

TESTING OF THE QUICKEST-ULTIMATE ALGORITHM TO SOLVE THE DISSOLVED CONVECTION EQUATION DURING A BORON DILUTION TEST AT THE PKL FACILITY

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Abstract

Rapid boron dilution transients have shown the need for accurate knowledge of the solute particle distribution in pressurized water reactors (PWR), since its concentration would affect the reactivity of the system. Particularly relevant are scenarios where a separation between high and low borated water takes place. For instance, low borated plugs can be formed in the loop seals of a PWR during small-break-loss-of-coolant-accidents (SBLOCA) where reflux-condensation conditions are kept for a long time. Since online boron concentration measurement is impractical in the primary system of PWR plants, the formation of such a plug would take place unnoticed by the operators. The thermal-hydraulic system code TRACE, developed by US-NRC, may be used to track the boron concentration along the system. However, in the TRACE code the dissolved solute convection equation is solved by employing a first-order upwind scheme. The use of such a scheme is known to introduce high numerical diffusion when a gradient of boron concentration flows through the system. In order to more accurately simulate rapid boron dilution transients by using TRACE, the high order explicit scheme QUICKEST together with the ULTIMATE limiter were implemented in the TRACE code. The model was tested in simple geometries and in the coupling between the TRACE code and a CFD code. A final step is presented in this paper where the new model is tested against an experiment on boron dilution carried out at the integral test facility PKL (AREVA), within the OECD/NEA PKL project.

Introduction

Boric acid is a soluble neutron absorber used in the primary coolant of pressurized water reactors in order to control the core reactivity. A significant reduction of the boron concentration in the core could cause a severe reactivity insertion and may lead to high power excursions, threatening the fuel integrity. Whereas in normal reactor operation the specified boron concentration is maintained by the volume control system, during accident conditions borated water would be injected by the emergency core cooling system.

Inadvertent boron dilution might occur in two different scenarios as pointed out by Teschendorff, 2001 [1]: Unintentional injection of unborated water from outside the primary cooling system or separation of primary coolant into highly borated water and almost boron-free water by evaporation and condensation. The latter type of events were first introduced by Hyvarinen in 1993 [2] and can occur during small break LOCAs where effective reflux-condensation conditions are established. Under such conditions, steam produced in the core flows to the steam generator U-tubes where it condenses, falling down to either side of the U-tubes. Since boric acid particles are retained in the liquid phase, the condensed liquid has no

boron. Hence, unborated water may be accumulated in the loop seals. If these conditions are maintained for a sufficient period of time, the loop seals and the cold legs will fill up with boron-free water. If at a later time, circulation in the cooling system is re-established, the plugs of low-borated water will be driven through the downcomer and lower plenum into the core with the risk of inserting undesired reactivity in the reactor core. To estimate the concentration and size of the plugs once they arrive to the core, computational tools are needed.

Due to the complexity of the phenomena involved during this process, computational fluid dynamics (CFD) codes have been employed for detailed analyses, and yielded good results in the reproduction of experimental data even in complex geometries [3]. However, the use of CFD is still limited to some areas of the primary system only, and its ability to simulate the formation of the plugs (mainly occurring during two phase flow) and the onset of natural circulation, which takes place along the transition from two-phase flow to subcooled flow, is still not yet demonstrated. Therefore assumptions and simplifications have to be made, in order to define appropriate boundary conditions for the CFD simulation. The boundary conditions are generally derived on the basis of simulations performed by thermal-hydraulic system codes.

Thermal-hydraulic system codes have proven their capability to simulate correctly most of the phenomena occurring during SBLOCAs [4]. In particular, simulations involving the onset of natural circulation or reflux-condenser conditions have been compared to experiments with satisfactory results [5]. In contrast to that, system codes are known to have relatively low accuracy when simulating the travelling of abrupt field changes (e.g. sharp fronts) because of high numerical diffusion generated by first order upwind models [6]. This is the case of a low concentration slug moving inside a highly borated medium. In addition, the mixing due to complex geometries is not taken into account. These are major obstacles for the accuracy of analyses for transients where boron plugs travel through the primary system.

