code and a main subroutine. The former sets the values of the parameters (in this case U, ν and Δs). The latter performs the calculations by calling another routine that iterates the finite-differences approximation over the whole range of time cycles. After generating the augmented file, a new driving main program was written, that now provides arrays for the dependent variable T(t,s) and its derivatives with respect to U, ν and Δs, also as a function of time and spatial position.

The values so obtained have been selected for two space positions and "steady-state" that in practice was assumed to be achieved at t=100 after the start of a transient calculation with constant boundary conditions. Table A.1 in Appendix A shows the comparison between the "exact" algebraic solution and its derivatives and the values from the analytical solution. The values obtained from the transient code generated with ADIFOR 2.0D and the new driver main program are nearly the same. This is coherent with previous experience and is due to the use of the chain rule of derivation and derivatives of intrinsic functions. These derivatives are handled exactly by ADIFOR 2.0D.

4 SENSITIVITY TO PARAMETERS IN SINGLE PHASE NATURAL CIRCULATION

In what follows, some summary information on the problem under analysis is given for the sake of completeness. As already mentioned, detailed description may be found in the authors' previous work.

4.1 Background

Figure 1 shows the geometry of a simple hydraulic system, adapted from Welander (1967). 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. When S tends to zero, the heat-transfer coefficient from/to the heat source/sink is increased to keep constant the total heat transferred. The reader is referred to the references for a detailed description of the governing equations.

The resulting dimensionless equations are:

$$\frac{dq}{dt} = \alpha \int_0^1 T \cdot ds \; - \; \varepsilon \cdot q \cdot |q|^{\xi-1} \qquad (t > 0), \tag{9}$$

for momentum and

$$\frac{\partial T}{\partial t} + q \frac{\partial T}{\partial s} = 0 \qquad (0 < s < 1, t > 0) \tag{10}$$

for energy balance, in which α and ε measure the driving (buoyancy) forces and the total friction in the loop respectively. To obtain Equations (9) and (10) advantage was taken from the observed anti-symmetry of the temperature distribution along the loop, allowing for solving the problem only in the interval s[0,1]. Appropriate boundary conditions are specified for the dimensionless temperature in $s = 0^+$ and $s = 1^-$. Again, details may be found in Welander (1967), Ambrosini and Ferreri (1998) and Ferreri and Ambrosini (1999) where, in addition to the original analysis of Welander, some conditions to ensure convergence of the numerical scheme toward the analytical solution have been developed.

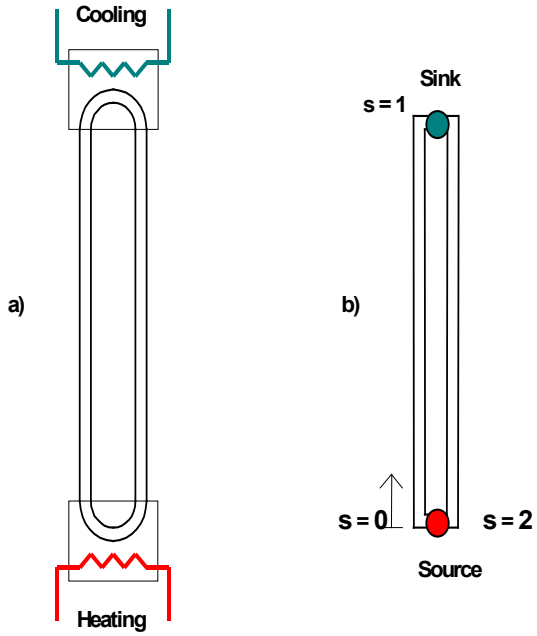

Figure 1 Sketch of the loop geometry (after Welander, 1967).

