

# Iodine source term assessment as result of iodine spiking and mass transfer phenomena during a SGTR transient using MELCOR 2.2 and CATHARE 2 codes

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## ABSTRACT

The European project denominated Reduction of Radiological Consequences of design basis and design extension Accidents (R2CA) was launched in September 2019, with a very broad participation: 11 countries, 17 participating organisations, including international organisations, utilities, regulators, technical support organisations, researchers and developers and was coordinated by IRSN. The main goal of the project was to assess the conservatism in the radiological releases calculations in nuclear power plant (NPP) studies.

The work here presented is focused on developing new calculation methodologies and updating computer code models to carry out more detailed assessments of source terms resulting from a steam generator tube rupture (SGTR) accident in the Design Extension conditions A (DEC-A) domain. For this purpose, participants in Work Package 2 (WP2) of R2CA developed and implemented simplified models in the Severe Accident (SA) and Thermal-Hydraulic (TH) codes that take into account iodine spiking and iodine transport phenomena within primary and secondary circuit. These methodologies will not only provide a better estimation of the radiological consequences, but should also serve to improve accident management procedures, innovative instrumentation development and early detection tools.

The new approaches are tested in a SGTR + Steam Line Break Outside Containment scenario without significant fuel degradation in a three-loop Western 1000 MW<sub>e</sub> PWR. During the transient, operators are also assumed to implement emergency operating procedures (EOPs) in line with Westinghouse EOPs to limit the release of radioactivity and control the evolution of plant parameters.

The calculations are performed by Tractebel and CIEMAT with the American SA tool MELCOR and Bel-V with the French TH code CATHARE.

The results highlighted some limitations of implemented models in predicting iodine behaviour as well as small discrepancies in the TH evolution of the transient, both of which were analysed and discussed in detail.

**Abbreviations:** AFWS, Auxiliary Feedwater system; CATHARE, Code for Analysis of Thermal Hydraulics during an Accident of Reactor and Safety Evaluation; CEA, Commissariat à l'énergie atomique et aux énergies alternatives; CF, Control Function; CIEMAT, Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas; CVCS, Chemical and Volume Control System; DBA, Design Basis Accident; DEC, Design Extension Conditions; ECCS, Emergency Core Cooling System; EOP, Emergency Operating Procedures; FL, Flow path; FP, Fission Product; HFP, Hot Full Power; HPSI, High Pressure Safety Injection; HS, Heat Structure; IRSN, Institut de Radioprotection et de Sécurité Nucléaire; LOCA, Loss-of-Coolant Accident; LOOP, Loss of Off-Site Power; LPSI, Low Pressure Safety Injection; MELCOR, Methods of Estimation of Leakages and Consequences of Releases; MFW, Main FeedWater; MSIV, Main Steam Isolation Valve; MSL, Main Steam Line; NPP, Nuclear Power Plant; PC, Partitioning Coefficient; PORV, Power Operated Release Valve; PWR, Pressurized Water Reactor; R2CA, Radiological Consequences of design basis and design extension Accidents; RCP, Reactor Coolant Pump; RCS, Reactor Coolant System; RHR, Residual Heat Removal System; RN, Radionuclide; RPV, Reactor Pressure Vessel; SA, Severe Accident; SG, Steam Generator; SGTR, Steam Generator Tube Rupture; SLBOUT, Steam Line Break Outside Containment; TH, Thermal-hydraulics; USNRC, United States Nuclear Regulatory Commission; WP, Work Package.

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## 1. Introduction

The principal radiological concern during a Design Extension Conditions A (DEC-A) transient results from the presence of radioactive iodine in the RCS coolant, the main source of which is the “iodine spiking”. This process occurs in the presence of defects in the fuel rod cladding, which generate leakage paths where the primary coolant can enter the fuel rod and volatile Fission Products (FPs) notably iodine can move into the Reactor Coolant System (RCS). Indeed, during steady-state operation, there is a reasonably low iodine activity level in the primary coolant (Lewis and Iglesias, 1995). Primary circuit depressurizations and temperature transients during shutdown promote the coolant ingress into the defected rod gap region. The incoming water causes a rapid dissolution of the iodine present in the gap and heats up. Once it reaches saturation temperature, it turns into vapor and flows back into the RCS, fairly rapidly increasing its iodine activity level by a factor of 50 to 100 (Tobin, 1984). The iodine spiking plays a key role in the radiological consequences assessment, especially for PWR where the high pressure primary coolant flows through the thousands of Steam Generator (SG) tubes, which represent the larger fraction of the RCS boundary surface. As a result, in the case of SGTR, iodine enters the SG side from where it can reach the environment through five different transport mechanisms, called partitioning, flashing, atomisation, bypass and liquid overflow.

Nowadays, several mathematical models have been developed (Tobin, 1984) (Lewis et al., 1997) to predict the iodine-spiking in PWR, but they are not yet available in most SA and TH codes. The partitioning mechanism (Cantrel and March, 2006), was also thoroughly studied to evaluate the iodine mass transfers from the containment sump to the containment atmosphere, during the ex-vessel phase of a SA. Therefore, dedicated models (Cousin and Bosland, 2017) are already implemented in some integral code (e.g. ASTEC, AC<sup>2</sup>), but they cannot be used to reproduce the phenomenon within primary and secondary circuits. Regarding the flashing and atomisation processes, only some TH codes have devoted model that simulate them.

To compensate for this shortcoming of SA and TH tools, in the frame of the WP2 of the R2CA project (Girault, et al., 2022) simplified models reproducing the iodine spiking and the transport mechanisms of iodine in the RCS and SG (partitioning, flashing) have been implemented in the reference codes. The models were tested by simulating a SGTR + Steam Line Break Outside the containment (SLBOUT) sequence and, considering operator actions in line with standard Westinghouse EOPs.

In this work, a comparative analysis of the results of SGTR + SBLOUT transient performed by Tractebel and CIEMAT with MELCOR and Bel-V with CATHARE is presented. The aim of this study is the improvement of radiological consequences assessment as well as accident management measures (operator actions) for accidental transients in the DEC-A domain.

The paper is organized as follows. The comparative study motivations is found in section 2. The description of the codes and models adopted by Tractebel, CIEMAT and Bel V are discussed in Section 3. The accident sequence progression is described in Section 4. The results analysis and the conclusions are respectively provided in Sections 5 and 6.

## 2. Code-to-code comparative study

The assessment of potential radiological consequences during DEC-A scenarios is important from a safety point of view because these accidents have a higher frequency of occurrence than SAs. Despite this, it is not common to analyse this kind of transients using SA and TH codes. In this study, three different approaches to evaluate the iodine source term during a DEC-A sequence are presented using two different software. The objectives of the benchmark are to identify needed developments in the codes and verify the capabilities of existing models in predicting the source term of a postulated accident under determined DEC-A

conditions. The code-to-code comparison carried out considers both the TH and radiological aspects of the accident. The results are assessed according to criteria, including RCS TH response, operator actions, kinetics and mechanism of iodine release, total amount and physical state (aerosol, gas, liquid) of iodine reaching the environment.

## 3. Code modelling and main assumptions

### 3.1. Tractebel

Tractebel has used the integral code MELCOR 2.2 release 18,019 (Humphries et al., 2021a) to perform the DEC-A calculations. The mesh scheme adopted to model the PWR1000 Like reactor is illustrated in Fig. 1. The core region, from the lower core plate to the top of the active fuel is discretized into 40 cells by means of four radial rings and 10 axial levels. Further 16 cells are used to describe the lower plenum region. MELCOR represents the core and associated structures as a projection in two dimensions with the COR package. TH phenomena taking place in the RCS are described by CVH, FL and HS packages which use a different nodalization respect to the one of the COR package. Indeed, 28 control volumes (CVH), 20 of which are energy-coupled with the 40 COR cells in the active fuel region, 48 flow paths (FL) and 18 heat structures (HS) are used to model the TH in the vessel region. Regarding the RCS, as clearly illustrated in Fig. 1 for the pressurizer loop, the primary circuit is discretized in 46 control volumes, seven for each hot, cross over and cold leg, eight for each primary side in the SGs, 1 control volume for the pressurizer, while 10 control volumes are used to model the secondary circuit, three for the riser, one for the SG dome, downcomer, separators, mixing volume, distribution ring, feedwater line and main steam line.

The TH phenomena are described in the MELCOR code using a full two-fluid approach rather than drift flow, so that hydrodynamic materials can move without residence time in the flow path, guided by a separate momentum equation for each field. The momentum equation is only one-dimensional and there is no momentum associated with a control volume, therefore multidimensional effects associated with advection of momentum cannot be calculated (Humphries et al., 2021a). In MELCOR all hydrodynamic material together with its energy, resides only in control volumes. The SGTR is modelled by two flow paths connecting primary and secondary sides of the SG and placed at the cold leg side tube sheet and in the cold box.