At the moment, analyses are moving toward coupled CFD and system codes calculations where the formation of the plugs is calculated by system codes and the displacement of the plug to the core is carried out by CFD analysis. Studies are being performed in this direction [7], however, even in this case, the accuracy issues of the solute transport models in system codes still need to be addressed. Efforts have been done in the past, aimed at improving boron transport models for codes like RELAP5 [8] and TRAC [6], but in the official releases of several best-estimate system codes (TRACE, RELAP5...) the solution of the dissolved solute convection equation is still based on first order schemes.

Recent advances at the Paul Scherrer Institut have been carried out to include the explicit QUICKEST scheme together with the ULTIMATE limiter in the TRACE code, to solve the solute convection-diffusion equation [9]. The new method has been tested in simple geometries and compared with CFD results [9]. In the present paper, a TRACE input deck of the PKL test facility [10] derived from a RELAP5 model [11] has been employed to simulate a test of the OECD/PKL-II project on boron dilution. In this work, the selected PKL experiment has been used to test the new solute tracker solution implanted in TRACE, and prove the robustness and performance of the new method in real transient conditions.

1. The new discretization scheme for the TRACE solute tracking equation

TRACE includes the capability of tracking a solute field, in order to simulate the presence of a soluble neutron poison in the coolant of the primary loop and, in this way, evaluate the reactivity feedback effects. Since the quantity of boron dissolved in the system is usually limited, the following assumptions are made in the modelling of solute transport [12, 13]:

- solute particles travel at the same local velocity of the liquid (so that knowledge of particle movement is not required);
- solute particles are present only in the liquid phase. If a maximum concentration is exceeded, they plate-out on the walls of the system;
- plating-out and re-dissolution occur at an infinite rate;
- the solute does not affect the hydrodynamics directly (liquid properties, liquid velocity field, heat transfer). However, the amount of dissolved or plated-out solute in the core affects the neutronic feedback, and therefore indirectly the liquid flow through the change in the reactor heat generation;
- plated-out solute affects only the neutronic reactivity feedback. In fact it may affect the surface friction and the wall heat transfer, but this is not modelled in TRACE;
- solubility is a function of the temperature only, and the dependence is considered linear over the defined temperature range.

According to the above hypotheses, the solute convection is governed by a one-dimensional convection equation, adapted to two-phase flow and appropriately constrained with the solubility limits. In differential form, the solute concentration follows the linearized Burgers equation [14]:

$$\frac{\partial \phi}{\partial t} + \frac{\partial (v_p \cdot \phi)}{\partial x} = \frac{\partial}{\partial x} \left(D \frac{\partial \phi}{\partial x} \right) + S$$

Where ϕ is the solute concentration, v_p is the speed of the particles (which is equal to the liquid velocity), D is the diffusion coefficient and S is a source/sink term. In addition to the previous assumptions, no modelling of boron diffusion is included in the TRACE code (i.e. $D=0$).

A first-order-upwind finite-volume semi-implicit scheme is used to solve the above equation in the original TRACE version. While such discretization is very robust and computationally efficient, its low accuracy and the introduction of significant numerical diffusion leave large room for optimization as regards to better tracking of sharp solute fronts. Several studies have pointed out the issue of high numerical diffusion introduced by thermal-hydraulic system codes [15].

To address the issue of the numerical diffusion, the third-order-upwind scheme QUICKEST [16,17], together with the ULTIMATE limiter [18], has been implemented in the solute convection equation of TRACE at the Paul Scherrer Institut [9], by following a strategy

similar to the one adopted in the past for RELAP [6]. The newly modified TRACE features low numerical diffusion of the solute tracker, together with the possibility of employing a user-defined physical diffusion coefficient for the dissolved solute; as a drawback, QUICKEST is an explicit method, thus the maximum time step is limited by the Courant number of the system. The solver is currently developed for one-dimensional components, and was extended to include the presence of side junctions, which introduces a quasi-two-dimensional component to the discretization.

