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METHODOLOGY FOR COUPLING THERMAL-HYDRAULIC FOR PRIMARY SYSTEM AND CONTAINMENT ANALYSIS

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Methodology for coupling thermal-hydraulic codes for primary system and containment analysis

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ABSTRACT

The present report describes a coupling methodology adopted to link a nuclear reactor thermal-hydraulic primary system code to a containment system code, set up in the frame of task LP2-E.1a of the AdP assigned to CIRTEN.

The codes to be coupled were chosen to be the RELAP5 Mod3.3 patch 3 and the Gothic version 7.2b(QA). The RELAP5 code was provided to the University of Pisa by ISPRA together with the FORTRAN source program, while the executable version of the Gothic code and limited rights to use it for the purposes of the present work were acquired from Numerical Applications, Inc. (NAI).

A procedure for exchanging information between the two running codes was also acquired from NAI. The procedure included a limited coupling between primary system and containment, allowing only for the exchange of information required to simulate a water blowdown from primary system to the containment at a single location in the plant.

Starting from this example, a procedure customised for more general applications was set up, in order to make possible the first validation calculations, to be described in a further report. The procedure is aimed at allowing bi-directional exchanges of mass and energy at multiple junctions, also including the exchange of noncondensable gases.

It must be remarked that the presentation reported herein is limited to a general description of coupling features, leaving details to unofficial internal documentation at the University of Pisa. A more detailed description is not possible in an open report without infringing the agreement signed by the University of Pisa with NAI for the delivery of the Gothic code, as a property of EPRI, in consideration of the proprietary nature of the information about the code features and structure.

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1. INTRODUCTION

The conceptual design of Gen. III innovative reactors at the end of the years 1980's and at the beginning of 1990's posed new challenges from the point of view of transient thermal-hydraulic analyses in the primary system and containment.

In fact, the classical approach of running containment calculations after the primary system ones, allowed by the substantial decoupling of phenomena in the two environments, was found unfeasible because several of the new engineered safety features established an unprecedented degree of coupling among them. Among the plant features that resulted in such a coupling, the following can be mentioned:

- presence of automatic depressurization systems that provide equalisation of primary system and containment pressure well before the primary system transient can be considered completed;
- the use of gravity driven injection systems, whose working principle is based on slight differences in pressure between primary system and containment, mostly due to the gravitational head generated by a water level;
- the need to demonstrate long term decay heat removal capabilities on the basis of relatively weak driving forces, involving flow paths embracing both the primary system and the containment.

All such features require a coupled approach for evaluating the behaviour of the reactor and of the containment during postulated accidents, since serial primary system and containment calculations would not provide correct sequence of events and scenario.

In addition, presently proposed medium sized reactors, characterised by an integrated design, share with passive Gen. III reactors the adoption of features that require coupled primary system and containment analysis capabilities. Therefore, setting up coupled tools for primary system and containment thermal-hydraulic analysis represents a increasingly important objective, also considering that primary system and containment codes have been optimised for their specific tasks and cannot be reliably used for the whole system.

The above considerations provide the motivation for the present activity aimed at coupling the RELAP5 Mod3.3 patch 3 [1-2] and the Gothic version 7.2b(QA) [3] codes. In a first step, it was not considered viable the coupling proposed as a specific task for CIRTEN in the AdP programme, as the Gothic code was provided to the University of Pisa only in its executable form. As a consequence, a first part of the activity was devoted to the acquisition from SIET of a coupled primary system and containment nodalization of the SPES3 facility for RELAP5 only, in the attempt to compare one-way serial calculations made with RELAP5 and Gothic. This part of the work was then terminated when a sample routine for coupling Gothic with RELAP5 was lately made available by NAI, restoring to the work to be done the initial intended objective. The first part of the work, that was not completed, is not reported in this document and is left as internal material at the University of Pisa, to be used as a background to plan for future activities.

The routine received by NAI, though implementing a strategy of coupling between the codes, was anyway limited in its capabilities, allowing only for the exchange of information required to assign a single water blowdown from a fixed junction in RELAP5 to an assigned volume in Gothic. Moreover the reference numbers of the break connection and the containment pressure were implemented in the coding, so that a new recompilation of the RELAP code should have been necessary after each modification of these parameters. The work performed on its basis involved therefore a generalisation of this single link to an arbitrary number of junctions injecting into the containment, to be arbitrarily defined by an external input data file. In addition to this extension, it was also considered necessary to achieve a two-way coupling, in which mass and energy could be exchanged by primary system and containment in both directions. This objective involved the need to treat the interchange of noncondensable gases from the containment atmosphere to the primary system and viceversa, which was not dealt with by the initial one-way water mass transfer allowed by the routine received from NAI.

Expectedly, the major encountered difficulties concerned the availability of variables from both codes to be exchanged through the interfacing process routine. In fact, the strategy of coupling involves in both codes the exchange of variables that are already available or can be made accessible as normal control variables, thus limiting the possible choices to a predefined set of variables indicated in the manuals of the two codes. This lead to some complication in the construction of the required information to be transferred between the codes and to some limitation in the obtained coupling capabilities.

The resulting coupling methodology is described in the present report, also highlighting the possible improvements that could be achieved in further work, necessarily requiring changes in the available versions of the codes to make more variables accessible by the interfacing routines.

Some calculation cases demonstrating the relevant capabilities achieved in the coupling of the two codes are reported in a companion document [4].

