

Multiscale analysis of the boron dilution sequence in the NuScale reactor using TRACE and SUBCHANFLOW

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ABSTRACT

In the 'High-Performance Advanced Methods and Experimental Investigations for the Safety Evaluation of Generic Small Modular Reactors' McSAFER H2020 European project the main aim pursued is to advance the research in safety analysis methods for water cooled Small Modular Reactors (SMRs). Hence, several light-water-cooled SMR concepts were selected along with the corresponding accident scenarios to be modelled to evaluate the potential application of advanced modeling tools based on the coupling of different codes and their benefits and drawbacks. In this study, the simulation of the postulated boron dilution scenario caused by the malfunction of the Chemical and Volume Control System (CVCS) in the NuScale reactor is performed using different modeling tools and approaches. More in particular, a TRACE-1D, a TRACE-3D and a TRACE-3D/SUBCHANFLOW (SCF) models have been developed to perform this analysis. Two cases have been carried out in this work: the first case is based on the calculation of the boron concentration evolution within the Reactor Coolant System (RCS) of NuScale to compute the time to loss of shutdown margin (SDM), and secondly, a best estimate calculation is performed to evaluate the plant response considering the reactivity feedbacks and the performance of the safeguards and safety systems of NuScale according to the public literature. These investigations have demonstrated that the applied modeling approaches and tools can capture the physics of the problem providing less conservative results than those obtained using the analytical methods presented in the DCA report of NuScale. In addition, it has been demonstrated that the NuScale design is robust against the consequences of the boron dilution transient and that no relevant asymmetrical effects appears due to the singular arrangement of the Helically Coiled Steam Generators (HCSGs) surrounding the riser.

1. Introduction

With the advent of the advanced design features implemented in the Small Modular Reactors (SMRs) such as the integral Reactor Pressure Vessel (RPV), the application of one dimensional thermal hydraulic (TH) tools to the safety analyses should be assessed carefully. Appropriate models and correlations should be carefully selected for each case considering the appearance of multi-dimensional phenomena associated with the new geometries or design concepts. Moreover, the small cores,

the peculiarities of both helical coiled and compact plate-type steam generators, and the passive safety systems used for the long-term removal of the residual heat, which are considerably different from the ones in large Gen II nuclear reactors, may require a careful selection of the numerical tools for safety evaluations (Queral et al., 2020).

In September 2020, the 'High-Performance Advanced Methods and Experimental Investigations for the Safety Evaluation of Generic Small Modular Reactors' McSAFER H2020 European project was launched pursuing the aim of advancing the research in safety calculations related

Abbreviations: SMR, Small Modular Reactor; RPV, Reactor Pressure Vessel; TH, Thermal Hydraulic; HCSG, Helically Coiled Steam Generator; CVCS, Chemical and Volume Control System; SCF, SUBCHANFLOW; RCS, Reactor Coolant System; NPM, NuScale Power Module; DHR, Decay Heat Removal System; SDM, Shutdown Margin; PWR, Pressurized Water Reactor; LOCA, Loss Of Coolant Accident; DWS, Demineralized Water System; BAS, Boron Addition System; IC, Isolation Condenser; LWR, Light Water Reactor; BWR, Boiling Water Reactor; VVER, Water-Water Energy Reactor; MTR, Material Testing Reactor; PZR, Pressurizer; BOC, Beginning of cycle.

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to SMRs (Sanchez-Espinoza et al., 2021) (Karlsruhe Institute of Technology, 2020). To do so, a very ambitious research program based on experimental investigations at European facilities along with the application of different multi-physics/-scale modeling approaches and advanced tools was defined to perform the analyses of the postulated scenarios for several SMR designs, such as NuScale, CAREM or SMART. For more details see (Sanchez-Espinoza et al., 2021).

NuScale is one of the most disruptive and mature designs close to deployment in USA and Europe. It is characterized by an inherently enhanced level of safety thanks to its improved design relying on natural circulation and the implementation of fully passive safety systems to assure the core coolability under all circumstances. NuScale got as first SMR-design the approval of the Nuclear Regulatory Commission; the begin of the first operation of a NuScale plant in the world is envisaged before 2030 (International Atomic Energy Agency, 2022).