To assess the potential impact of ‘iodine-spiking’ and ‘iodine partitioning’ processes on the source term, specific models were developed and implemented in the deck by Tractebel.

As previous mention, MELCOR does not include a model describing the iodine spiking process, so it was reproduced using twenty RN1\_VS flags, which simulate a time-dependent source of I<sub>2</sub> in each control volume of the core region activated at the time of SCRAM.

In contrast, MELCOR has an “iodine pool” model (RN package) which can simulate the iodine mass transfer from liquid to gas phase by partitioning. This model, however, is valid for volumes where the pressure is below 1.0E + 06 Pa and the liquid temperature lower than 423 K, corresponding to conditions that may be found in a PWR containment during a SA (Humphries et al., 2021b). Since the initial TH conditions in the affected SG may not be within the above temperature and pressure ranges, it was decided not to use it, but to develop a new model of iodine partitioning. The new model assumes that all iodine escaping from the damaged fuel rods as a result of SCRAM is molecular iodine (I<sub>2</sub>), and through a series of Control Functions (CFs), a mass flux of iodine ( $\Phi$ ) is injected above the SG liquid level. The magnitude of  $\Phi$  depends on the different concentration of I<sub>2</sub> in the liquid and gas phase within the SG. According to the “Two Film” model (Whiteman, 1923), the difference in concentration in the two phases is the driving force behind this process, which can be represented through a partition coefficient denoted as PC, and defined as follows (Chandrasekaran et al., 1985).

$$PC = \frac{I_2 \text{ activity concentration in liquid phase at the interface } \left[ \frac{Bq}{m^3} \right]}{I_2 \text{ activity concentration in gas phase at the interface } \left[ \frac{Bq}{m^3} \right]} \quad (1)$$

The “Two Films” model does not consider any phase change at the gas–liquid interface and assumes that volatile species reach equilibrium at the interface. Therefore, the iodine mass transfer flow can be described (Herranz et al., 2009) by the equation (2).

$$\Phi = A_{int} \cdot K_L \cdot (C_L - C_g \cdot PC) \quad (2)$$

Where  $\Phi$  is the mass transfer flow rate (kg(I<sub>2</sub>)/s),  $A_{int}$  the interfacial area (m<sup>2</sup>),  $C_g/C_L$  are the concentration of I<sub>2</sub> in gas/liquid phase (kg(I<sub>2</sub>)/m<sup>3</sup>),  $K_L$  is the overall mass transfer coefficient calculated using the following formula:

$$\frac{1}{K_L} = \frac{1}{k_L} + \frac{PC}{k_g} \quad (3)$$

Where  $k_L, k_g$  are individual mass transfer coefficients in the liquid/gas side (m/s) equal to 1.10<sup>-3</sup> m/s and 2.10<sup>-3</sup> m/s respectively (Cousin and Bosland, 2017), and  $PC$  is the partition coefficient which is set conservatively to 100 in the first case analyzed in agreement with the lower limit value of the experimental data presented in (Postma and Tam, 1978) and with the guidelines in the NRC Standard Review Plan (NUREG-0800, 1981).

Since the main motivation for this analysis is to accurately determine the potential amount of iodine/activity released into the environment, Tractebel has decided to conduct a sensitivity study by adopting two other different values of  $PC$ .

This is because the actual value of  $PC$  is uncertain, since it depends on water temperature, water pH, iodine concentration and TH conditions. Consequently, assuming a constant value of 100 without taking into account conditions within the SG does not seem to be realistic, even based on more recent studies (Cantrel and March, 2006).

Therefore, the second sensitivity case considers the effect of liquid

phase temperature in the SG (equation (4) on the value of  $PC$  (Cousin and Bosland, 2017).

$$PC = H = 231.385 \cdot \exp(1.65017 \cdot 10^{-4} \cdot (T - 571.24) \cdot (T - 273.15)) \quad (4)$$

In addition, as demonstrated in SISYPHE experiments (Cantrel and March, 2006), in the case of evaporative conditions (expected in the first phase of the transient within the damaged SG), the previous  $PC$  is no longer valid and the iodine mass transfer model must also consider diffusion/convection processes. Therefore, the third sensitivity case considers evaporation conditions, and the  $PC$  used is that inferred from the SISYPHE test measurements and shown in Equation (5).

$$PC = \frac{C_L}{C_g} = \frac{H \cdot \left( 1 - \frac{\beta \cdot Q_e}{A_{int} \cdot Q_L \cdot k_L} \right)}{\left( 1 + \frac{\alpha \cdot Q_e}{A_{int} \cdot Q_L \cdot k_g} \right)} \quad (5)$$

Where  $Q_e$  is the evaporation mass flow rate of steam (negative in case of condensation) (kg.s<sup>-1</sup>),

$\rho_{st}, \rho_L$  are densities of steam and liquid phase (kg.m<sup>-3</sup>), and  $\alpha/\beta$  are two dimensionless coefficient, set equal to 0.19 and 6.6 in (Cantrel and March, 2006). The mass flux for the third case is defined in equation (6):

$$\Phi = \frac{A_{int} \cdot k_L \cdot k_g}{\left( H \cdot k_L + k_g + \frac{\alpha \cdot Q_e}{A_{int} \cdot Q_L} - \frac{\beta \cdot Q_e \cdot H}{A_{int} \cdot Q_L} \right)} \left( H \cdot C_g - C_L - \frac{\alpha \cdot Q_e \cdot C_L}{A_{int} \cdot Q_L \cdot k_g} - \frac{\beta \cdot Q_e \cdot H \cdot C_g}{A_{int} \cdot Q_L \cdot k_L} \right) \quad (6)$$

Since, the evaporation rate at the liquid–gas interface is not calculated by MELCOR, this case required an additional implementation of a set of CFs to determine the average evaporation rate  $Q_e$  within the damaged SG. Partitioning models work whenever the concentration of I<sub>2</sub> in the SG liquid phase exceeds that of the SG gas phase multiplied by the value of  $PC$  and stops otherwise. Their main limitations are listed here after:

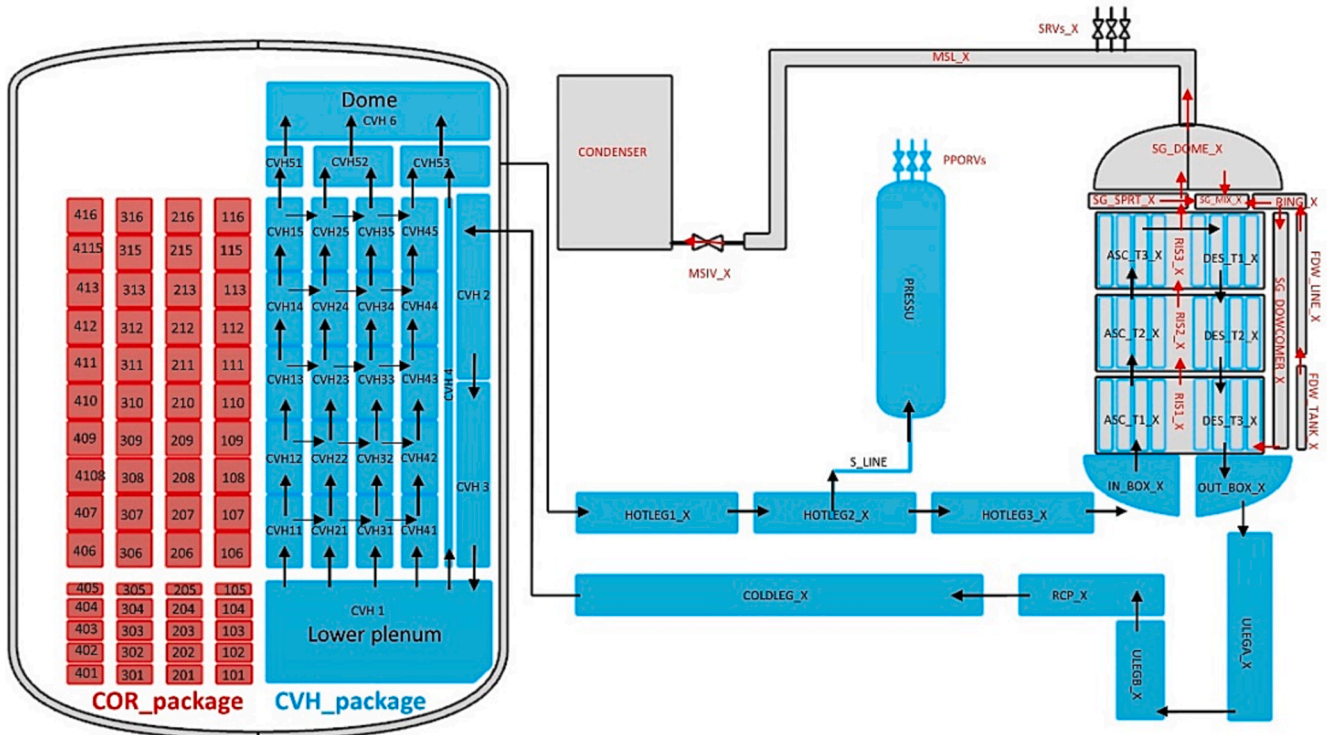


Fig. 1. RCS and vessel nodalization adopted by Tractebel (Pressurizer loop).