2. GENERAL STRATEGY OF COUPLING

2.1 Addressed links between primary system and containment

As mentioned in the Introduction, the routine received from NAI addressed a single one-directional link from RELAP5 to Gothic, simulating a water blowdown into a Gothic volume.

The situation is depicted in Figure 1, showing that the initial coupling strategy related the transfer of mass and fluid enthalpy from a RELAP5 junction connected to a time dependent volume to a boundary condition flow path in Gothic, returning to the time dependent volume in RELAP5 the value of the containment pressure, to be used as a "back-pressure" for the junction.

In this coupling methodology, the RELAP5 junction must have as "TO" volume the time dependent volume, in order to obtain a positive flow rate when the flow enters the containment volume. The transfer of variables between the two codes involved the use of an inter-processing coupling routine written in C language, to be linked to RELAP5 after compilation, allowing the exchange of vectors of variables from Gothic to RELAP5 and viceversa, through appropriate changes to the TRAN routine managing the time advancement in RELAP5.

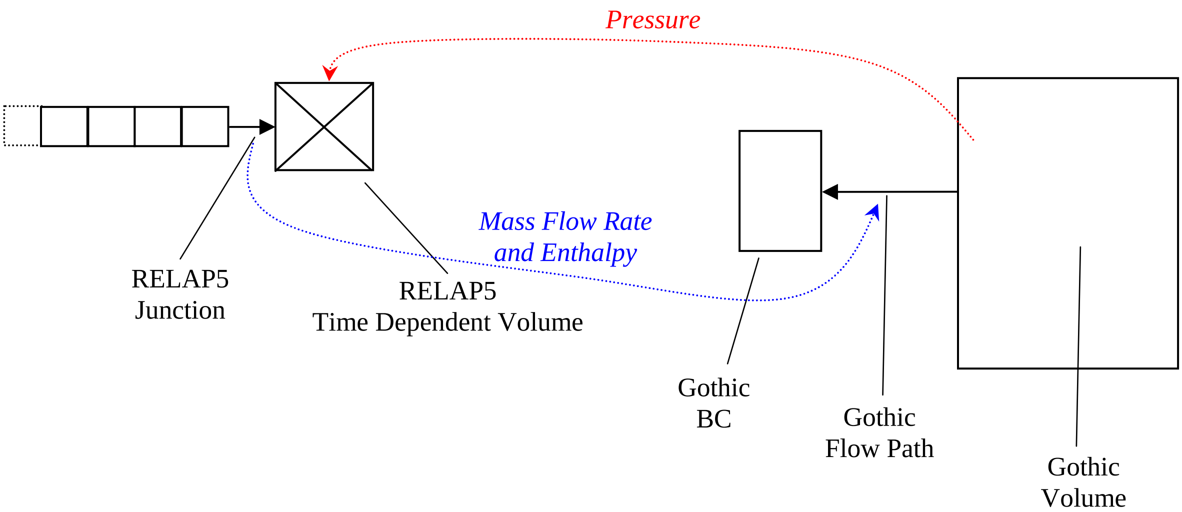


Figure 1. Arrangement of the initial coupling routine for the transfer of variables related to a water blowdown

In this regard, it must be noted that the compilation and link phases of RELAP5 routines under Windows requires a rather complex procedure, to be made under simulated Linux environment, not always described in full detail in the accompanying notes. Thanks to the kind availability of NAI, some of the required steps were clarified, leading to a successful compilation process.

Such process resulted anyway too time consuming for use during methodology improvement and debugging. In the aim to speed up the procedure, the FORTRAN routines of RELAP5 generated by the original step-by-step method in a machine-dependent format were loaded under a workspace of the Compaq 6.6 compiler, to allow for fast implementation of any change required during the methodology development.

In the original procedure, the variables read from RELAP5 (flow rate and enthalpy) were assigned to a Gothic boundary condition that provided the necessary in-flow into the Gothic volume, while the back pressure from the containment volume was directly written into the general vector of variables defined in RELAP5 (the "FA" vector) in the appropriate location. The former of these two choices was maintained also in the methodology developed by the University of Pisa, while the second one resulted too limiting for the intended purposes.

In fact, the main objectives of the improvement work made by the University of Pisa were:

- to make possible the simultaneous management of multiple junctions and time-dependent volumes, whose identification labels could be defined in a separate input file;
- to allow not only for forward flow from primary system to containment, but also for backward flow, as required, for instance, for simulating a gravity driven injection from a containment pool (e.g., the IRWST in the AP1000 reactor);
- to deal with exchanges involving not only water but also noncondensable gases.

The use of multiple junctions resulted possibly the easiest of the above objectives to be achieved, just requiring an attentive definition of vectors of labels and variables to be assigned at each link between RELAP5 and Gothic, after reading an additional input file specifying junction and volume labels.

On the other hand, making possible backward flow through the RELAP5 time-dependent volume to the related junction involved the assignment of thermodynamic properties in the volume itself, well beyond the initial redefinition of pressure. In this aim, writing the values of internal energy of the two phases, void fraction and noncondensable quality in the "FA" vector resulted inefficient, unless the routine updating all the thermodynamic properties in time dependent volumes was called. As a consequence, the previous way of transferring data to RELAP5 (i.e., writing into the “FA” vector) was abandoned, in favour of a transfer of data via a new common area to the RELAP5 routine TSTATE, where the thermodynamic conditions of the time dependent volumes are evaluated. The data were then directly assigned to the time dependent volumes involved in the link, that are identified in the RELAP5 input deck by the following choices:

- the value of “t” in the “εbt” label of the time dependent volume must be defined as “6”, thus activating the option for the definition of pressure, internal energy of liquid and gas, void fraction and noncondensable quality by a table; these values, starting from some user-selected time, must be assigned on the basis of the containment volume conditions;
- in this purpose, in the table defining the values of “P”, “Uf”, “Ug”, “voidg” and “quala” (i.e., pressure, liquid and steam/gas internal energy, void fraction and noncondensable gas quality) there must be a sharp transition (to be made in a single timestep) from physical values of pressure to integer (though expressed in floating point format) and negative values; this change is interpreted by the modified RELAP5 routines as the shift from the calculation of time dependent volume properties on the basis of the input table to the assignment of these properties on the basis of the Gothic volume properties connected to the “junction” whose order is identified by the absolute of the negative pressure.