2. Analysis of the PKL I tests

The OECD/PKL-I program is a continuation of the previous OECD/SETH project [10] which addressed, among others issues, boron dilution transients. Within the project, a series of boron dilution related experiments were carried out at the PKL test facility. The PKL, located in Erlangen (Germany), is a large scale experimental power plant facility designed to simulate pressurizer water reactors under accidental conditions. The facility replicates the entire primary system and most of the secondary system (except for the turbine and condenser) of a 1300-MW PWR plant, with elevations scaled 1:1 and volumes and power reduced by a factor of 145. The number of rods in the core and the number of U-tubes in the steam generators (SG) were scaled by a factor of 145 as well. Unlike many experimental facilities with only two available loops (one to simulate the broken loop and the other to simulate the intact three loops), PKL simulates all four loops separately. The experiments performed in the PKL test facility address the issue of boron dilution from the thermal-hydraulic point of view, and are a good reference to both validate and improve thermal-hydraulic codes.

The studies on boron dilution within the OECD/PKL I project consisted of two tests:

- Test F1.2 was designed to analyze the rate of boron dilution under reflux-condensation conditions depending on the mass inventory in the primary system. The test follows a series of consecutive steady states with different mass inventories, while a high SG level is maintained in the U-tubes. In this way, it is possible to determine at what U-tube levels and mass inventories the accumulation of condensate in the loop seals occurs [19]. This test focuses on the process of formation of the boron diluted slugs and not on its transport through the system. Therefore, the use of a second order scheme in this case is not needed.
- Test F1.1 is instead a continuation of the E series of the SETH project [20] related to SBLOCA with boron dilution. In this case the test is configured such to resemble a PWR Westinghouse design, e.g. steam generator cool down rate of about 50 K/h and Emergency Core Cooling (ECC) injection into all 4 cold legs. The main objective of the test is to gather the maximum amount of low borated water in the loop seals (LS), and study the restart of natural circulation providing the minimum boron concentration at the reactor pressure vessel inlet [21]. This test is used in this paper to test the new method.

2.1 Description of the TRACE Nodalization

The TRACE nodalization has been fully developed based on a well tested RELAP5 model of the PKL test facility, previously developed at the Technical University of Catalonia (UPC) [5,21] with the support of the Spanish Nuclear Regulatory Body (Consejo de Seguridad Nuclear). The model changes have been kept to the minimum extend to allow cross comparison between the two codes. A diagram of the nodalization is shown in Fig. 1. All walls and surfaces are modeled by heat structures to take into account any heat loss or heat exchange. The core fuel rods and other heaters (upper head and pressurizer) are modeled by means of heat structures, as well. Most auxiliary, safety and control systems are modeled by means of FILL (i.e. velocity or mass flow-rates boundary conditions) and BREAK (i.e. pressure boundary conditions) components.