- They assume that 100 % of iodine escaping from the defect fuel rod is molecular iodine ( $I_2$ ), when the most probable chemical form released from the spiking is CsI which is less volatile than  $I_2$  and soluble in the water (Beahm et al., 1992);
- They do not consider the reduction of iodine inventory in the primary coolant as a result of the partitioning process of  $I_2$  from the liquid to the gas phase;
- They are applied to aqueous solution with very low iodine concentrations, for which PC is quite low (Lin, 1981);
- The initial temperature within the SG could be higher than those used to validate the  $I_2$  partitioning model (Whiteman, 1923) (Cantrel and March, 2006);
- the SGTR transient may proceed on a faster time scale than that required for partitioning equilibrium to be reached.

Based on these statements, the models implemented may lead to an overestimation of the amount of iodine released into the environment. The sensitivity cases performed by Tractebel based on the PC value adopted are illustrated in Table 1.

### 3.2. CIEMAT

CIEMAT has used the last release of the integral code MELCOR 2.2, the 18019. MELCOR is a fully integrated, engineering-level computer code that models the progression of SAs in nuclear power plants (NPPs) (Humphries et al., 2021a). In particular, a broad spectrum of accident phenomena in both boiling and pressurized water reactors is treated in MELCOR in a unified framework. These include TH response in the RCS, reactor cavity, containment, and confinement buildings; core heat up, degradation, and relocation; core-concrete attack; hydrogen production, transport, and combustion; FP release and transport behaviour (Humphries et al., 2021a). The Radionuclide (RN) package calculates the release and transport behaviour of FP vapours, aerosols and other trace species, including release from fuel and debris, aerosol dynamics with vapour condensation and re-vaporization, deposition on structure surfaces, transport through flow paths, and removal by engineered safety features. The RN package operates on the basis of material classes, which are groups of elements with similar chemical properties. The radionuclide initial inventory is based on the ORIGEN code results (Humphries et al., 2021b). The reference NPP (3 loops PWR 1000 MWe) is modelled with a total of 32 control volumes, 46 flow paths and 66 heat structures. The RCS (28 control volumes) is modelled in two loops (Fig. 2), one of which combines the two intact coolant loops, and the other corresponds to the one of the Pressurizer and the failed SG. The Reactor Pressure Vessel (RPV) is modelled into 5 interconnected control volumes: annulus, lower plenum, channel, bypass and upper-plenum. In plant model, compartment connections are modelled as flow paths, some of which are controlled through valves. The core region is divided in 4 radial rings and 15 axial nodes. The first three rings represent the fuel and the fourth ring represents the core bypass region. In the modelling, two control volumes (channel and bypass) and 12 HSs are used.

The safety systems Auxiliary Feed Water (AFW), High Pressure Safety Injection (HPSI) and Low Pressure Safety Injection (LPSI) are

**Table 1**  
Tractebel sensitivity cases.

Case	$I_2$ Partition coefficient
Tractebel_PC100	PC = Constant equal to 100
Tractebel_No_Evap	PC = $H = 231.385 \cdot \exp(1.65017 \cdot 10^{-4} \cdot (T - 571.24) \cdot (T - 273.15))$
Tractebel_Evap	$PC = \frac{H \cdot \left(1 - \frac{\beta \cdot Q_e}{A_{int} \cdot q_L \cdot k_L}\right)}{\left(1 + \frac{\alpha \cdot Q_e}{A_{int} \cdot q_{st} \cdot k_g}\right)}$

modelled through MELCOR control functions. The double ended rupture of the steam line is modelled using three flow path regulated as control valves (through the use of CF), one modelling steady state operation and the other two describing the water discharge to the environment once the SLBOUT occurs. The rupture of three SG tubes is modelled by a flow path that connects primary and secondary sides of the SG and is placed at the cold leg side tube sheet.

In the analysis of the FP behaviour the following key assumptions were made (Humphries, 2021b), (NUREG-800, 1981):

- Reactor operation with initial coolant activity concentration of  $3.7 \cdot 10^7$  Bq/kg DE  $^{131}I$ .
- Initial noble gases activity concentration of  $3.7 \cdot 10^7$  Bq/kg DE  $^{131}I$ .
- A spiking phenomenon is assumed to occur right at the reactor trip and only for the molecular iodine.
- The spiking model assumes that the iodine release rate from the fuel to the primary coolant increases to a value 500 times greater than the release rate corresponding to the iodine concentration at the equilibrium value stated in the NPP Technical Specifications. Note that this assumption does not lead to a “spike”; instead, it assumes a continuous and monotonous iodine accumulation until the event is terminated. In other words, this might be seen as a bounding case of iodine spike (Reisi Fard, 2011).
- No radioactivity is considered in the affected SG at the beginning of the accident.
- Three distinct mechanisms for transport of the iodine to the environment, i.e flashing, atomization and partitioning were modelled with the application of the flashing and fog formation model in the case of pool entering a volume through a flow path (Humphries, 2021b) using MELCOR control functions. The radioactivity release through the partitioning effect is considered using the constant PC = 100 between the pool and steam volumes in the affected SG. The radioactivity release due atomisation and flashing is assumed to be released into the steam volume of the affected SG.

### 3.3. Bel-V

CATHARE-2/V2.5\_2/mod8.1 developed by CEA, EDF, AREVA, and IRSN (Daron, 2019) is a TH system code that solves the conservation laws for water and steam for a wide variety of single and two-phase flow conditions. The adopted CATHARE 2 model of the 3-loop PWR is based on a fully 1-D nodalization. It includes the primary and secondary sides, three primary cooling loops and their associated safety injection systems, and a detailed representation of the RPV components and structures (Fig. 3).

Particular attention is given to the SG nodalization where three U-tubes lengths (short, medium and long) with detailed ascending and descending nodes are considered (Fig. 3). In total, the nodalization contains around thousands of hydraulic nodes and hundreds heat transfer structures. The control systems like the pressuriser heaters, level control, safety and relief valves are also modelled.

The CATHARE code has the capabilities to simulate radioactivity transport from the primary to the secondary side and its release to the environment. This last feature will not be used in the current work. A manual assessment of the radioactivity release is considered based upon specific formula and the calculated key TH parameters.

The radioactivity release into the RCS due to iodine spiking is considered to take place after the SCRAM. Dilution through clean water injected by the HPSI, accumulators, Control Volume Chemical System (CVCS) pump and other minor systems is taken into account. All radioactivity in the SG is coming exclusively through the SG tube break and is released only through the SLBOUT (otherwise accumulated in the SG).

For the calculation of the FP and radioactivity release into the environment, simple calculations using Excel and VBA have been implemented. The main assumptions used are listed hereafter:



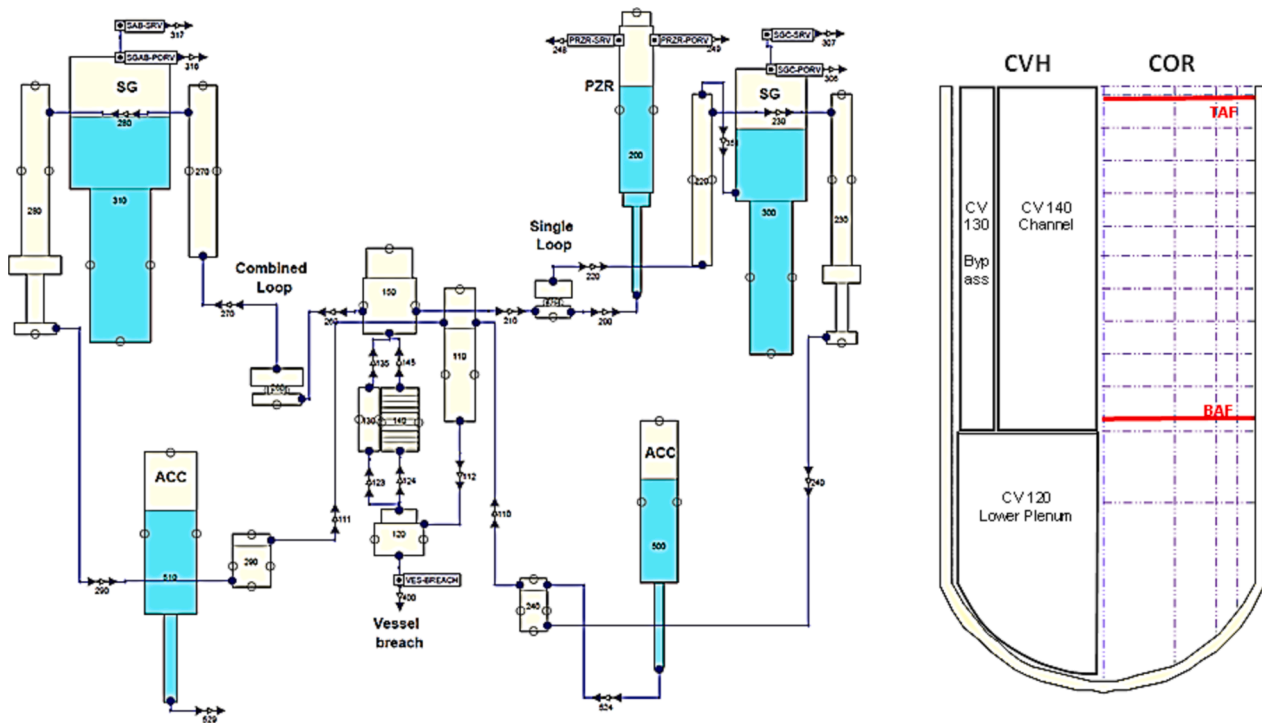


Fig. 2. RCS and vessel nodalization adopted by CIEMAT.

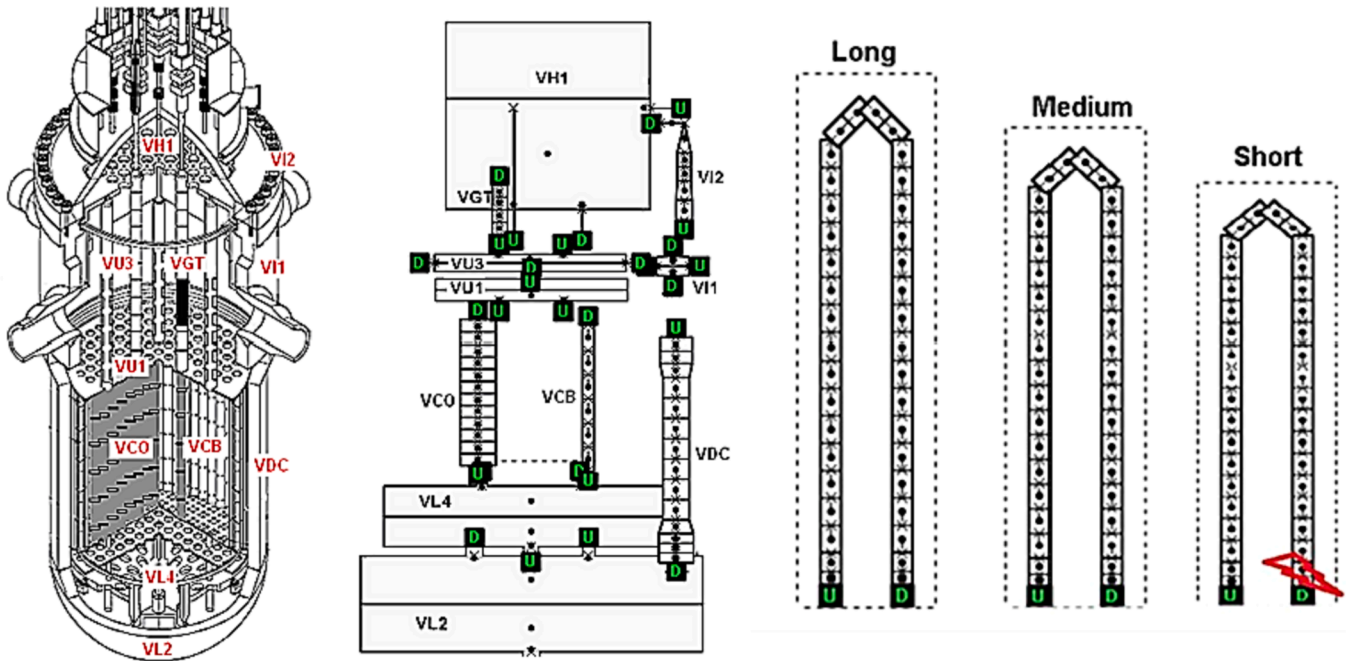


Fig. 3. CATHARE vessel modeling and SG U-tube representation.

- The radioactivity release due to spiking is considered to be instantly diluted in the RCS
- The flow through the SG tube break is considered isenthalpic, and the radioactivity is released with vapor directly into environment through the main steam line break
  - The radioactivity release by flashing is assumed to be 100 % released into environment independently of the flow rate through main steam line break, but only during the time of the break simulation
  - The radioactivity release by atomisation is assumed to be 100 % released into environment, independently of the flow rate through main steam line break, but only during the time of the break simulation
  - The radioactivity released into environment by partitioning is calculated using the flow rate obtained by subtracting the vapor released by flashing and atomisation from the vapor flow rate through the main steam line break
- The radioactivity release with the liquid phase once the SG is overfilled is taken into account.

- Distribution of the radioactivity in the SG is recalculated at each time step, using the constant partitioning coefficient (PC = 100) and the SG liquid and vapor masses (i.e. dilution of the secondary coolant in SG is taken into account automatically by using real-time SG masses).

The calculations are based on the activity and mass transfer modelling with a time step of 0.001 s thus making the results sensitive to the instant dilution assumption.

#### 4. Accident scenario description

The selected scenario is a SGTR double-ended break on 3 U-tubes which taking place simultaneously with SLBOUT, when the reactor is at Hot Full Power (HFP). The SGTR is situated within the SG on the pressurizer loop at the bottom of the shortest U-tube bundle on the cold leg side while the SLBOUT is positioned before the Main Steam Isolation Valve (MSIV) and therefore cannot be isolated.

The scenario also assumes that together with the opening of the SGTR and SLBOUT, a Loss of Off-Site Power (LOOP) occurs. Despite the LOOP, all Emergency Core Cooling Systems (ECCS) as well as AFWS remain available and no core uncover is expected. The general sequence of operator actions reproduced in this transient are determined from the Westinghouse EOPs (Dekens et al., 1985).

The SGTR + SLBOUT accident progression is explained as following. The combined effect of the three events leads to reactor shutdown and primary pump shutdown. Subsequent to the SCRAM and LOOP, operators trigger the three trains of High Pressure Safety Injection (HPSI) systems which begin to inject cold water in the primary circuit. Almost at the same time, the operator in agreement with EOPs, starts regulating the AFW flow towards the SGs. No action is performed on the damaged SG until 1200 s, when the SG is identified and the operator isolates it by stopping the dedicated AFWS. About 1000 s after the AFWS isolation, operators begin cooling down the primary circuit with a maximum gradient of 56 °C/h by controlling the opening and closing of the SG Pilot Operated Relief Valves (PORVs) in intact SGs. The aim of this operation is to cool down and establish a subcooling margin in the primary circuit. During this phase, the operator monitors the liquid level in the pressuriser, keeping it at around 30 % through the controlled opening/closing of a Pressurizer PORV. Next, operators turn off one by one the HPSI trains to reduce the primary-to-secondary coolant refrigerant losses and approach the conditions necessary to connect the primary system to the residual heat removal system (RHRS) (i.e.  $P = 28 \text{ bar}_a$   $T = 450 \text{ K} = 177 \text{ °C}$ ). The transient terminates when the connection of the primary circuit to the RHRS.

It is important to note that in this accidental sequence, the position of the SGTR aims to maximize the overfilling phenomenon in the affected SG, while the occurrence of the SLBOUT before the MSIV has the purpose to maximize the amount of coolant that can flow into the environment even after containment isolation.

Therefore, three transport mechanisms are expected that make the largest contribution to the source term.

The first one is the partitioning mechanism. Indeed, following the opening of the SGTR, most of the refrigerant escaping from primary circuit mixes with the water in the SG secondary side. As the water continues to boil, because of heat input from the primary circuit, the iodine partitions between liquid and gas phase and is transported, with the steam, out of the SG and ultimately to the environment.