In this work, the boron dilution sequence initiated by the malfunction of the Chemical and Volume Control System (CVCS) is simulated (Kliem et al., 2020) with different modeling approaches based on the system code TRACE and the subchannel code SUBCHANFLOW (SCF). In that sense, the computational approaches considered in this study are based on the application of the:

- system code TRACE to describe the NuScale plant behavior under accidents using the point kinetics model along with 1D and 3D modeling approaches and,
- multiscale coupled code TRACE/SCF consisting of a 3D representation of the RPV by TRACE except for the core region, which is represented by the quasi-3D subchannel code SCF.

This paper is organized in eight sections. Section 2 describes the functioning of a generic NuScale Power Module (NPM), where special attention is paid to the Decay Heat Removal System (DHRS). In Section 3, the main features associated with the physics involved in the boron dilution sequence in NuScale are discussed. Then, a brief description of the main capabilities of the TH tools used in this work is given in Section 4. Afterwards, the TH models specifically developed to perform the boron dilution calculations are presented in Section 5 along with the main hypotheses considered. Sections 6 and 7 present the results of the two analyses performed in this study, the calculation of the time to loss the shutdown margin (SDM) considering the power as constant, and the ‘best-estimate’ case relying on the point kinetics model to compute the power evolution during the transient. Finally, the conclusions drawn from this study are presented in Section 8.

2. NuScale power module description

This section is divided into two subsections: firstly, the general functioning and the main design features of the NPM are described. Then, the DHRS performance under transient conditions is presented.

2.1. Fundamentals

The NPM primary side is characterized by the integral PWR design of the RPV where the whole RCS circuit including the helical steam generator tubes is allocated eliminating Large/Medium Break Loss-Of-Coolant-Accidents (LOCAs) by design. Hence, only small leaks of coolant could occur due to the rupture of the piping of the CVCS or by the penetrations made in the RPV for the instrumentation tubes and the control rod drive mechanisms. As can be seen in Fig. 1, the RPV consists of three sections with different diameters for the lower, transition, and upper sections respectively. Furthermore, a small core loaded with 37 17x17 fuel assemblies generates a rated thermal power of 160 MW (NuScale Company LLC, 2020a), which is removed by the natural circulation-driven mass flow rate inside the RCS (NuScale Company LLC, 2020b).

With regard to the flow path within the RCS, the water inventory

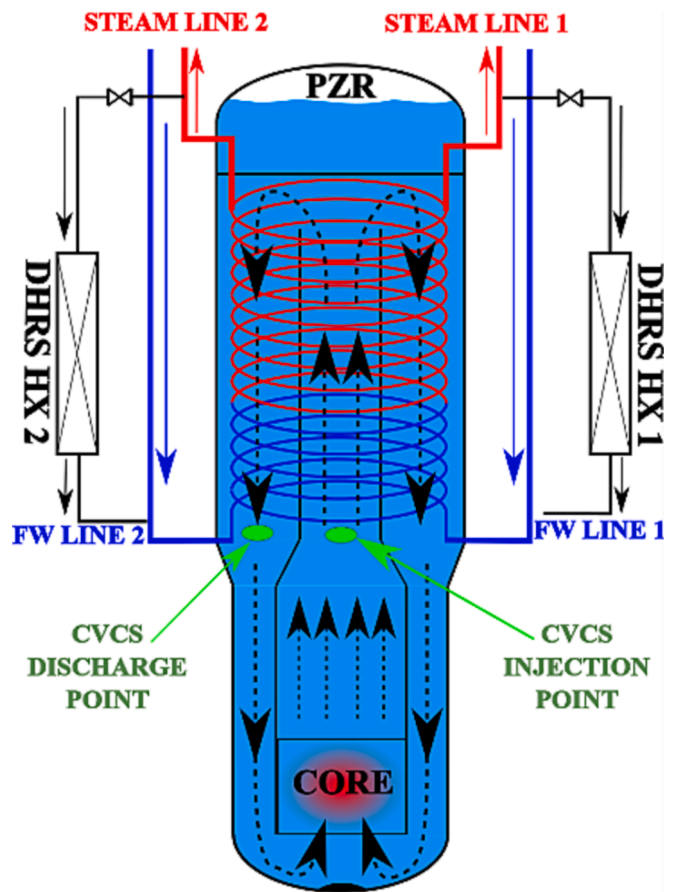


Fig. 1. RPV scheme of NuScale including DHRS piping.