The above choices make it possible (with some limitations to be described later on) to transfer in backward flow to RELAP5 water and/or noncondensable gases through the same junction that is injecting water to Gothic in forward flow. However, this arrangement was found not suitable for the simultaneous injection to Gothic of water and noncondensable gases from RELAP5. This is because in Gothic it is possible to define two types of boundary conditions:

1. a boundary condition in which pressure, temperature, liquid volume fraction, steam volume fraction and flow rate are assigned;
2. a boundary condition in which pressure, water/steam mixture enthalpy, steam volume fraction and flow rate are assigned.

Unfortunately, the second option is suitable only for water and steam injection to the containment volume, without noncondensable gases, since void fraction at the junction is evaluated with the assumption of water-steam thermal equilibrium; when noncondensable gases are present an unrealistic interpretation of the flow enthalpy might therefore result.

On the other side, the use of the first option is unsuitable for water and steam injection, as it requires a single value of the mixture temperature and this is neither available from the RELAP5 code, nor it can easily be built assuring the conservation of energy flowing through the junction.

The above situation lead to the remarkable complication that *a given RELAP5 junction must be coupled with* *two* *boundary conditions and flow paths of Gothic*, to allow for the following functions to be accomplished:

- first boundary condition and flow path: injection of water/steam mixtures from RELAP5 to Gothic in the case of *forward flow* and extraction of steam/water plus noncondensable gas mixtures from Gothic to RELAP5 in the case of *backward flow*;
- second boundary condition and flow path: injection of noncondensable gas from RELAP5 to Gothic in the case of forward flow only.

In summary, each RELAP5 junction connected to Gothic must be coupled with two Gothic boundary conditions. The resulting situation for two RELAP5 junctions connected to Gothic is represented in the Gothic working screen as shown in Figure 2; the couples of flow paths 1 and 3, on one side, and 2 and 4, on the other side, are at same physical heights and correspond to only two RELAP5 junctions. Flow paths 1 and 2 accomplish with the transfer of water/steam only in forward flow and of the whole water/steam plus noncondensable gas mixture in backward flow; flow paths 3 and 4 are activated only for forward flow and transfer only the noncondensable gas.

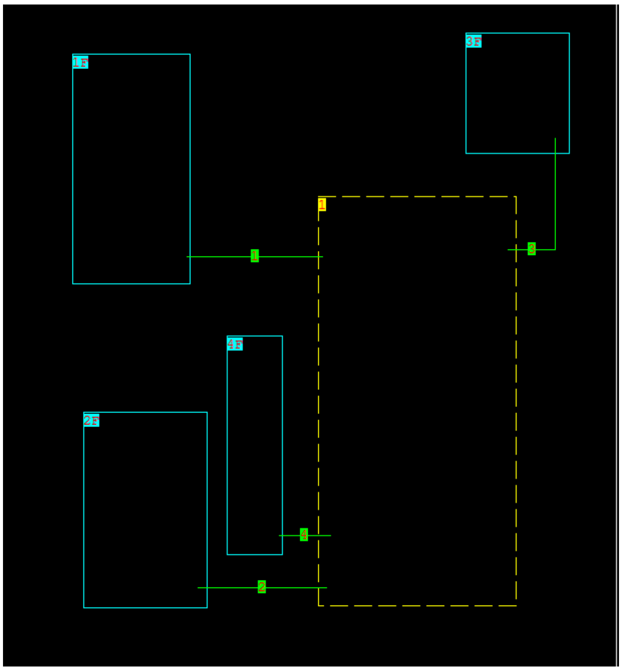


Figure 2. Arrangement of Gothic volumes, flow paths and boundary conditions corresponding to two RELAP5 junctions connected to Gothic

By the way, it is necessary to clearly declare that at the present time it is possible to transfer only a single noncondensable gas that, in the tests performed for the first assessment of the updated routines, was chosen to be air. In fact, transferring a mixture of two or more noncondensable gases would require a transfer of information between the two codes that at the moment is not feasible by the accessible variables.

According to the above description, the flow of information between the two codes at each link between a RELAP5 junction and Gothic is depicted in Figure 3. By comparison with Figure 1, it can be noted the greater complexity of the links and the improved capabilities introduced in the present work with respect to the initial coupling routine received from NAI.