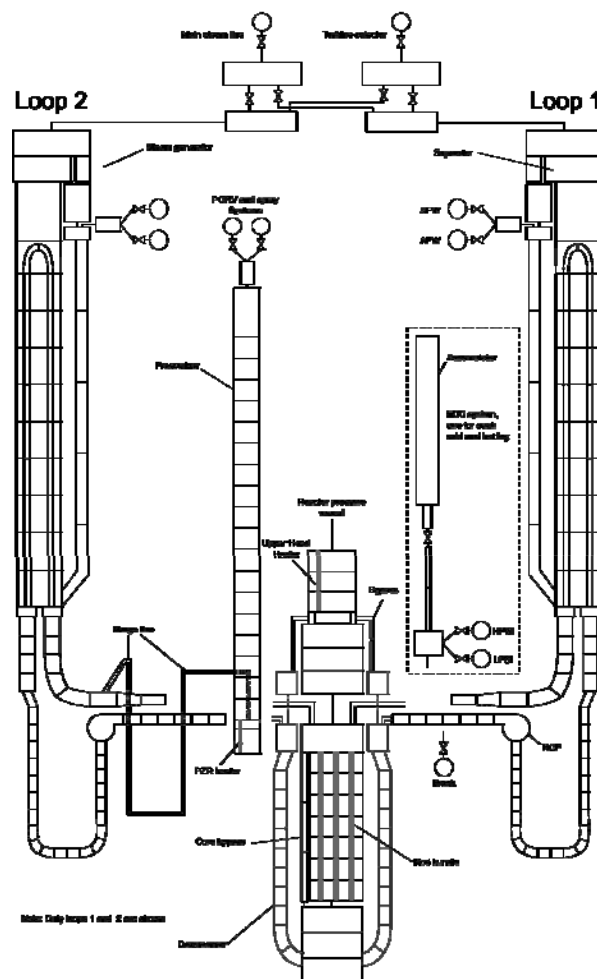


Figure 1 Nodalization for the PKL Test Facility

The core region is nodalized by a single pipe with 7 axial cells. The downcomer (DC) is modeled with two separate pipes, since recirculation was detected in some experiments. On the other hand, the downcomer of the SGs are simulated with a single pipe as the required detail in the secondary system is not as high as for the primary side. There are four bypass pipes from the upper plenum (UP) to the DC, which are nodalized with two different lines to allow the reproduction of asymmetric phenomena.

The discretization used in the nodalization consists of 438 hydraulic volumes and 1356 heat structures mesh points.

A steady state calculation (zero transient) was performed to check the stability of the developed TRACE nodalization. The initial conditions of the PKL facility prior the conditioning phase of Test F1.1 were successfully achieved with the TRACE model. Table 1 displays the deviation from the experiment of both RELAP5 and TRACE simulations. Most parameters are in close agreement with the experimental data, the core outlet temperature is 3 degrees higher, and the natural circulation flow is slightly under-estimated. These differences were already present in the RELAP5 calculation.

Table 2 Steady state conditions for PKL test F1.1, RELAP5 and TRACE deviation from the experiment is shown

	Deviation from experiment	
	RELAP5	TRACE
Primary pressure	0.15 bar	0.16 bar
Hot leg temperature	+3 K	+3 K
Cold leg temperature	+0.5 K	+0.8 K
Loop mass flow	-7 %	-5 %
Pressurizer level	10 %	0 %
Main steam pressure	0.0 bar	0.0 bar
Main steam temperature	0.0 K	0.0 K
SG level	2 %	3 %

The RELAP5 model was also used to check the pressure drops along the primary system and heat losses. Since the k-factors used in both models were the same and these provided the same pressure drops, it can be concluded that the treatment of friction losses in the two codes is similar. Finally the nodalization was tested by comparing the simulation of Tests F1.1 and F1.2 with the experiment and the RELAP5 model [11]. In the present paper the calculation on Test F1.1 is used to test the new solute tracker implemented in TRACE.

2.2 Test F1.1

Test F1.1 is a boron dilution transient with a small break located in cold leg 1. Each High Pressure Safety Injection (HPSI) pump injects symmetrically in all loops (cold leg injection). Unavailability of Low Pressure Safety Injection (LPSI) and accumulators is supposed. In addition, one of the HPSI pumps is not operable.