within the core is heated and flows upwards through the central hot riser. At the top of the riser, the flow is redirected radially to the annular region, where the HCSG tubes are located. The primary coolant leaving the HCSG lower part, is colder and denser since the feedwater inside the helical coiled tubes was heated up. Consequently, the denser coolant flows downwards through the downcomer by gravity. Finally, the flow is again redirected from the downcomer to the central region in the lower plenum reaching the core inlet plane and closing the RCS loop (NuScale Company LLC, 2020b).

Regarding the secondary side, two dedicated feedwater and steam lines can be found in each NPM with the corresponding isolation valves (two for each steam line and two for each feedwater line) (NuScale Company LLC, 2020c). Therefore, the heat generated in the core is removed by two HCSGs (with two trains each) with a total number of 1380 tubes. However, in NuScale the HCSGs are not mounted as independent units as it is commonly found in other SMR designs. In this case, the helical tube bank is arranged within the annular region between the inner surface of the RPV and the outer surface of the upper riser tube in such a way that they are symmetrically intertwined surrounding the riser itself, see Fig. 1. Because of it, non-symmetrical behaviors are almost fully eliminated within the RPV (NuScale Company LLC, 2020d).

Given the important role of the CVCS in this study, it should be noted that this system oversees, among other tasks, the management of the chemistry of the primary coolant and, more in particular, the control of the boron concentration in the RCS (NuScale Company LLC, 2020e). For this purpose, the injection and discharge points of the CVCS makeup and letdown lines are located above the core to ensure that the core is covered with liquid water in case of penetration failure (NuScale Company LLC, 2020e). More specifically, the CVCS injection point can be found at the height around the upper riser inlet and, the discharge point is located at the same height but in the annular region between the RPV

and the riser itself, see Fig. 1. In addition, CVCS counts on two redundant variable-speed makeup pumps (positive displacement kind), which provide the RCS with the coolant with the proper boron concentration achieved by the contributions to the makeup flow of the Demineralized Water System (DWS) and the Boron Addition System (BAS) lines, (NuScale Company LLC, 2020e). In that sense, it should be noted that the main source of unborated water in the NPM is the DWS system (the one which makes the boron dilution sequence more challenging to the safety systems). Furthermore, although CVCS is not a safety system, two automatic, fail closed and safety-related redundant DWS isolation valves are implemented in the CVCS so that the consequences of the inadvertent injection of unborated water in the RCS can be successfully avoided or stopped (NuScale Company LLC, 2020e).

2.2. DHRS system description

The DHRS system is a passive safety system designed to remove the decay heat generated within the core under certain conditions after a reactor trip. In particular, DHRS actuation is required when the core cooling is not achievable by the normal performance of the secondary side under non-LOCA conditions (NuScale Company LLC, 2020d).

Each train of the DHRS system includes an isolation condenser (IC) consisting of the correspondent piping connected to the steam and feedwater lines along with a heat exchanger with 80 vertical tubes and two collectors attached to the outer surface of the CNV of the NPM and submerged in the reactor pool. It is worth to mention that both DHRS trains are mounted at each NPM and connected independently to each steam line, see Fig. 1. Therefore, each secondary side loop has a dedicated DHRS train, which is connected to the correspondent steam line before the MSIVs at the top, and to the feedwater line after the FWIVs at the bottom. In addition, two redundant DHRS actuation valves are located immediately after the connection with the respective steam line (NuScale Company LLC, 2020d). The safety signals in NuScale demanding the DHRS actuation are summarized in Table 1.