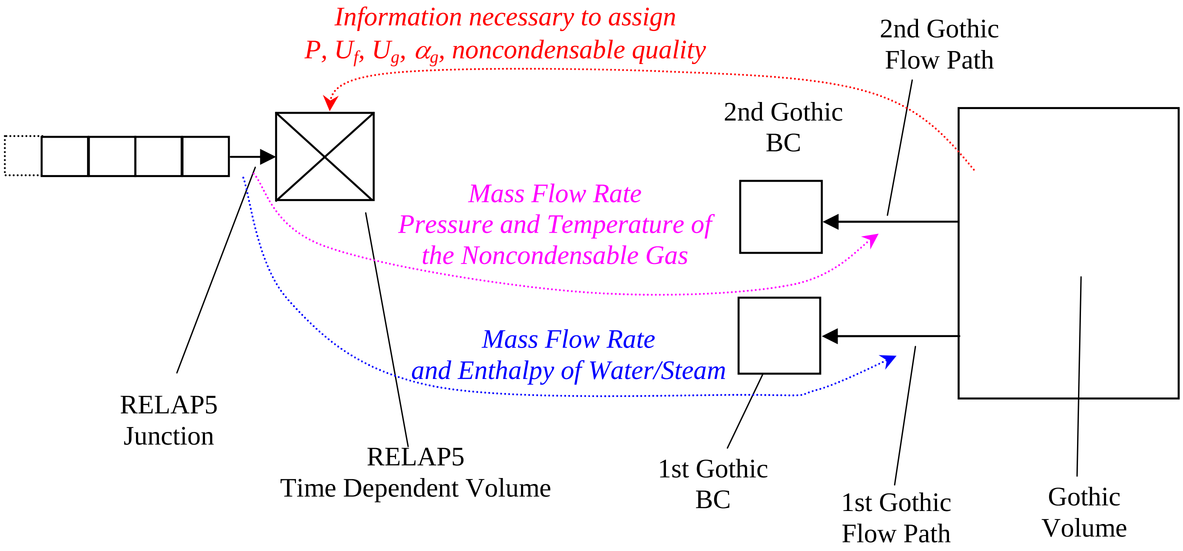


Figure 3. Arrangement of RELAP5 and Gothic elements and flow of information between the codes at each RELAP5 junction connected to Gothic in the presently adopted methodology

Notwithstanding these improvements, it must be remarked that the obtained coupling is still imperfect. This is due partly to the essential differences in the thermal-hydraulic balance equations and modelling assumptions of the two codes, to the lack of availability of precise information on details of their use in both codes and to the objective to limit the complexity of the coupling in this first attempt. In particular, it must be remarked that:

- in the case of countercurrent liquid and gas flow at the RELAP5 junction, the information transferred to Gothic may be inaccurate, as it is based on the overall flow rate calculated by the code and on the averaged fluid enthalpy evaluated on the basis of a dynamic quality calculated using the absolute value of phasic velocities; the result may not correspond exactly to the energy flow through the junction calculated by RELAP5 in such a complex (but relatively less interesting) case;

- for flow from the Gothic lumped parameter volume to the RELAP5 junction, RELAP5 calculates the flow rate on the basis of the information on pressure, phasic internal energies, void fraction and noncondensable gas fraction assigned to the time dependent volume; since a "built in" information on the void fraction calculated by Gothic at each flow path in the case of outflow is not accessible, it was necessary to reconstruct this information on the basis of primary information on junction elevation, junction height span and the location of the liquid level in the volume; at the moment, it cannot be granted that this reconstruction exactly matches with the information internally calculated by Gothic.

In general, the following considerations apply in relation to the preservation of mass and energy in the transfers from Gothic to RELAP5 and viceversa:

- <u>the exchanged mass flow rate is always calculated by RELAP5</u> and its value is applied to Gothic flow paths injecting or extracting a corresponding rate of mass;
- however, the mass flow rate is instantaneously assigned to Gothic making use of an explicit coupling in which the time advancement steps are not the same for the two codes: exact preservation of mass and energy would require an integration in time of the flows of mass and energy, depending on the relative magnitude of the two time steps, that was not considered a priority in the present work;
- as explained above, the value of the flow averaged enthalpy at the RELAP5 junction/Gothic flow path is evaluated according to the absolute value of junction velocities and cannot correctly deal with countercurrent flow conditions;
- the liquid and vapour/gas flows calculated by RELAP5 for negative flow rate (i.e., from Gothic to RELAP5) are based on the reconstructed information of void fraction at the flow path and on the best presently possible understanding about the variables to be accessed in Gothic for phasic enthalpies; whatever may be the accuracy of this information, it is anyway obvious that extraction of mass from the Gothic volume will probably occur on the basis of an homogeneous flow assumption (slip ratio equal to unity) while RELAP5 will calculate by its own means a slip condition between the phases, with the related enthalpy flows.

The above mentioned possible inaccuracies could be decreased in their extent or eliminated in the future. A first action in this regard could be to obtain from NAI a version of the code in which more details are available at the flow paths in order to achieve a more qualified exchange of information in the transfer of data from Gothic to RELAP5. A second action could be to separate liquid, steam and gas flows entering Gothic making use of three flow paths, in order to better account for conditions of countercurrent flows; this choices will anyway considerably complicate the procedure of preparation of a coupled calculation.

2.2 Information flow management

As mentioned in the discussion of the coupling methodology reported in the previous sections, access to relevant variables in both codes is possible mainly through the variables stored in vectors that can be called as control variables. This was a convenient choice for RELAP5, avoiding to intrude too much in the structure of the code (an always risky action), and a definitely obliged one for Gothic, owing to the unavailability of the FORTRAN source program of the code.

The transfer of information from RELAP5 to Gothic and viceversa is accomplished by the use of the *ipc.c* routine that must be linked with the RELAP5 code, after compilation, and provides the function of inter-process communication. Without disclosing the detailed features of the routine, it can be anyway declared that the routine allows to transfer lists of variables “from” and “to” the external process (i.e., RELAP5). The variables to be written to the output list or read from the input one must be defined in the input deck of Gothic, via the appropriate windows available to the user, and assigned or used for the intended purpose. In this process of interfacing variable definition, care must be obviously taken to preserve the exact order in which the variables will be read and adopted in either code.