4.2 Sensitivity to parameters using ADIFOR

The analysis will focus on the results obtained using the implicit coupling of the momentum and energy equations and the forward-time, upwind-space finite-difference method (FTUS) for the momentum equation. It may be argued that the consequences of using this approximation on the results are well known, i.e. obtaining an $O(1,1)$ solution in the space and time increments. What was not too evident was the quantification of these effects (and those of the coupling) on the stability limits on natural circulation systems. To fix ideas, the approximation given by Equations (11) and (12) will be used:

$$T_i^{n+1} = (1 - C_{OU})\, T_i^n + C_{OU}\, T_{i-1}^n \qquad (i=2, \ldots, N-1) \tag{11}$$

$$T_N^{n+1} = \left(1 - C_{OU} - \frac{\Delta t}{\Delta s} F_{nod}(q^n)\right) T_N^n + C_{OU}\, T_{N-1}^n - \frac{\Delta t}{\Delta s} F_{nod}(q^n)\, T_1^{n+1}$$

$$T_N^{n+1} = -T_1^{n+1}$$

where C_{OU} is the Courant number $C_{OU} = \dfrac{q \cdot \Delta t}{\Delta s}$ and $\Delta s = \dfrac{1}{N-1}$ is the space increment, with N being the number of nodes. The function $F_{nod}(q)$ is the above mentioned source-sink heat transfer multiplier, introduced to provide steady-state convergence to the exact solution.

The momentum equation is discretized in time as follows:

$$q^{n+1} = q^n + \left(\alpha \cdot \Delta s \sum_{i=1}^{N-1} \frac{T_i^{n+1} + T_{i+1}^{n+1}}{2} - \varepsilon \left| q^n \right|^{\xi-1} \cdot q^{n+1} \right) \Delta t \tag{12}$$

In this way, a map may be obtained, as reported in Ambrosini and Ferreri (1998). The value of $\Delta\rho$ given by:

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

where $\rho(\mathbf{A})$ is the spectral radius of the matrix relating the perturbations in the state variables at time $(n+1)\Delta t$ and $n\Delta t$ after linearization. $\Delta\rho$ 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. The zones are delimited by the neutral stability boundary (NSB), that is a natural boundary curve for this analysis.

Figure 2 shows the stability map in the plane of α and ε, the system global parameters. It has been obtained using 11 nodes ($\Delta s = 1/10$), $C_{ou}= 0.8$ and $\xi = 1.75$. The selection of these values for C_{ou} and ξ is not arbitrary. Despite the very low number of nodes, they ensure low numerical diffusivity while keeping the calculations stable on one hand and turbulent flow friction on the other. The theoretical NSB corresponds to Welander's analysis and is coincident with the one obtained from spectral analysis (see Ambrosini and Ferreri, 1998).