From the physical point of view, the mass flow rate in the DHRS is driven by the density gradient in the DHRS loop and the difference in height between the bottom of the DHRS ICs and the bottom of the HCSGs. Hence, when the isolation of the NPM is demanded, the MSIVs and FWIVs are eventually closed, and the DHRS actuation valves open creating the two DHRS natural circulation loops. The overheated steam from the HCSGs outlet flows directly to the DHRS piping and, consequently, to the DHRS ICs. When the steam reaches the DHRS submerged pipes and the ICs, it is condensed because of the cooling effect of the reactor pool. For that reason, it becomes denser flowing downwards to the feedwater lines by gravity reaching eventually the HCSGs inlet region again.

3. Description of the boron dilution sequence in the NuScale power module

The boron dilution sequence in NuScale can be caused by the malfunction of the CVCS or by the failure of the human action of the operator associated with the control of the boron concentration in the RCS. The main source of unborated water within an NPM is identified as the DWS (NuScale Company LLC, 2020g).

Table 1
DHRS actuation signals (NuScale Company LLC, 2020f).

Actuation signal	Setpoint	System Automated Function
High Pressurizer Pressure [MPa]	13.790	Demands the DHRS actuation valves.
High Narrow Range RCS Hot Temperature [K]	594.261	
High Main Steam Pressure [MPa]	5.516	Primary and secondary MSIVs
Low AC Voltage to Battery Chargers [-]	-	Primary and secondary MSIBVs FWIVs and feedwater regulating valves

Consequently, it is highly important to take into consideration that the boron dilution sequence begins with the injection of unborated water within the RCS due to a malfunction of the CVCS. Therefore, a boron dilution front is formed in the CVCS makeup injection point and then, that dilution front goes through the different RCS regions over and over following the flow path explained in Section 2. When the dilution front reaches the core region, an insertion of positive reactivity takes place due to the reduction of boron concentration. For that reason, the shutdown margin is significantly reduced. Hence, the time to loss that margin needs to be evaluated. As a result of the core boron concentration reduction, the core power is increased and the reactor is eventually tripped by any SCRAM signal which, in turn, also demands the closure of the DWS's isolation valves finishing the unborated water injection within the RCS. Finally, it should be noted that the decay heat generated in the core can be successfully removed by the actuation of the DHRS system and the reactor pool becomes the ultimate heat sink maintaining the plant conditions under control in the long-term.

4. Modeling tools description

In this section, a brief description of the simulation tools applied in this study is performed making special emphasis on the features of the coupled TRACE/SCF tool.

4.1. The system code TRACE

The TRAC/RELAP Advanced Computational Engine (TRACE) code (U.S. NRC, n.d.) is developed and maintained by the U.S. Nuclear Regulatory Commission (NRC) as the reference code for analyzing the steady-state and transient behaviour of Light Water Reactors (LWR) of Generation II and III (PWR, BWR, VVER). The TRACE code has been designed to perform best-estimate analyses of loss-of-coolant accidents, operational transients, and other accident scenarios for light water reactors. It is based on a component approach to model the reactor systems in which the capability to model TH phenomena in both one-dimensional (1D) and three-dimensional (3D) domains is implemented including a set of heat transfer correlations for the wall/coolant heat transfer and interphase heat transfer covering the whole boiling curve (horizontal and vertical flow regimes) i.e. the pre- and -post CHF heat transfer. It solves a system of six conservation equations for mass, momentum and energy for a two-fluids in one or three dimensions. Dedicated models describes the transport of boron in the liquid phase. It also includes correlations to describe the heat transfer in helical coiled steam generators (U.S. NRC, n.d.).

Although the execution time of TRACE simulations is highly case dependent, it can be generally optimized thanks to the usage of the first-order upwind for solving the spatial difference and the stability-enhancing two-step (SETS) numerical method for the time integration (SETS allows the material Courant limit to be exceeded allowing the optimization of the time-step size in slow transients). However, this numerical method cannot be applied when a high-order spatial numerical method is selected. It is the case when e.g. boron dilution sequences are analyzed. Instead, a semi-implicit method that imposes the Courant limit is used leading to an increased computational time.