A description of the variables transferred through the codes *at each RELAP5 junction linked to Gothic* is reported hereafter.

From RELAP5 to Gothic

The variables transferred from RELAP5 to Gothic are five per each RELAP5 junction linked to Gothic and must be assigned in the order reported below:

1. the water/steam mass flow rate: this value must be assigned to the first of the two junctions injecting mass into Gothic;
2. the flow averaged enthalpy of the water/steam mixture: this is the specific enthalpy to be assigned to the above flow;

3. the noncondensable gas mass flow rate: this flow rate must be assigned to the second junction, injecting only gas;
4. pressure in the RELAP5 volume upstream the junction: this is necessary to define the thermodynamic properties of both the water/steam and of the noncondensable gas to be injected into the Gothic volume;
5. temperature in the RELAP5 volume upstream the junction: also this variable is necessary to define the thermodynamic properties of the noncondensable gas to be injected into the Gothic volume.

As it can be noted, assigning these variables, that are read from the “FA” vector choosing within the list of “minor edit” variable requests, implies to define the codes of the junction and of the volume upstream the junction in the adopted RELAP5 nodalization; this information must be provided in the “relaptogothic.dat” file that is read by the modified TRAN routine of RELAP5 at the start of the calculation.

It must be noted that in the original routine provided by NAI, only the two first variables in the above dotted list were assigned.

From Gothic to RELAP5

The variables transferred from Gothic to RELAP5 are ten per each RELAP5 junction linked to Gothic and must be assigned in the order reported below:

1. pressure in the containment volume;
2. specific enthalpy of liquid in the containment volume;
3. specific enthalpy of steam in the containment volume;
4. specific enthalpy of the noncondensable gas in the containment volume;
5. liquid level in the containment volume;
6. elevation of the junction from the bottom of the containment volume;
7. height span of the junction in the containment volume;
8. density of the liquid phase in the containment volume;
9. density of the vapour (gas plus steam) phase in the containment volume;
10. mass fraction of steam in the containment volume.

The containment volume may be a single lumped GOTHIC or one of the nodes of a subdivided volume, when a more accurate definition of containment side variables is needed. As it can be argued from their definitions, all the above variables are required to define the backpressure downstream a junction injecting into a Gothic volume and the thermodynamic properties of the fluid upstream a junction extracting fluid from a Gothic volume.

It must be emphasised that all these variables must be converted from the SI units (supposed to be adopted in RELAP5) to British units or to multiples of SI units adopted in the Gothic code, also depending on the input choices. Hereafter, it will be anyway implied that SI unites are always adopted in both RELAP5 and Gothic input decks, since the present limited qualification was performed only with these options.

2.3 Time advancement management

The coupling between the two codes is made on the basis of a time-explicit coupling, in which the conditions calculated by either code are used by the other for the next time step advancement. The synchronisation between the two codes is performed by the interfacing C routine, by passing the elapsed time of the RELAP5 and GOTHIC codes as the first element of the two vectors needed for the inter-processing exchange of information. As the interfacing C routine that manages the time advancement was not modified with respect to the original version received by NAI, being of proprietary nature, it is not possible to describe its detailed structure in this report.

As above mentioned, though this was not possible in the present phase of the work, improvements in the reliability of the information transferred between the two codes, by proper time integration, could be advisable in the future.

3. DESCRIPTION OF INVOLVED ROUTINES AND CODE FEATURES

3.1 Involved RELAP5 Routines

The main RELAP5 routines involved in the coupling between the two codes are two:

- the TRAN routine, controlling the transient advancement;
- the TSTATE routine, for updating the time dependent volumes and junctions at each time step.

The following main changes were introduced in the original TRAN routine for purpose of coupling RELAP5 with Gothic:

- read statements for defining:
    - the units to be used in the Gothic code input file (SI assumed up to now);
    - the number of RELAP5 junctions linked to Gothic;
    - the labels of the linked junctions and of the related upstream volumes in the RELAP5 nodalization; both these labels must be entered as integers having the same format of the parameters to be assigned in minor edit requests related to junctions and volumes;
- assignment of the indices of the variables to be read in RELAP5 from the “FA” vector, making use of calls to the SCNREQ routine;
- calculating the five variables to be passed to Gothic, i.e.:
    - the partial mass flow rates and enthalpies of water/steam and noncondensable gases and the pressure to be assigned to the first Gothic flow path assigned to each linked RELAP5 junction;
    - the pressure and the temperature of the volume upstream the junction, for letting Gothic calculate the thermodynamic properties of the noncondensable gas injected at the second Gothic flow path assigned to each linked RELAP5 junction;
- assigning the variables to be passed from RELAP5 to Gothic to the vector used by the C routine passing information to the Gothic code;
- reading the 10 variables to be passed from RELAP5 to Gothic in the vector used by the C routine passing information from the Gothic code;

- preparing the "univec" vector of five components to be passed in a common area to the TSTATE routine for defining pressure, liquid and gas specific internal energies, void fraction and noncondensable gas quality.

The passage of information must be made at the first time-step and at each subsequent one.