The second one is the flashing mechanism. Since, the SGTR break flow passes from the high primary temperature and pressure to the lower secondary temperature and pressure, a fraction of the water flashes to steam. The iodine associated with the flashing fraction, does not mix with liquid phase in the SG, and is directly transported by the gas phase through the SLBOUT to the environment. Finally, once the SG shell side is overfilled the contaminated liquid coolant can flow out into the environment through the SLBOUT.

The key events of the SGTR + SLBOUT and their timing calculated by

the WP2 participants are illustrated in Table 2.

### 5. Result comparison

#### 5.1. Thermal-hydraulic results comparison

Simultaneously with the onset of the accident ( $t = 0 \text{ s}$ ), LOOP occurs and the primary pumps shut down along with reactor SCRAM. After MFW isolation, AFW is activated for all SGs (Table 2) and the water level inside them is monitored. Then, as illustrated in Fig. 4, the initiation of SGTR + SLBOUT results in abrupt depressurization in the affected SG, named SG1, and a more gradual depressurization in the intact SGs (SG2 and SG3). The loss of primary fluid through the SGTR and subsequently through the SLBOUT causes also an initial depressurization of the primary circuit as seen in Fig. 5. All three cases analyzed predict a similar evolution of the above parameters. The rapid initial pressure drop in the primary circuit lasts less than 300 s, after which it rapidly stabilizes around 100 bar<sub>a</sub> up to 2500 s. The pressure settling is due to the intervention of the three HPSI trains that are able to compensate the loss of coolant through the SGTR. The HPSI mass flow rates are illustrated in Fig. 6 and as can be seen their behaviour is in agreement with the evolution of the pressure in the primary circuit.

The operation of the three trains of the HPSI system maintains a significant pressure difference within the damaged SG (~100 bar), which is the driving force behind the displacement of the primary coolant in the secondary circuit through the SGTR (Fig. 7). Tractebel, Bel V and CIEMAT predict similar release kinetics and cumulative masses of coolant reaching the shell side of the SG.

The larger mass flow rate through the SGTR (Fig. 8) computed by Tractebel and CIEMAT is due to the modelling adopted to describe the SG and SGTR. Indeed, the Tractebel and CIEMAT SG model describes the SG tube bundle radially by a single volume in contrast to Bel V model that discriminates three different tube lines (short, medium, long). The use of a single volume imposes to reproduce the double ended SGTR with two breaks one in the bottom volume of the tube bundle and one in the cold box as carried out by Tractebel or more simply through a single break in the SG tube bundle volume as performed by CIEMAT, instead of two breaks in the short tube line. Therefore, the SGTR in MELCOR calculations affects all the TH within the SG tube bundle, rather than just one SG tube line, and leads to higher SGTR mass flow rates. However,

**Table 2**  
SGTR + SLBOUT key events and calculated by timings.

N°	Tractebel Time [s]	CIEMAT Time [s]	BELV Time [s]	Key event
1	$t < 0$	$t < 0$	$t < 0$	Steady-state hot full power
2	$t = 0$	$t = 0$	$t = 0$	SGTR + SLBOUT
3	$t = 0.73$	$t = 0.24$	$t = 1.0$	LOOP + SCRAM, CVCS, heaters and Reactor Coolant Pump (RCP) unavailable
4	$t = 0.73$	$t = 2.18$	$t = 2.0$	MFW isolation opening EOP procedure
5	$t = 2.0$	$t = 2.18$	$t = 2.0$	MSIV closure
6	$t = 20.9$	$t = 20.18$	$t = 20.9$	HPSI injection
7	$t = 110.7$	$t = 110$	$t = 110.0$	AFW to all SGs
8	$t = 1210$	$t = 1210$	$t = 1210$	SG-1 AFW turned off
9	$t = 2290$	$t = 2290$	$t = 2290$	Operator starts the cooldown via the intact SGs (56 K/h)
10	$t = 2400$	$t = 2400$	$t = 2400$	Operator starts primary depressurization
11	$t = 2488$	$t = 2420$	$t = 2535$	LPSI 1/3 activation HPSI 1 turned off
12	$t = 2548$	/	/	Accumulators isolation
13	$t = 3008$	$t = 3000$	$t = 3055$	HPSI -2 turned off
14	/	$t = 3190$	$t = 3200$	Accumulator start injecting ( $P_{\text{prim}} < 45 \text{ bar}_a$ )
15	$t = 3408$	$t = 3440$	$t = 3500$	HPSI -3 turned off
16	$t = 3688$	$t \sim 3800$	$t \sim 3800$	Met RHR connection conditions
17	$t = 4288$	$t = 5000$	$t = 5000$	End of calculation

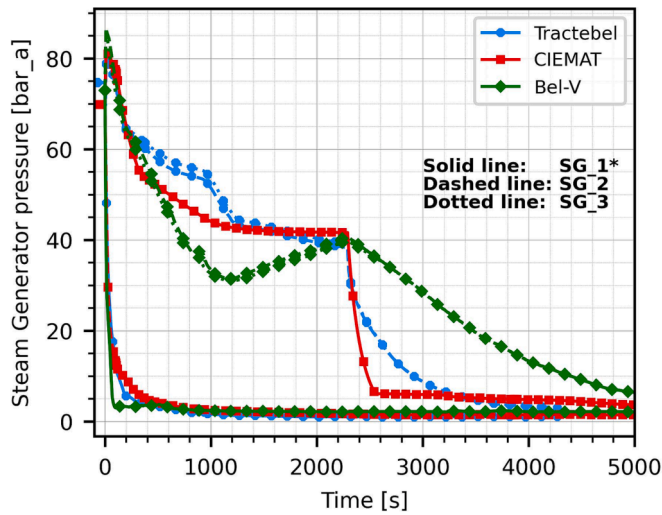


Fig. 4. SGs pressures.

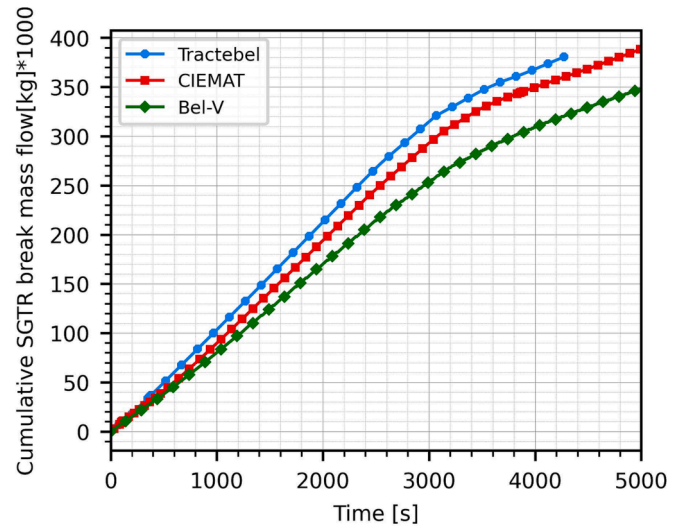


Fig. 7. Cumulative flow rate SGTR.

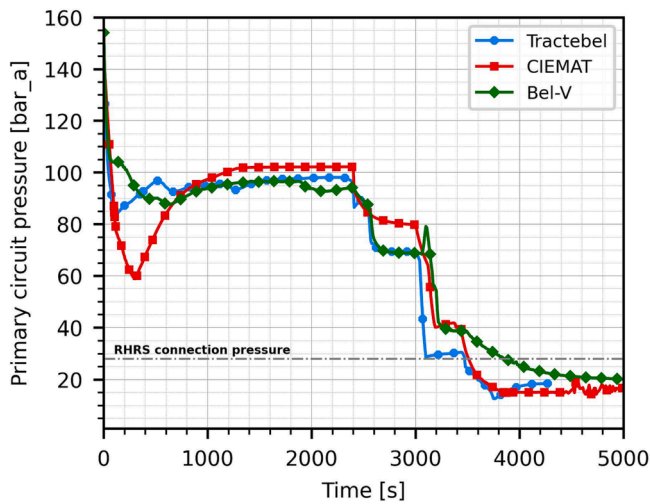


Fig. 5. Primary circuit pressures.

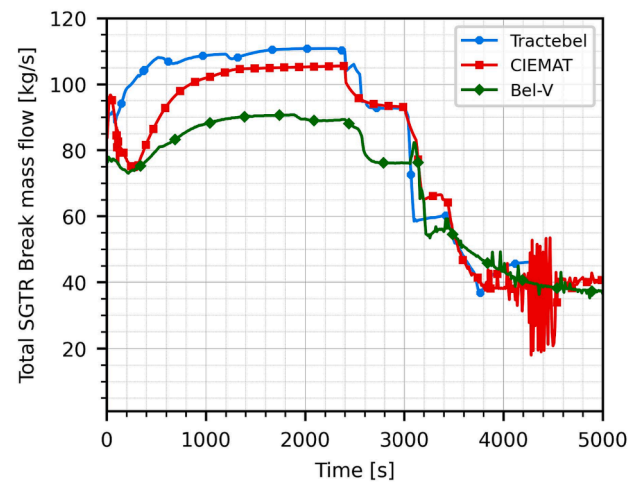


Fig. 8. Mass flow rate SGTR.