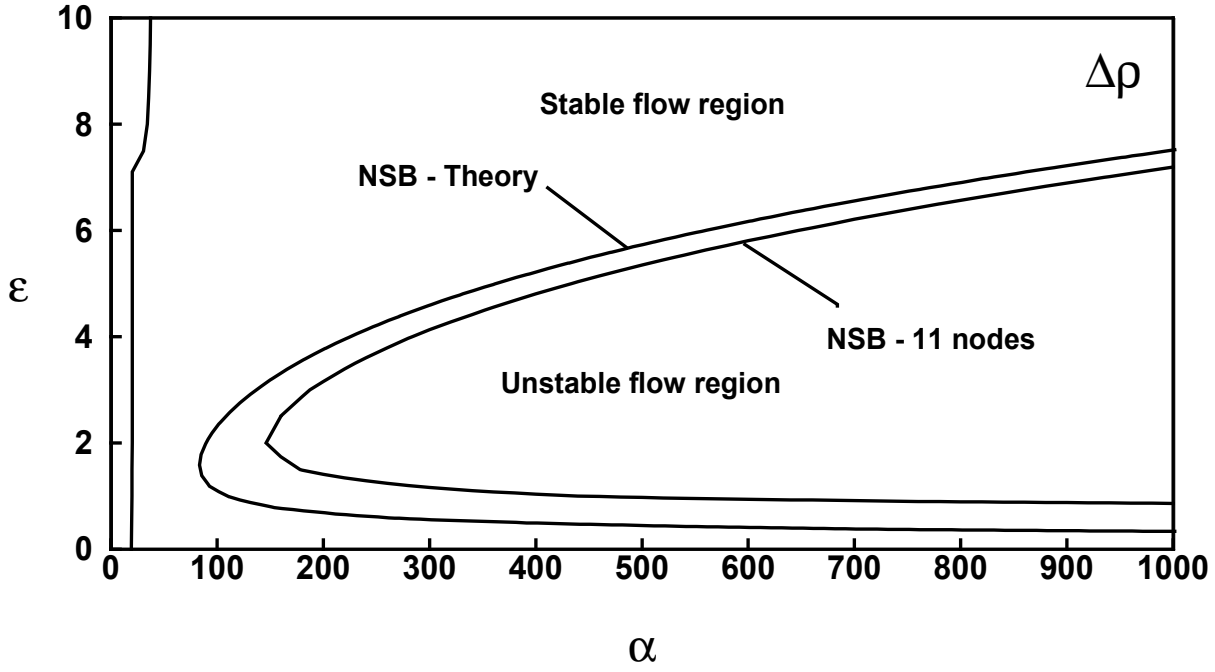

Figure 2 Map of $\Delta\rho$ for the first-order, explicit momentum, implicit temperature coupling, C_{OU}=0.8 and ξ=1.75, Δs = 1/10 [1]

The interest in the analysis to follow is showing how the solution depends on C_{ou} and ξ. The above mentioned set of parameter values in the dependence domain will be denoted as $(\,)_O$.
This implies calculating the following derivatives:

$$\left.\frac{\partial \Delta\rho}{\partial C_{OU}}\right)_O \quad \text{and} \quad \left.\frac{\partial \Delta\rho}{\partial \xi}\right)_O .$$

In these cases, the value of Δs will be fixed; however, Δs will be also varied in turn trying to investigate how the computed trends confirm the results of the author's previous analyses on the sensitivity to noding.
In order to improve the reliability of the obtained conclusions, it was decided to check every exploratory calculation made with the help of ADIFOR using finite-difference approximations of the derivatives; this prudent approach was rewarding, because it allowed eliminating some reasonable looking, wrong results.

The influence of ξ will be considered in the first place. Figure 3 shows the map of $\left.\frac{\partial \Delta\rho}{\partial \xi}\right)_O$ as a function α and ε considering Δs=1/10. In this map, the numerical neutral stability boundary is shown as a reference. It may be observed that this derivative is not always negative. This is due to the shift in the NSB for increasing values of ξ. Figure 4 shows the same map, but considering Δs = 1/30. Now the negative area is more smoothly defined. A reasonably converged solution with respect to nodes number corresponds to Δs=1/100, which was obtained also by finite-differences as a further check. In this case the zero curve remains unchanged, with small changes in the values of the derivative.