The modification made to the TSTATE routine is just the following:

```
         elseif (itype .eq. 7) then
c
c  input is (P,uf,ug,voidg,xa)
c
c
c----UNIPI-------------------start---------------
c
       write(46,*) ' in tstate 1', (prop(iii), iii = 11, 15)
       if(prop(11) .lt. 0.0d00) then
                iunipi = iabs(idint(prop(11)))
c
                if(iunipi.gt.1000) then
                      iunipi = iunipi - 1000
c
       write(46,*) ' iunipi = ', prop(11), iunipi
                      prop(11) = univec(1,iunipi)
                      if(univec(6,iunipi).lt.0.0d00) then
                             prop(12) = univec(2,iunipi)
                             prop(13) = univec(3,iunipi)
                             prop(14) = univec(4,iunipi)
                             prop(15) = univec(5,iunipi)
                      endif
c
                else
c
                             prop(11) = univec(1,iunipi)
                             prop(12) = univec(2,iunipi)
                             prop(13) = univec(3,iunipi)
                             prop(14) = univec(4,iunipi)
                             prop(15) = univec(5,iunipi)
c
            endif
c
       write(46,*) ' in tstate 2', (prop(iii), iii = 11, 15)
       endif
c
c----UNIPI-------------------end---------------
c
```

In order to make these FORTRAN lines, added in the subroutine TSTATE for processing the case in which "t" in "εbt" is equal to 6, work properly it is necessary that a sudden change from physical values of pressure to negative and integer values is assigned in input for the time dependent volume. As an example, the following table is assigned to the "ccc" time dependent volume to shift from the imposed conditions of a classical "option 6" component to the assignment of the values of pressure, internal energies, void fraction and noncondensable gas quality in the containment volume to which the first junction listed in the "relaptogothic.dat" is linked:

```
*                  εbt
ccc0200            006
*                  Time      Press       Uf       Ug      Voidg     Quala
ccc0201             0.0       1.e5     41000.  370000.      1.0       1.0
ccc0202             5.0       1.e5     41000.  370000.      1.0       1.0
ccc0203        5.000001        -1.     41000.  370000.      1.0       1.0
ccc0204           1.e06        -1.     41000.  370000.      1.0       1.0
```

The above lines mean that, after 5 s of transient calculation, the control of the properties in the time dependent volume is assigned to the corresponding Gothic containment volume conditions, in place of the values listed in the table. Obviously enough, if instead of the first junction linked to Gothic the second or the *n*-th junction are addressed, pressure must be assigned to "-2." or "-*n.*" at the prescribed time.

As a variant of the above input choice, the following definitions can be also adopted:

```
*               εbt
ccc0200         006
*               Time      Press       Uf      Ug     Voidg    Quala
ccc0201          0.0       1.e5    41000. 370000.      1.0      1.0
ccc0202          5.0       1.e5    41000. 370000.      1.0      1.0
ccc0203     5.000001     -1001.    41000. 370000.      1.0      1.0
ccc0204        1.e06     -1001.    41000. 370000.      1.0      1.0
```

with the negative values of pressure taking the values -1001., 1002., …, -100n., with a similar meaning as in the case of -1., -2., …, -n.. This choice is adopted in order to specify that only the backpressure will be taken from the containment calculation to be assigned in the time dependent volume for forward flow, while the full set of variables P, U_f, U_g, α_g and quality of the noncondensable gas will be assigned for backward flow, as in the previously described case. This option was introduced to avoid local numerical problems with very dynamic blowdown cases in which it was found difficult to assign coherent values of all the thermodynamic values calculated by Gothic to be passed to RELAP5. This option could be removed in the future once a proper understanding of the reasons leading to the encountered problems will be achieved.

In transferring the value of the internal energy of the noncondensable gas, it must be considered that the zeroes of this quantity are defined in different ways for each noncondensable gas in the two codes. This difficulty, that was fully expected on the basis of previous experience in the coupling of similar codes, was overcome by making the two codes calculate the internal energy of air at 0 °C and assuming that the difference observed in the internal energies computed by the two codes at that temperature is sufficiently representative of the difference at *any* temperature. The latter assumption, evidently, was made trusting in the physical reliability of the properties included in both codes that, despite of the difference in the reference temperature, should anyway follow known experimental data for air properties in sufficiently close agreement. Obviously enough, at the present stage there was no other possible choice than relying in such an assumption, since an exact equalisation of property evaluation in both codes is out of the scope of any code coupling activity between existing codes. The difference in air specific internal energy calculated by RELAP5 and Gothic was provisionally assigned the value

157422.92 J/kg, while waiting for more detailed information to suggest a better qualified value.

An additional limitation in the coupling methodology is related to the evaluation of the specific internal energy of the liquid at the RELAP5 time dependent volume. In the case of a water pool containing also bubbles, the internal energy of the liquid may be greater than the saturated liquid value, being interpreted by the RELAP5 code as a flow of metastable superheated liquid. Since RELAP5 allows only for a limited superheating to be dealt with in time dependent volumes, an upper limit to U_f was assigned at 800 kJ/kg, that resulted as a suitable value for RELAP5 in the range from 0.01 to 1 MPa of containment pressures. This simplification was accepted on the basis of the following considerations:

- supersaturated conditions in pools are normally restricted to limited time ranges in postulated accidents (e.g., the blowdown phase), where downstream junction conditions, with the possible exception of back pressure, are rather unimportant, unless there is a drainage of a pool containing bubbles towards a primary system component (a somehow rare case);
- a proper account of such multi-phase situations allowed in Gothic, to be made coherent with the two-phase flow model of RELAP5, would require the transfer of a huge amount of information from Gothic to RELAP5, considerably complicating the process of data transfer; by the way, it is not completely clear at the moment if such information is available in the form of accessible variables in Gothic.