4.2. The subchannel code SUBCHANFLOW

SCF is a fast running and flexible subchannel simulation tool. It can handle rectangular, hexagonal, and plate fuel bundles as well as the whole core geometries built from these. The code is based on the legacy COBRA code family (Coolant Boiling in Rod Arrays) (Basile et al., 2010; Rowe, 1973; Wheeler et al., 1976). Modeling is concentrated on the main physical phenomena occurring in subchannel flow for steady state and transient conditions in consideration of fast and stable execution. In a basic option, steady state and transient problems are solved with an iteration-based COBRA like fully implicit solver, so the flow is restricted

to upward direction with lateral exchange. In addition, a solver based on the semi-implicit SOLA method is available which allows low mass-flow rates, downward flow and buoyancy driven flow (Hirt et al., 1975). Coolant properties and state functions are implemented for water using the IAPWS-97 formulation. In addition, property functions for liquid metals (sodium and lead) and gases (helium, air) are available. Two phase flow (boiling) is implemented for water and sodium. The heat transport from the nuclear heated fuel rods to the fluid is based on a cylindrical 1D radial heat conduction model including the gap conduction between the fuel pellets and the cladding. As boundary conditions, the total mass-flow rate or a channel-dependent mass-flow rate can be selected. It is possible to distribute the flow automatically to the parallel channels depending on the friction at the bundle inlet. In addition, a pure top-bottom pressure difference boundary can be used. Fluid temperature at the inlet and pressure at the outlet always have to be prescribed as boundary conditions. An iterative steady-state numerical procedure is available to determine the power at which critical heat flux conditions appear during the simulation.

In SCF, profit is taken from the many valuable empirical correlations for pressure drop, heat transfer coefficients, void generation, etc., collected over the last decades. Consequently, it does not follow the general trend to describe two-phase flow by simulating the processes on a microscale basis e.g., separate conservation equations for liquid droplets, films or vapor bubbles. In addition, a three-equation two-phase flow model that is a mixture equation for mass, momentum, and energy balance is implemented in SCF. The constitutive relations are expressed as mixture equations for wall friction and wall heat flux as well as a two-phase flow slip velocity correlation. Boron transport can be tracked conserving strong concentration gradients. The main calculation routines are allowed to be controlled by a series of C programming language functions interfaces. They permit to use SCF as an external recompiled library, to exchange all the data necessary for coupled neutron physics calculations. The input is oriented to a text-based user interface using comprehensive keywords and simple tables. All data are given in SI units apart from temperatures which are input in °C and converted to Kelvin degrees internally. Extensive validation work is performed using data of relevant experiments for PWR, BWR, and MTRs (Almachi and Sanchez Espinoza, 2022; Imke and Sanchez, 2012).

4.3. TRACE/SCF coupled tool

The TRACE/SCF multiscale tool developed at KIT has been applied to the analysis of the boron dilution sequence in the NuScale reactor by the UPM research group. It is based on the ICoCo (Interface for Code Coupling) standard and the SALOME platform (Zhang et al., 2021). This is a server-client system where TRACE and SCF are in charge of performing the corresponding calculations, ICoCo is responsible for inter-code data exchange, and SALOME is the supervisor which synchronizes the calculation of both codes.

4.3.1. ICoCo interface

ICoCo is a standard Application Protocol Interface (API) for code coupling developed by CEA within the framework of the European NURISP project to handle various code coupling tasks. It is a very flexible, modular object-oriented generic interface (framework) for code coupling. It does not contain any calculation code. Therefore, ICoCo provides only the corresponding functions and methods (setDataFile, initialize, computeTimeStep, solveTimeStep, getOutputMEDField, setInputMEDFields...) to the involved codes along with the description of the activities performed by them. For example, some methods allow to insert various input and output ports to the coupled codes making the interaction between the selected codes very flexible and convenient. On the other hand, ICoCo relies on the MEDCoupling library (also implemented in the SALOME platform) to perform the meshes and fields mapping between codes in coupled calculations for the data exchange between them. For further information see (Zhang, 2020).

4.3.2. SALOME platform

The SALOME platform is an open-source software for numerical pre- and post-processing activities, but it can be also used as the environment to perform code coupling and relevant simulations. The platform was initiated by CEA, EDF, and OpenCascade. It has been employed in a wide range of engineering fields (CEA/DES et al., n.d.). SALOME allows performing efficient code coupling using a very powerful mesh interpolation tool included in the built-in module MED, known as the MEDCoupling libraries (CEA/DES et al., n.d.). The SALOME built-in module YACS is in charge of the development as well as the execution of the coupling codes.