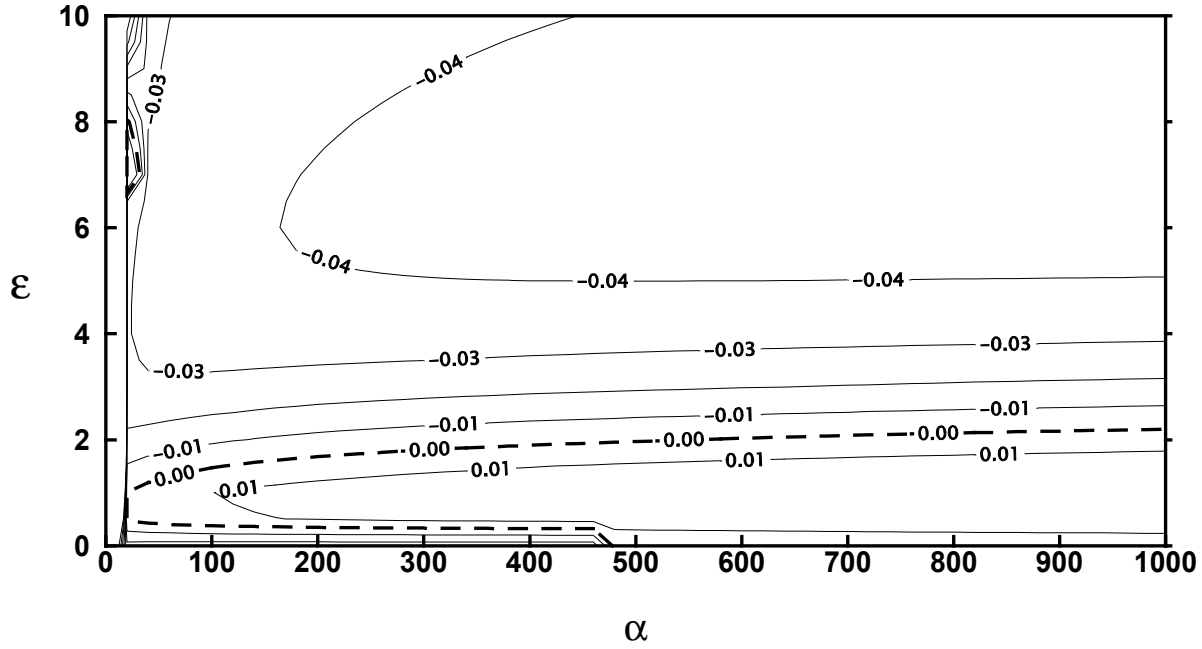

Figure 3 Sensitivity map of $\Delta\rho$ to the friction law exponent ($\partial\Delta\rho/\partial\xi$) for the first-order, explicit momentum and implicit temperature coupling. [C_{OU}=0.8, ξ=1.75 and Δs=1/10]

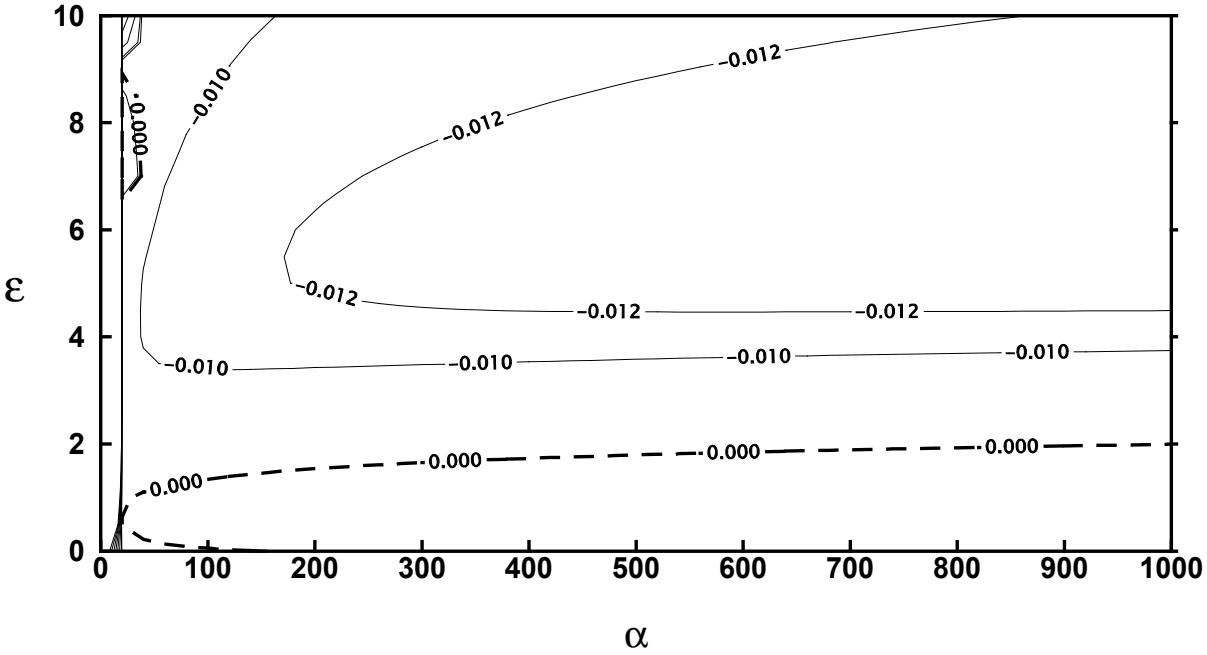

Figure 4 Sensitivity map of $\Delta\rho$ to the friction law exponent ($\partial\Delta\rho/\partial\xi$) for the first-order, explicit momentum and implicit temperature coupling. [C_{OU}=0.8, ξ=1.75 and Δs=1/30]