While accepting the above compromise, that could lead to an imperfect energy balance between Gothic and RELAP5 in limited time windows, it is hoped that a future version of Gothic will provide direct access to the variables that may make easier the treatment of such conditions in the coupling between Gothic and RELAP5.

3.2 Gothic InterProcess Communication features

Gothic is equipped with the capability to run its process simultaneously with external processes. This InterProcess Communication (IPC) feature allows the identification of the process to be run simultaneously with Gothic together with its input file and to run it starting the process from the Gothic side.

The variables to be read and written from and to the external process must be defined in the appropriate panels available in Gothic (through *IPC Read* and *IPC Write*) and must be listed strictly in the same order that is used in the modified TRAN routine to assign the respective variables, reported in Chapter 2.

3.3 Interfacing routine

As mentioned in the previous sections, an interfacing routine written in C language is provided with the code, allowing for the transfer of information from and to the external process. There was no need to customise this routine for the particular needs of present work and the version received in the example purchased from NAI was retained.

4. RUNNING COUPLED CALCULATIONS

4.1 Data to be defined on RELAP5 side

As mentioned in the previous chapters, the strategy of coupling between the two codes includes the link of multiple junction and time dependent volume couples in RELAP5 to a doubled number of corresponding flow paths linked to boundary conditions in Gothic. At the moment a quite redundant number of such junctions is made possible in the coupling (up to 100), but this is obviously a limitation that can be easily removed whenever needed.

The only required change in a RELAP5 input deck regards the time dependent volumes downstream the junctions linked to Gothic and was described in Section 3.1 Involved RELAP5 Routines. It is even more stressed that the negative integer number (though assigned as a floating point) suddenly appearing in the pressure table (in a single time step) must be assigned considering the order of junctions and "from" volumes appearing in the "relaptogothic.dat" ASCII file, that is read by the modified TRAN routine at the start of the calculation. An example of such file is reported hereafter:

```
UNITS
'SIUnits'
NJUN
2
JVAR           JFROM
105000000      100200000
205000000      200200000
```

The above lines in the file specify the following:

- the SI units are selected for the Gothic input deck; this choice is recommended since it is the only one checked up to now;
- two junction and time dependent volume couples are linked to Gothic, being identified by 105000000 and 205000000; it must be recalled that:
    - <u>the junctions must have the corresponding time dependent volume defined as the "TO" volume</u>; in this respect the above definitions require the presence in the RELAP input deck of two time dependent volumes (e.g., 110 and 210 in this example, but the numbering may be absolutely arbitrary) containing lines similar to the following ones:

```
*              εbt
1100200        006
*              Time      Press      Uf      Ug     Voidg    Quala
1100201         0.0       1.e5   41000. 370000.      1.0      1.0
1100202         5.0       1.e5   41000. 370000.      1.0      1.0
1100203    5.000001        -1.   41000. 370000.      1.0      1.0
1100204       1.e06        -1.   41000. 370000.      1.0      1.0
```

and

```
*                 εbt
2100200           006
*                 Time       Press       Uf       Ug      Voidg     Quala
2100201            0.0        1.e5    41000. 370000.        1.0       1.0
2100202            5.0        1.e5    41000. 370000.        1.0       1.0
2100203       5.000001         -2.    41000. 370000.        1.0       1.0
2100204          1.e06         -2.    41000. 370000.        1.0       1.0
```

in which the mandatory specifications are the option ‘t’ in the ‘εbt’ field, to be assigned at ‘6’, and the presence of integer negative numbers assigned to pressure, putting a link between the first and the second junction in the “relaptogothic.dat” file to the time dependent volumes containing -1. and -2. in pressure specification after some selected time;

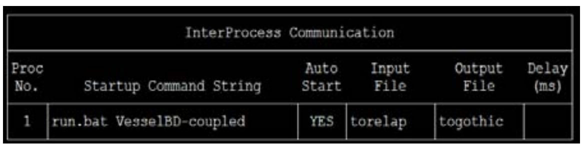
- o the “FROM” junction volume must be also specified, to let the TRAN routine assign the proper values of temperature and pressure for calculation of forward flow of noncondensable gases; in the above example, the FROM volumes are the volumes 20 in the pipe components 100 and 200 respectively;
- o the donwnstream (i.e., “TO”) time-dependent volume should represent the containment volume on the side of RELAP5; its properties will be read from the volume or the node of a subdivided volume connected to the corresponding boundary condition flow path in Gothic and assigned during calculation advancement.

Variants of this arrangement are possible for specific cases, as it will be shown in the companion report on the first coupling assessment [4], but they must be conceived clearly understanding their implications in the logical process adopted by the coupling routines.

4.2 Data to be defined on Gothic side

As already mentioned in the previous sections, the actions to be performed on the Gothic side are related to the assignment of the process name and of the requested variables.

Figure 4 shows the assignment of the batch file running RELAP5 (“run.bat”) with the argument of one of the sample input files (“VesselBD-coupled.i”). This assignment is necessary in order to know which external process has to be run in conjunction with Gothic.


InterProcess Communication

Proc No.	Startup Command String	Auto Start	Input File	Output File	Delay (ms)
1	run.bat VesselBD-coupled	YES	torelap	togothic	

Figure 4. Assignment of the external process on the Gothic side

On the other hand, several control variables must be prepared for exchanging data between the two processes as shown in Figure 5. Some of them will be assigned to the boundary conditions as shown in Figure 6.