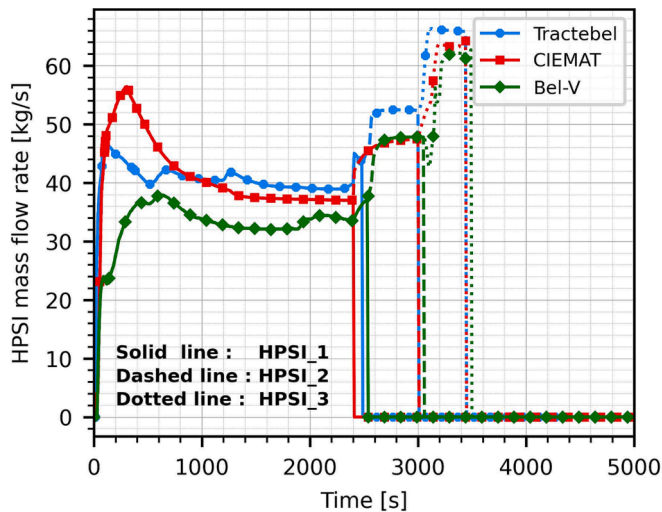


Fig. 6. HPSI mass flow rate.

this simplified representation of the SGTR scenario reduces CPU time by 90 percent and provides a result similar to that of more detailed modeling.

Around 1200 s, the SGTR is identified, and the affected SG is isolated by stopping the dedicated AFW system, but no particular impact in the TH parameters is observed. The pressurizer PORVs and SG PORVs are assumed to be operating even in the presence of the LOOP, since they are powered by diesel generators. Therefore, after 2200 s, operators according to the EOPs open two SG PORVs in the intact SGs (Fig. 9), trying to increase the amount of heat removed from the primary circuit and reduce its pressure. The cumulative releases of the PORVs in the intact SGs predicted by CIEMAT and Bel V are quite similar, i.e. around 10 tons, in disagreement with Tractebel which calculates about 50 tons (Fig. 9). In the case of CIEMAT, this result can be explained by the fact that a small amount of steam discharged through the SG PORV causes an abruptly depressurization in the SG (Fig. 4). This indicates that the size adopted by CIEMAT to model SG upper volume normally called SG dome is rather smaller in comparison to that used by other participants. Indeed, as supported by Fig. 11, when the damaged SG is filled of water (due to SGTR) the maximum mass of water contained within is around 100 t in the CIEMAT case against 140 t and 160 t for Bel V and Tractebel respectively. In the case of Tractebel, the larger size of the SG dome with



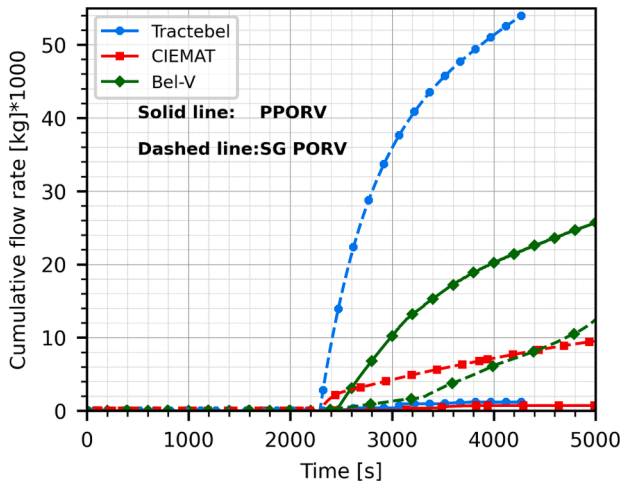


Fig. 9. Intact SGs PORVs and PPORVs steam mass flow.

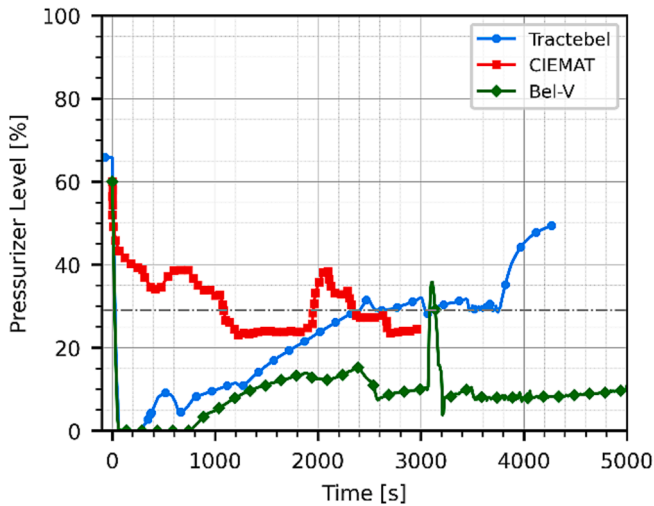


Fig. 10. Pressurizer level.

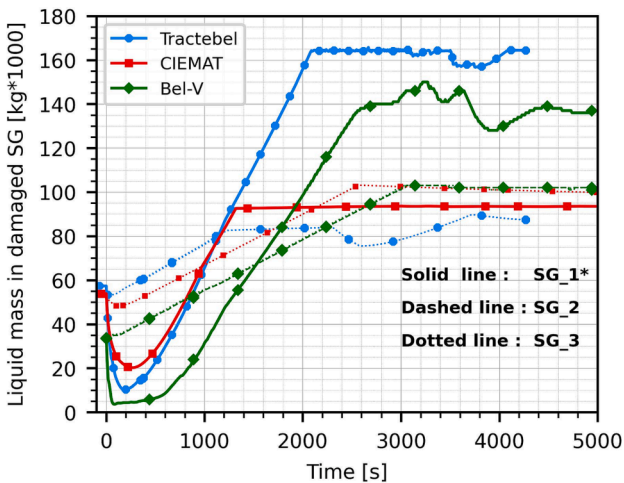


Fig. 11. Liquid mass in the SGs.

respect to CIEMAT justifies the discrepancy observed in the results (50 tons vs 10 tons). This is because the Tractebel SG has a higher inertia and more steam must be released to depressurize it. On the contrary, the

difference between Tractebel and Bel V results is related to the fact that, Tractebel assumes an instantaneous total opening of the SG PORV, while Bel V considers that the SG PORV opens and closes cyclically to meet the maximum cooling limits of the primary circuit coolant of  $56^{\circ}\text{C/h}$ , thus significantly reducing the total amount of vapour discharged through the valve. According to the EOPs, the opening of the pressurizer PORV only serves to keep the level inside the pressurizer around 30 %. Interestingly, to control the water level in the pressurizer, the Bel V case discharges 27000 kg of steam into the containment versus 1200 kg of the Tractebel and 723 kg of the CIEMAT cases (Fig. 9). In fact, as showed in Fig. 10, unlike the Tractebel and CIEMAT cases, in Bel V the water level in the pressurizer never reaches the requested 30 %. Therefore, Bel V keeps the PPORV open from 2400 s up to the end of the transient. It is not clear the reason why the level of water in the pressurizer does not increase in the Bel V case despite the injection of HPSI into the primary circuit as well as the high pressurizer water level throughout the transient calculated by CIEMAT.

The continuous operation of the three HPSI trains eventually causes high water level in the damaged SG, as seen in Fig. 11, where the overfilling of the affected SG occurs around 2000–2300 s in Tractebel and Bel V cases respectively and around 1300 s for CIEMAT.

As long as the affected SG was not filled with water, only vapor could pass through the SLBOUT (Fig. 12). Once the SG is filled, the primary coolant in liquid form, together with the fission and corrosion products dissolved in it, can reach the SLBOUT and be released directly into the environment. In order to significantly reduce the primary-to-secondary leakages as well as the SG water level, operators start to sequentially turn off the three HPSI trains from 2400 s (Fig. 6). The three primary pressure step changes seen in Fig. 5 are precisely due to the stopping of the three HPSI trains. The last two phases are less pronounced in the Bel V curve because the accumulators are assumed to be activated just then instead of being isolated as recommended by the EOPs.

Calculations are considered terminated, when the primary circuit conditions meet RHRS requirements i.e., coolant temperature below  $177^{\circ}\text{C}$  and pressure less than 28 bar<sub>a</sub>, which occurs between 3500 and 4000 s in all cases analyzed. A brief overview of the calculated TH response shows that despite the implementation of EOPs (with some delay), the amount of contaminated primary refrigerant reaching the environment is on the order of hundreds of tons (close to the initial primary coolant inventory). Therefore, even if the reactor coolant activity is rather low, the liquid-phase FP release must be quantified in a SGTR + SLBOUT scenario.