The change of $\Delta\rho$ as a function of C_{OU}, $\left.\frac{\partial\Delta\rho}{\partial C_{OU}}\right)_O$, is shown in Figure 5. It was obtained using the same set of parameters. Decreasing C_{OU} should lead to further damping in zones of positive derivatives. This is coherent with the analysis shown in Ambrosini and Ferreri (1998), where a set of calculations was made imposing a fixed time interval that lead to more damped solutions. It was due to low Courant numbers when considering a fixed number of nodes and constant ξ. Figure 6 shows the map considering Δs=1/30. Now, a shift in the zero

curve towards the right of the map may be observed. Once again, it is interesting to resort to "converged" maps. The map so obtained showed further bending of the zero curve, leading to positive and negative zones in the map.

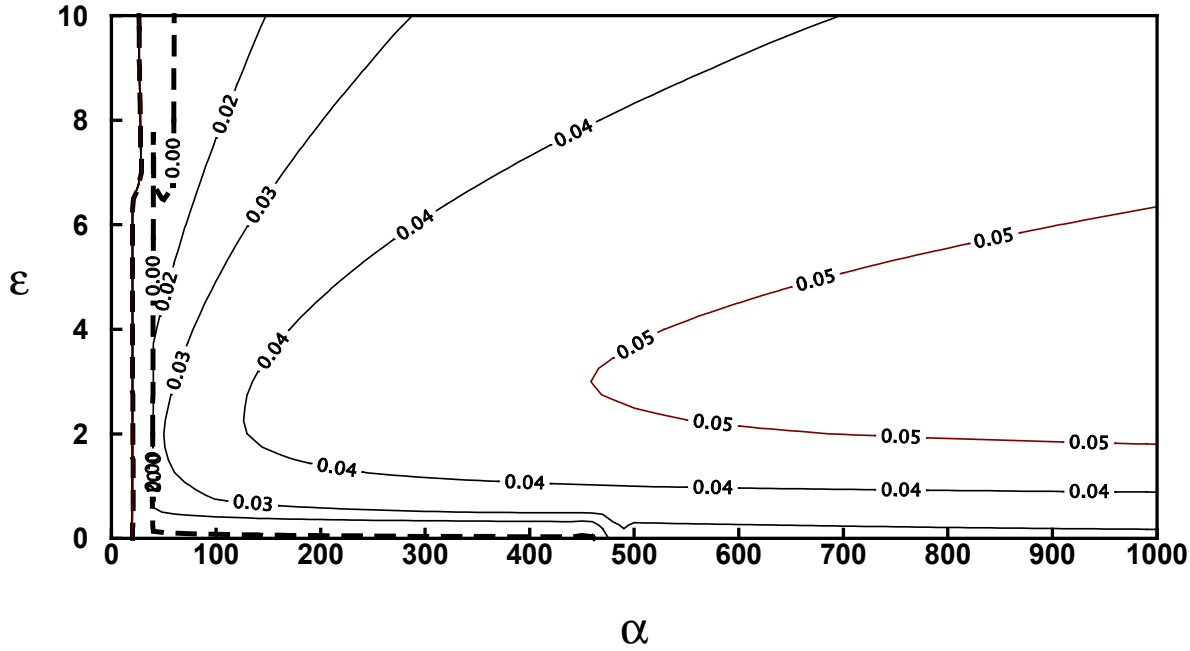

Figure 5 Sensitivity map of $\Delta\rho$ to cell Courant number ($\partial\Delta\rho/\partial C_{OU}$) for the first-order, explicit momentum and implicit temperature coupling. [C_{OU}=0.8, ξ=1.75 and Δs=1/10]