Since the maximum operating pressure of the PKL test facility is 45 bar, it is not possible to simulate the entire transient of a normal PWR starting from nominal operating pressure (ca. 160 bar). Hence, in the test the transient starts at a primary pressure of less than 45 bar, and with the initial conditions corresponding to those that would prevail in a real plant at this time of the transient. The initial conditions for Test F1.1 consist of a partially emptied primary system at a pressure of 39 bar, with highly borated water in the core and unborated water in the loop seals. In order to reach such conditions, a conditioning phase is performed during which the primary mass inventory is reduced to 50%, and reflux-condensation conditions are

established in the primary system. During this phase slugs of boron-diluted condensate are formed in the LSs. The conditioning phase was also simulated by TRACE, in order to analyze the process of formation of the unborated slugs.

The hardware configuration of test F1.1 is described in reference [21]. The main characteristics are listed here:

- Small break ($21 \text{ cm}^2/145$) in cold leg 1 between the reactor coolant pump (RCP) and the reactor pressure vessel (RPV).
- Low pressure injections: unavailability of LPSI and accumulators.
- High pressure injections: primary feed by 1 out of 2 HPSI pumps, injection of highly borated water via header symmetrically into all 4 cold legs.
- Steam generators secondary side: cooldown of all 4 SGs at 56 K/h using all main steam relief control valves (MS-RCVs) (SGs interconnected via main steam header).

During the first part of the test, the primary and secondary pressures decrease following the secondary cool-down. Since the amount of injected water is greater than the discharged mass, the primary system refills. When the primary system is refilled, primary pressure recovers and natural circulation is established. At this moment, the boron-diluted slugs are transported to the vessel through the cold legs. Secondary pressure continues falling bounded by the cool-down, while primary pressure stabilizes at a certain pressure until the end of the transient.

2.2.1 Results

The RELAP5 results shown in this section were obtained with a modified version of RELAP5 mod3.3, where a second order scheme is used to solve the solute transport equation [8]. Figure 2 shows the break mass flow along with the primary and secondary pressures obtained with the modified versions of RELAP5 and TRACE. The primary and secondary pressures present a quite good agreement with the experimental data in both cases. The break flow is also well simulated, the only difference being a slightly overestimation by both codes during the last part of the transient (e.g. after 7000 s in Figure 3).

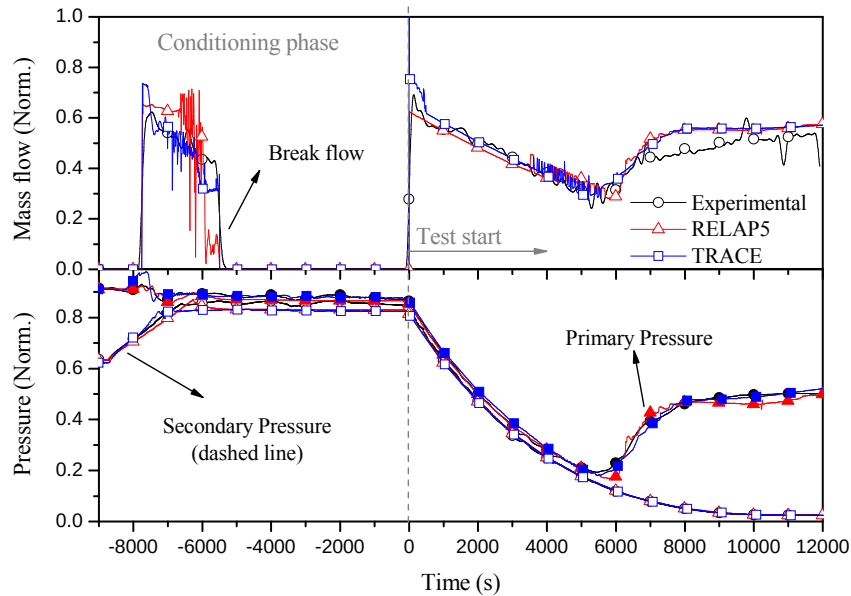


Figure 4 Break mass flow (top) and primary and secondary pressures (bottom) for Test F1.1