## 5.2. Source term results comparison

The quantity of iodine escaping from the primary circuit depends on

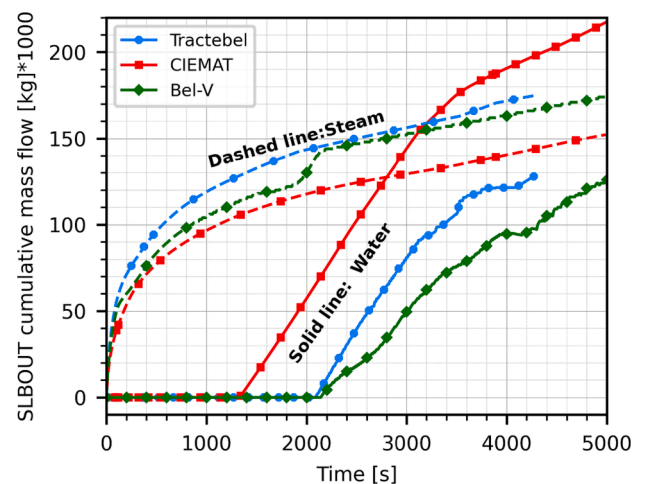


Fig. 12. Cumulative liquid mass flow rate SLBOUT.



two main factors. The first is the TH response of the RCS, as the refrigerant moves from the SG tube side to the SG shell side due to the pressure difference between the primary and secondary circuits. The second is the iodine concentration in the RCS following the SCRAM caused by the prolonged release of the iodine spiking. Tractebel and Bel V have determined the iodine spiking based on utility experience, and in agreement with the pre-spiking (initial primary circuit contamination), so that the spiking and the pre-spiking are proportional and are a consequence of the same number of fuel defects. In contrast, CIEMAT has assumed a bounding and constant value of the iodine spiking release. CIEMAT's choice is in line with (NUREG-0800, 1981), which recommends modeling the spiking so that the iodine concentration in the RCS increases 500 times over its equilibrium concentration. However, these two distinct approaches lead to large discrepancies of around one order of magnitude between the iodine activities entering the RCS, as shown in Fig. 13. In Fig. 11 it is possible to see that at the beginning of the transient the mass of coolant inside the shell side of the SG decreases abruptly and the SGTR is supposed to be above or only slightly below the water level. In these conditions, iodine can be transported by steam to the environment through the SLBOUT. Therefore, in the very early phase of the accident the main mechanism governing the iodine release is expected to be the flashing. After that, and during the filling phase of the affected SG the dominant release mechanisms becomes the partitioning. Finally, when the SG is overfilled the coolant in liquid phase will transport the iodine dissolved in it through the SLBOUT (Fig. 12).

Regarding the flashing release, since the coolant in the SG at the beginning of the transient is only slightly contaminated, no significant release of radioactivity is expected, and its contribution should be less relevant than the other two. Furthermore, the MELCOR code assumes that FPs can be transported in gas/steam or liquid phase and does not directly model the flashing release mechanism. Consequently, only Bel V with CATHARE has taken into account this phenomenon, and its contribution is around 20 % of the partitioning (not illustrated).

In contrast, the effect of the PC value on iodine transport and release is directly investigated in the three Tractebel cases. CIEMAT and BelV calculations instead adopted a constant value of PC equal to 100 (as in Tractebel\_PC100).

Fig. 14 shows the integrated iodine released to the atmosphere, before the overfilling of the damaged SG. As expected, taking into account the boiling conditions in the SG, the iodine mass reaching the environment due to the partitioning significantly increases. Indeed, as confirmed in Fig. 15, by considering diffusion and convection processes in the determination of the PC (Tractebel\_Evap), its value decreases, resulting in an increase of iodine concentration in the gas phase of the

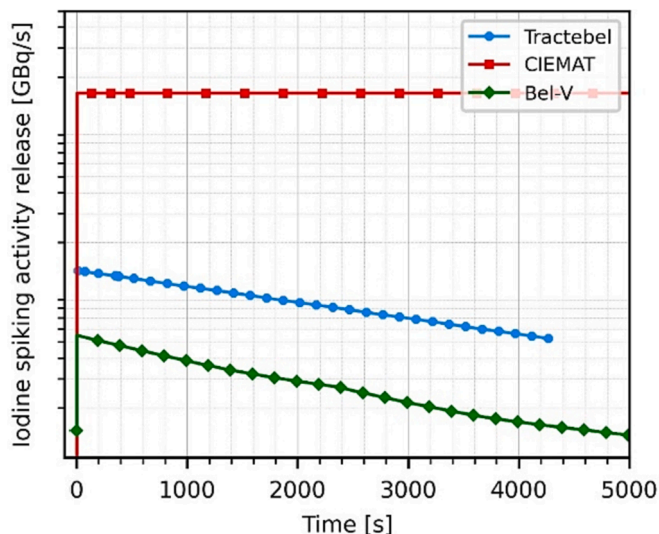


Fig. 13. Iodine activity due to spiking.

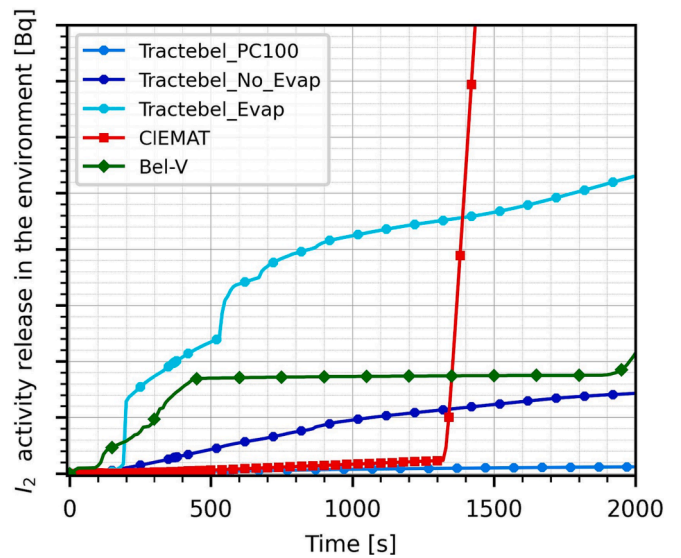


Fig. 14. Iodine activity released into the environment (short term).

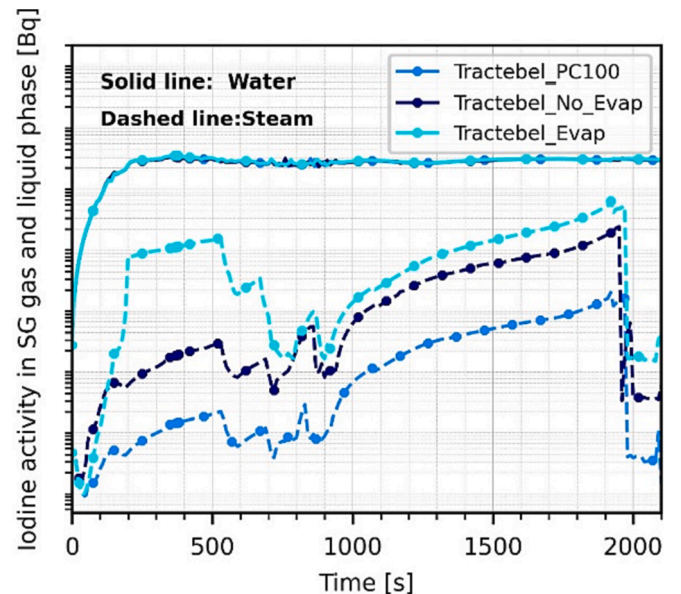


Fig. 15. SG Iodine activity repartition liquid/gas.

affected SG. This is particularly pronounced in the first phase of the transient, when there is intense evaporation of water within the SG. On the other hand, when only the effect of liquid temperature is taken into account to determine the PC (Tractebel\_No\_Evap) value, this is on average lower throughout the transient with respect to the case with PC = 100.

Once the SG is filled with water, iodine starts flow out through the SLBOUT dissolved in the liquid, as illustrated in Fig. 16. CIEMAT, due to the conservative assumptions adopted, predicts a cumulative iodine release an order of magnitude higher than that calculated by Tractebel and BelV.

Because of the transient characteristics, the cumulative activity released in the early phase of the accident (0–2000 s) due to partitioning is overridden by the activity released with the liquid in the late phase of the accident (2000–5000 s). However, in the event of an isolable steam line break, the contribution of the partitioning would become the dominant one.