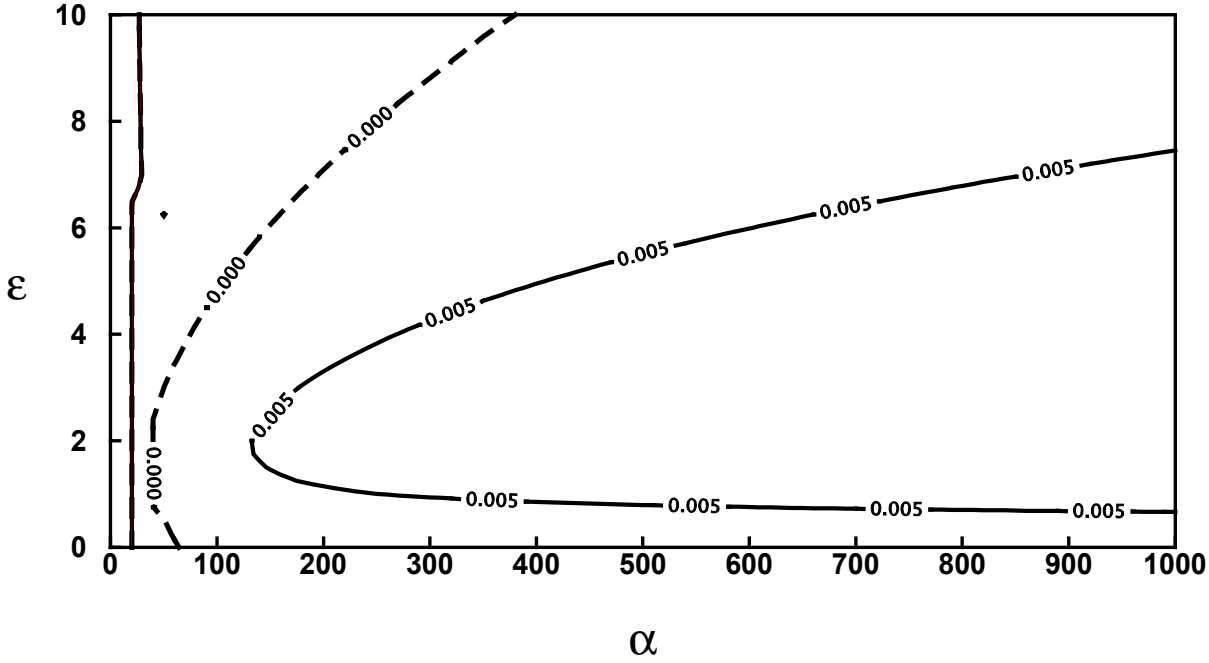

Figure 6 Sensitivity map of $\Delta\rho$ to cell Courant number ($\partial\Delta\rho/\partial C_{OU}$) for the first-order, explicit momentum and implicit temperature coupling. [C_{OU}=0.8, ξ=1.75 and Δs=1/30]

The above shown analysis were the main goal of this paper. However, as already mentioned, the effects of Δs on the neutral NSB were also addressed. Authors' previous work was mainly devoted to this aspect of the computations and the effects of different approximations were assessed. The derivative of $\Delta\rho$ in terms of Δs for

$\Delta s=1/100$, $C_{ou}= 0.8$ and $\xi = 1.75$ showed convergence. However, the same derivatives computed using ADIFOR were not coincident. Further analysis is needed to clearly understand the reasons of this discrepancy.

5 CONCLUSIONS

The use of the automatic differentiation tool ADIFOR 2.0D proved to be useful to determine the influence of parameters on the neutral stability boundary maps of natural circulation flows. This is not the most usual use of this tool, since it involves tracing the influence of parameters on the spectral radius of the discrete problem. However, the results obtained confirmed exactly the numerically simulated derivatives maps. In this way, the influence of the cell Courant number and a variable related to the exponent in the friction law was assessed. Experience showed that checking results with finite-differences may be rewarding to get insight on the results. (this seems to be a common practice among practitioners of numerical modeling using these techniques).

The use of ADIFOR is straightforward when applied to predictive codes that give a result as a function of a set of parameters. However, it is essential to know the details of the code to be differentiated and to explicitly calculate the steady-state conditions corresponding to the addressed fixed point. This is particularly difficult when dealing with unstable steady-state conditions, which cannot be achieved asymptotically by transient calculations with constant boundary conditions.