The start of the natural circulation coincides with the increase of primary pressure and break flow. This event occurs almost simultaneously in the three traces shown (around 6000 s in Figure 2). The predictions of the boron concentration along loop 4 are shown in Figure 5, where the modified TRACE version is compared with the original TRACE and the RELAP5 codes. The boron dilution phenomenon occurring during the conditioning phase in the LS was correctly simulated by all code versions, as shown in the bottom plot of Figure 6. The difference between the two TRACE models during this period is very small because diffusion does not play a role during reflux-condensation conditions. Later on, after the start of the test the two TRACE versions also show very similar trends, since numerical diffusion and the physical diffusion term introduced in the QUICKEST-ULTIMATE scheme follow similar patterns (second order derivative).

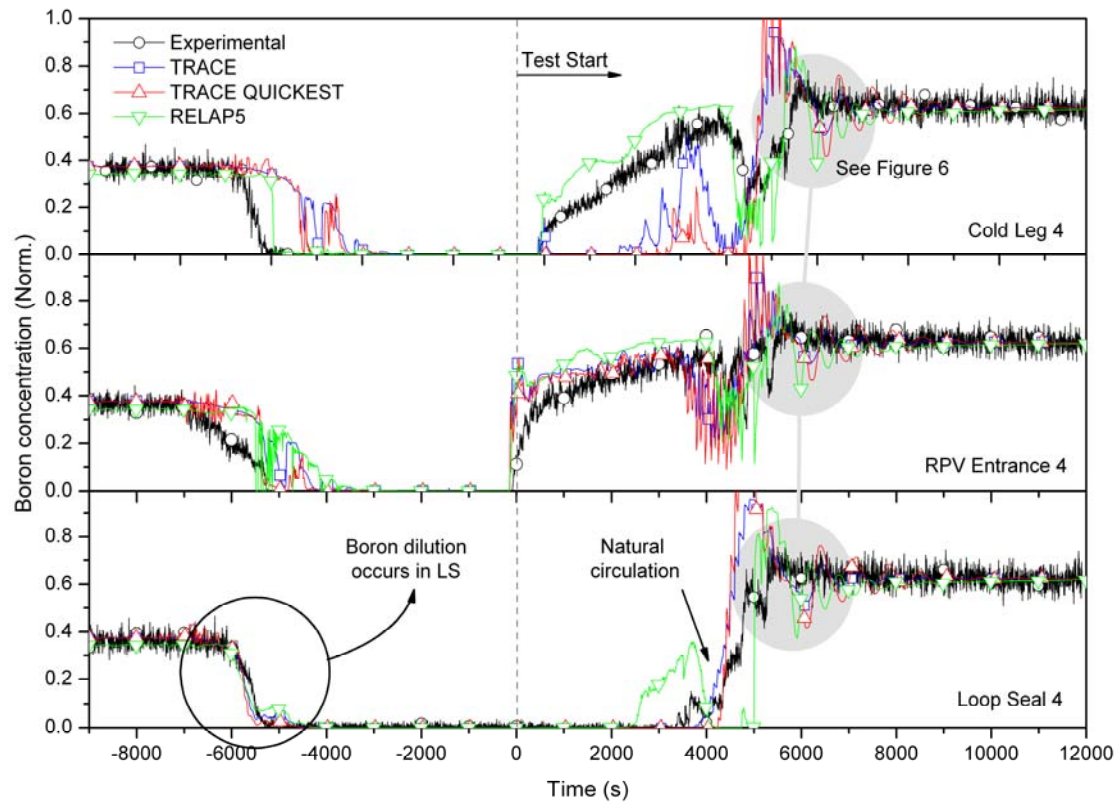


Figure 7 Boron concentration along loop 4 for Test F1.1. The new TRACE model is compared to the original TRACE model and the RELAP5 modified version

Figure 4 shows a detail of the boron concentration along the loop when the natural circulation is established, and thus the slightly unborated slug circulates around the system. One can appreciate the differences between the amplitude of the concentration oscillations, and that similar minimum values are obtained with the two second order schemes (RELAP5 and TRACE). Higher diffusion is seen with the original TRACE version, even though the equation used in that model supposes no diffusion at all, this result was expected due to the highly diffusive solver used in the original TRACE version. In addition, whereas the original TRACE results are affected by the time step and the spatial discretization, the results with the new method are not altered by such changes (see ref. [9] for further details). On the other hand, it must be noted that, coinciding with the start of natural circulation (around 5000 seconds in Figure 3), the boron concentration is suddenly very high for a short period of time indicating that, perhaps the numerical flow limiters are not adjusted properly.