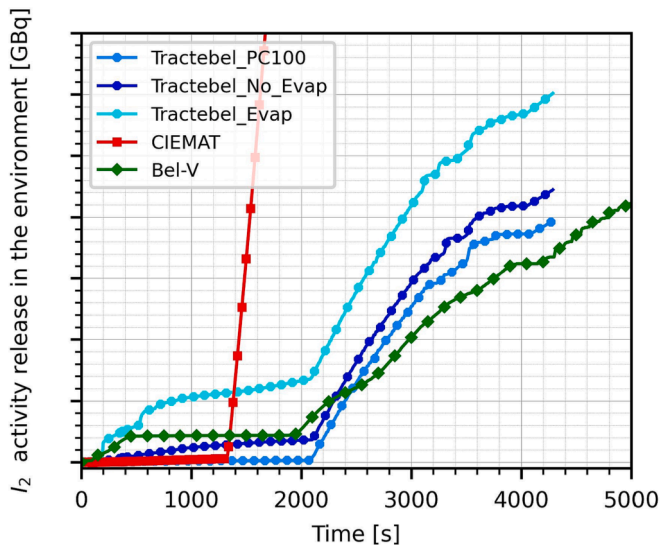


Fig. 16. Iodine activity releases into the environment (long term).

## 6. Summary and conclusion

In this article, two MELCOR and one CATHARE calculations reproducing a SGTR + SLBOUT transient to evaluate the iodine source term were performed. The main interest was to identify and model the main transport mechanisms responsible for iodine release under DEC-A conditions and to assess their impact on the source term.

The TH results showed some discrepancies in the results, mainly due to different modelling of SGs and implementation of procedures. Despite this, they provide similar indications in the progression of the accident.

The SGTR + SLBOUT with LOOP is characterised by the fact that, in the initial phase, iodine is released into the environment mainly through partition and flashing mechanisms in the steam phase. Once the damaged SG is filled with water, the iodine dissolved in the coolant reaches the environment in the liquid phase through the SLBOUT. The latter mechanism contributes between 80 and 99 % to the iodine source term.

The results have demonstrated that the methodologies adopted by the participants to assess the iodine source term have a significant impact on the kinetics and cumulative release of iodine into the environment. In particular, CIEMAT, using the conservative assumption suggested in (NUREG-800, 1981) to evaluate the iodine spiking, calculates a source term (one order of magnitude) greater than Tractebel and Bel V, that with the use of a fairly similar initial spiking iodine contribution provide quite close results.

Regarding the partitioning mechanism, it was noted that, by evaluating the PC as a function of temperature and evaporation conditions within the SG, iodine activity in the gaseous phase increases significantly, resulting in the emission of radioactivity into the environment significantly greater than the case with a PC intake equal to 100 in the first phase of the accident (releases in gas phase). Overall, the contribution of partitioning to the source term is increased by up to 20 % (Tractebel\_Evap).

Tractebel and Bel V provide similar total cumulative iodine release into the environment. This is explained by the fact that the cases analysed differed from each other mainly in the modelling of partitioning and flashing transport mechanisms, which, as stated above, provide secondary contribution to the radioactivity release.

Finally, from an operational point of view, to reduce iodine release, HPSI trains must be deactivated sequentially as soon as possible, verifying after deactivation each train that the pressurizer level remains above 30 %. The purpose of sequentially deactivating the HPSI trains is to depressurize the primary circuit as quickly as possible to reduce the

SGTR mass flowrate and therefore the FP releases. This also allows to reach the 28 bar threshold to be able to do the connection to the Residual Heat Removal System.

## CRedit authorship contribution statement

**P. Foucaud:** Supervision, Conceptualization, Methodology, Software, Data curation, Writing – original draft, Visualization, Validation. **M. Di Giuli:** Conceptualization, Writing – original draft, Software, Data curation, Visualization. **M. Salmaoui:** Supervision. **A. Bousbia Salah:** Writing – original draft. **R. Iglesias:** Writing – original draft. **A. Malkhasyan:** Writing – review & editing. **L.E. Herranz:** Writing – review & editing.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Data availability

The data that has been used is confidential.

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Views and opinions expressed in this paper reflect only the author's view and the European Commission is not responsible for any use that may be made of the information it contains.

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## References

- Beahm, E. C., Weber, C. F., Kress, T. S. and Parker, G. W., 1992. Iodine chemical forms in LWR severe accidents. Final report (No. NUREG/CR-5732; ORNL/TM-11861). Nuclear Regulatory Commission, Washington, DC (United States).
- Cantrel, L., March, P., 2006. Mass transfer modeling with and without evaporation for iodine chemistry in the case of a severe accident. *Nucl. Technol.* 154, 170–185.
- Chandrasekaran, T., Lee, J. Y. and Willis, C. A. (1985). Calculation of releases of radioactive materials in gaseous and liquid effluents from pressurized water reactors. (No. NUREG-0017-Rev. 1). US NRC.
- Cousin, F. and Bosland, L., 2017, “ASTEC V2.2 SOPHAEROS module: Theoretical Manual”, Report n° IRSN/2017-00215, Institut de Radioprotection et de Sûreté Nucléaire, Cadarache.
- Darona J., 2019, “CATHARE 2 v25\_3mod8.1 code: Dictionary of operators and directives”, DEN/DANS/DM2S/STMF/LMES/NT/2018-63810/A. Note technique CEA, Cadarache.
- Dekens, J. P., Bastien, R., Prokopovich, S. R., 1985. The emergency response guidelines for the Westinghouse pressurized water reactor (No. IAEA-TECDOC-334), Vienna.
- Girault N.; Mascari, F.; Kaliatka, T., 2022. The R2CA project for evaluation of radiological consequences at design basis accidents and design extension conditions for LWRs: motivation and first results. Proceedings of the 10th European Review Meeting on Severe Accidents Research (ERMSAR2022 ID:332), Karlsruhe (Germany), May 16–19, 2022.

- Herranz, L.E., Fontanet, J., Cantrel, L., 2009. Modeling liquid–gas iodine mass transfer under evaporative conditions during severe accidents. *Nucl. Eng. Des.* 239 (4), 728–734.
- Humphries, L., Beeny B., Gelbard F., Louie D., Phillip J., 2021a. “MELCOR Computer Code Manuals-Vol. 1: Primer and User’s Guide-Version 2.2. 18019”, SAND2021-0252O, Sandia National Laboratories (USA).
- Humphries, L., Beeny B., Gelbard F., Louie D., Phillip J., 2021b. “MELCOR Computer Code Manuals, Vol. 2: Reference Manual–Version 2.2. 18019”, SAND2021-0241O, Sandia National Laboratories (USA).
- Lewis, B. and Iglesias, F., 1995. An Iodine Spiking Model for Pressurized Water Reactor Analysis, Vol. 1 (Theory Manual) and Vol. 2 (User’s Manual), Electric Power Research Institute report, Knoxville, (USA).
- Lewis, B., Iglesias, F., Postma, A., Steininger, D., 1997. Iodine spiking model for pressurized water reactors. *J. Nucl. Mater.* 244 (2), 153–167.
- Lin, C., 1981. Volatility of iodine in dilute aqueous solutions. *J. Inorg. Nucl. Chem.* 43 (12), 3229–3238.
- NUREG-0800, Rev 2. 1981 Standard Review Plan for the Review of Safety Analysis Reports for Nuclear Power Plants, Chapter 15, section 15.6.3, <https://www.nrc.gov/reading-rm/doc-collections/nuregs/staff/sr0800/index.html>.
- Postma, A. and Tam P., 1978, “Iodine behaviour in a PWR cooling system following a postulated steam generator tube rupture accident”, US NRC, NUREG 0409.
- Resi Fard, M., 2011 NUREG-0933 Resolution of Generic Safety Issues: Issue 197: Iodine Spiking Phenomena (NUREG-0933, Main Report with Supplements 1–34) <https://www.nrc.gov/sr0933/Section%202.%20Task%20Action%20Plan%20Items/b65r2.html>.
- Tobin, K., 1984. “A mathematical model of iodine spiking in pressurized water reactors”, Doctoral dissertation, Virginia Polytechnic Institute and State University. [https://vtechworks.lib.vt.edu/bitstream/handle/10919/88579/LD5655.V855\\_1984.T625.pdf?sequence=1&isAllowed=y](https://vtechworks.lib.vt.edu/bitstream/handle/10919/88579/LD5655.V855_1984.T625.pdf?sequence=1&isAllowed=y).
- Whiteman, W.G., 1923. The two-film theory of gas absorption. *Chem. Metal. Eng.* 29.