In this respect, the goal of applying this technique to large thermal-hydraulic systems codes seems a really challenging one. This is due to multiple sources of derivative discontinuities, coming from physical correlations and intrinsic functions. Tabular data may pose further difficulty to the analysis, not to speak about numerical induced oscillations like the ones observed on flow rate. The task will surely require a huge effort. A non-trivial additional limitation may be that codes must be fully developed and documented. Nevertheless, the cost of generating sensitivity results using a *brute-force* approach is so high that getting a set of dependent variables results with respect to some parameters from an augmented code may be rewarding. Anyway, a cost/benefit analysis should be performed to justify a project like this.

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APPENDIX A

COMPARISON OF ALGEBRAIC AND NUMERICAL SOLUTIONS

The algebraic analysis of equations (6) and (8) and its derivatives is shown here. Table A.1 shows the comparison of the calculated values of $\partial T/\partial \Delta s$, $\partial T/\partial U$ and $\partial(T)/\partial \nu$ as a function of the position and Δs, U and ν. Note that by "exact" we mean the values obtained from equation (8). The corresponding numerical solution, obtained from (6), is affected by truncation error. It is, nevertheless, the exact value of the algebraic solution as computed using equation (5), the only errors being those originating in the rounding to machine precision.

	CASE_#1.1	CASE_#1.2	CASE_#2.1	CASE_#2.2	CASE_#3.1	CASE_#3.2
M	11	11	21	21	51	51
Δs	0.1	0.1	0.05	0.05	0.02	0.02
i	6	10	11	19	26	46
P_G	1	1	0.5	0.5	0.2	0.2
T_i^{SS} (Eq.6)	0.030303	0.499756	0.0170459	0.444277	0.0103739	0.401812
$T_{e,i}^{SS}$ (Eq.8)	0.0066929	0.367851	0.0066929	0.367851	0.0066929	0.367851
$\partial T/\partial \Delta s$	-0.734619	-2.48778	-1.11702	-5.90542	-2.1388	-16.7193
$[\partial T/\partial \Delta s]_e$	-0.332403	-3.67609	-0.664806	-7.35218	-1.66201	-18.3805
$\partial T/\partial U$	-0.734619	-2.48778	-0.558512	-2.95271	-0.42776	-3.34387
$[\partial T/\partial U]_e$	-0.332403	-3.67609	-0.332403	-3.67609	-0.332403	-3.67609
$\partial T/\partial \nu$	7.34619	24.8778	5.58512	29.5271	4.2776	33.4387
$[\partial T/\partial \nu]_e$	3.32403	36.7609	3.32403	36.7609	3.32403	36.7609

	CASE_#4.1	CASE_#4.2	CASE_#5.1	CASE_#5.2	CASE_#6.1	CASE_#6.2
M	101	101	201	201	1001	1001
Δs	0.01	0.01	0.005	0.005	0.001	0.001
i	51	91	101	181	501	901
P_G	0.1	0.1	0.05	0.05	0.01	0.01
T_i^{SS} (Eq.6)	0.0084466	0.385499	0.0075471	0.376853	0.006860	0.369681
$T_{e,i}^{SS}$ (Eq.8)	0.0066929	0.367851	0.0066929	0.367851	0.0066929	0.367851
$\partial T/\partial \Delta s$	-3.80693	-35.0114	-7.13347	-71.724	-33.7274	-365.77
$[\partial T/\partial \Delta s]_e$	-3.32403	-36.7609	-6.64806	-73.5218	-33.2403	-367.609
$\partial T/\partial U$	-0.380693	-3.50114	-0.356673	-3.5862	-0.337274	-3.6577
$[\partial T/\partial U]_e$	-0.332403	-3.67609	-0.332403	-3.67609	-0.332403	-3.67609
$\partial T/\partial \nu$	3.80693	35.0114	3.56673	35.862	3.37274	36.577
$[\partial T/\partial \nu]_e$	3.32403	36.7609	3.32403	36.7609	3.32403	36.7609

TABLE A.1 Analytical and exact algebraic solutions and their derivatives computed for L = 1, U = 0.1 and ν = 0.01 (P=10)