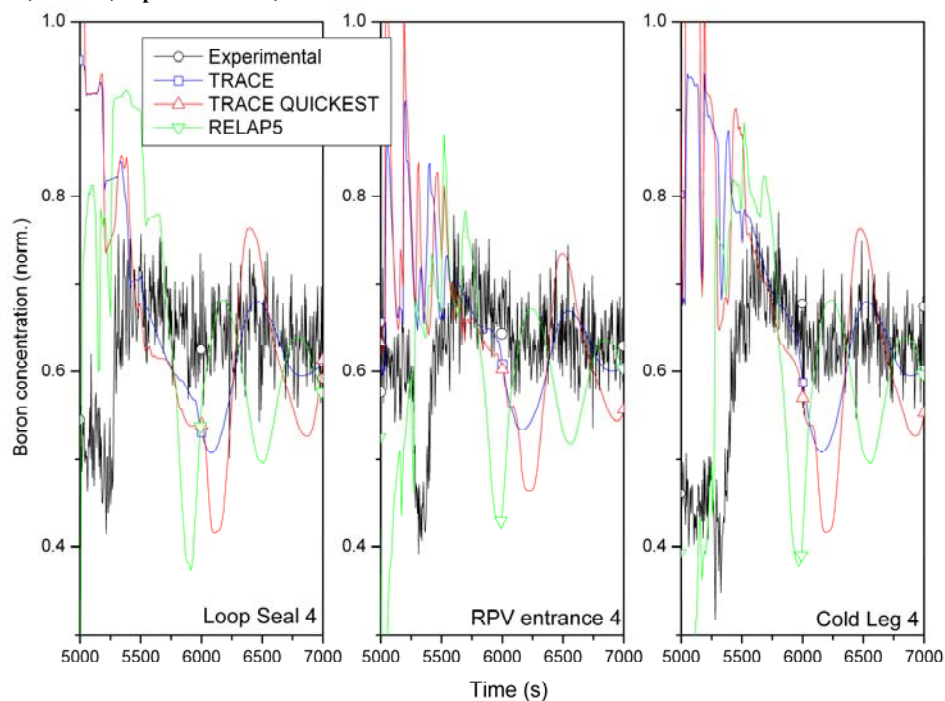


Figure 8 Detail of the Boron concentration along loop 4 once the natural circulation is established, Test F1.1

3. Conclusion

The QUIKEST-ULTIMATE algorithm has been implanted in the USNRC code TRACE to solve the dissolved convection equation for the tracking of solute particles. In order to test the robustness and applicability of the new method, a simulation of a SBLOCA with boron dilution experiment performed at the PKL test facility, has been carried out. The nodalization of the PKL facility used was derived from a RELAP-5 input deck developed at the UPC. The overall performance of the nodalization showed a good agreement with the experiment and the results in the thermal-hydraulics part were not altered by the use of the new method. The new algorithm has helped to reduce significantly numerical diffusion and permits the addition of a physical diffusion term to the equation. The oscillations observed after the restart of the natural circulation (i.e. the circulation of the slug through the system) were in close agreement with the RELAP-5 simulation which was solved with a second order scheme as well. However, the diffusion observed in the experiment was much higher. This is reasonable since system codes do not take into account the mixing due to the structures and geometry, especially where 3-dimensional effects are important.

4. Acknowledgments

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