Control Variables

CV #	Description	Func. Form	Initial Value	Coeff. G	Coeff. a0	Min	Max	Upd. Int. Mult.
1C	Backpressure	ipc_wri	0.	1.	0.	-1e+03	1e+032	0.
2C	flow_enth_qua	ipc_rea	0.	1.	0.	-1e+03	1e+032	0.
3C	Flow_njul	sum	0.	1.	0.	-1e+03	1e+032	0.
4C	Enth_jun1	sum	0.	1.	0.	-1e+03	1e+032	0.
5C	FLow_NC_jun1	sum	0.	1.	0.	-1e+03	1e+032	0.
6C	Bk_press_jun1	sum	0.	1.	0.	-1e+03	1e+032	0.
7C	Tgas_jun1	sum	0.	1.	0.	-1e+03	1e+032	0.
8C	Flow_jun2	sum	0.	1.	0.	-1e+03	1e+032	0.
9C	Enth_jun2	sum	0.	1.	0.	-1e+03	1e+032	0.
10C	Flow_NC_jun2	sum	0.	1.	0.	-1e+03	1e+032	0.
11C	BK_press_jun2	sum	0.	1.	0.	-1e+03	1e+032	0.
12C	Tgas_jun2	sum	0.	1.	0.	-1e+03	1e+032	0.
13C	avbar	sum	0.	1.	0.	-1e+03	1e+032	0.
14C	rhonc	sum	0.	1.	0.	-1e+03	1e+032	0.
15C	albar	sum	0.	1.	0.	-1e+03	1e+032	0.
16C	hliqin	sum	0.	1.	0.	-1e+03	1e+032	0.

Figure 5. Assignment of various useful control variables on the Gothic side

Fluid Boundary Conditions - Table 1

BC#	Description	Press. (kPa)	FF	Temp. (C)	FF	Flow (kg/s)	FF	S P	J O	ON Trip	OFF Trip	Elev. (m)
1F	Gravity injecti	1.	6C	E1.0	4C	1.0	3C	N	N			9.5
2F	Tank	1.	11	E1.0	9C	1.0	8C	N	N			0.5
3F	Gravity_NC	1.	6C	1.0	7C	1.0	5C	Y	N			9.5
4F	Tank_NC	1.	11	1.0	12	1.0	10	Y	N			0.5

Figure 6. Assignment control variables to boundary conditions on the Gothic side

Finally, the 10 variables to be passed to RELAP5 at each junction can be considered in Figure 7, referring to the case of two RELAP5 junctions both linked to a single lumped Gothic volume (cV1), that also serves as a list of the exact sequence of control variables to be passed to RELAP5 per each linked junction (see, e.g., the list of control variables from 2 to 11 and from 12 to 21 in the Figure).

Function Components
Control Variable 1C
Backpressure
ipc_write
Y=G*ipc_write(ProcX1,a2X2,a3X3,...,anXn)

#	Gothic_s Name	Variable location	Coef. a
1	Proc	cp1	1.
2	P	cV1	1.
3	Hl	cV1	1.
4	Hs	cV1	1.
5	Hm	cV1	1.
6	Poolel	cV1	1.
7	Eljncl	cJ1	1.
8	Htjncl	cJ1	1.
9	Rl	cV1	1.
10	Rv	cV1	1.
11	Smassf	cV1	1.
12	P	cV1	1.
13	Hl	cV1	1.
14	Hs	cV1	1.
15	Hm	cV1	1.
16	Poolel	cV1	1.
17	Eljncl	cJ2	1.
18	Htjncl	cJ2	1.
19	Rl	cV1	1.
20	Rv	cV1	1.
21	Smassf	cV1	1.

Figure 7. Assignment of 10 variables for each of two junctions adopted in sample calculations

4.3 Procedure to be followed for calculation preparation

In order to run the calculation, the following steps must be performed:

- preparing the RELAP5 input deck, with particular attention to the junctions to be linked to Gothic and to the identification of the “FROM” volume (of any allowed kind) and the “TO” time dependent volume;
- preparing the Gothic input deck, with particular attention to:
  - the 2 boundary conditions and the related flow paths corresponding to each linked RELAP5 junction;
  - the assignment to the flow paths of the 3 variables for “forward” flow of water/steam flow rate and of the 2 variables for noncondensable gas “forward” flow;
  - the assignment of the 10 variables required to be transferred to RELAP5 per each linked junction;
- preparing the “gothictorelap.dat” file, taking care in assigning a sequence of junctions and “FROM” volumes coherent with the specifications adopted in defining the time dependent volumes in RELAP5;
- running the calculation from the appropriate Gothic control panel.

5. CONCLUSIONS AND FUTURE DEVELOPMENTS

The performed work allowed to achieve coupling capabilities between the Gothic and the RELAP5 codes. Summarising, the coupling capabilities that were achieved are related to the analysis of gas-steam and liquid injection into or extraction from a Gothic containment volume, driven by the calculation of flow rates at RELAP5 junctions.

As it will be shown in a companion Report [4], this allows, for instance, the analysis of superheated water blowdown from a primary coolant loop to the containment system, together with gravity driven injection.

The achieved capabilities extend those allowed by the sample interfacing routine received from NAI, allowing for bi-directional mass and energy exchanges with the treatment of noncondensable gases (air at the moment). Nevertheless, this first form of coupling between the codes could be improved and made easier whenever the Gothic code will be equipped with a wider range of accessible variables calculated at flow paths, as local pressure, void fraction as a function of water level and the specific enthalpies of each flow field.

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