The development of the TRACE/SCF coupling code in SALOME can be summarized in the following steps (Zhang et al., 2021):

1. Develop ICoCo for TRACE and implement them together into SALOME.
2. Develop ICoCo for SCF and implement them together into SALOME.
3. Develop the interpolation tools to handle the field mapping between different meshes of TRACE and SCF. Implement the interpolation tools into SALOME.
4. Construct the scheme for coupling simulation in SALOME for the selected transient.

In this work, the domain decomposition approach is applied, and the data exchange is only performed at the core inlet and the core outlet (two planes) regions. The fields to be exchanged between the codes are listed below:

TRACE → SCF:

1. Core Inlet:
 - o mass-flow rate,
 - o coolant temperature
 - o boron concentration.
2. Core Outlet:
 - o pressure.

SCF → TRACE:

1. Core Inlet:
 - o pressure.
2. Core Outlet:
 - o mass-flow rate,
 - o coolant temperature,
 - o boron concentration.

5. Description of the modeling approaches

In this section, the main features of the TH models of the NuScale SMR built to perform the calculation of the boron dilution sequence are briefly explained. Regarding the modeling approaches applied in this study, three different modeling constraints were imposed on each step of the study as follows:

1. The full-plant TRACE model (RPV, steam lines, feedwater lines, DHRS, etc.) is only based on 1D components referred to as TRACE-1D model.
2. In the full-plant TRACE model, the RPV and core is based on 3D model (VESSEL components); hereinafter it is named as TRACE-3D model.
3. In the full-plant TRACE model under point 2, the TRACE core model is replaced by the SCF model; hereinafter it is referred to as TRACE-3D/SCF model.

It is worth to be noted that the development of the different models listed above is based on public data sources, see (NuScale Company LLC, 2020h, 2020a, 2020d, 2020i, 2020e, 2020c, 2020b, 2020f, 2019a, 2019b, 2016a, 2016b), however, certain values have been estimated by expert judgment. In the models, the RCS is divided into different volumes and regions according to the NuScale DCA, see (NuScale Company LLC, 2020a, 2020d), as listed below:

1. The core region is divided into Lower/Upper Core Plates, Fuel Assemblies and Bypass volumes.
2. Hot leg region is formed by the Lower Riser, the Transition Riser, and the Upper Riser volumes.

3. The HCSG primary side region is formed by the outer volume of the HCSG tubes.
4. The cold leg consists of Upper DC, Transition DC, Lower DC and Lower Plenum volumes.
5. Pressurizer (PZR) region.

The key-features implemented in the three different models are briefly described below:

- The modeling of the RCS flow path has been achieved using a 1D PIPE component for each of the regions identified previously for the TRACE-1D model in the first step of this study, see Fig. 2. For the second and the third cases of this study, the same nodalization scheme of the RCS (apart from the core region) is used. However, two 3D cylindrical VESSEL components have been implemented in the RCS models considering two radial rings (one for modeling the central region and the other one for the annular region between the inner RPV surface and the outer surface of the central region (riser and core barrel)) and four azimuthal sectors, see Fig. 3. Finally, to do the modeling of the region where the HCSGs are located, the dedicated kind of PIPE and VESSEL ‘Tube Bank Crossflow’ available in TRACE is selected respectively (U.S. NRC, n.d.).
- The active core height (2 m long) is nodalized with 20 axial levels and one hydraulic cell per axial level for the TRACE-1D case. However, a radial nodalization scheme of the core with 37 hydraulic cells is additionally implemented in the 3D Cartesian VESSEL and in the SCF core models for the TRACE-3D and TRACE-3D/SCF approaches, see Fig. 3 and Fig. 4. By doing so, a ‘fuel assemblies to hydraulic channels’ ratio of 1:1 nodalization criterion is met in the 3D core models since the NuScale core is formed by 37 fuel assemblies, as it was commented in Section 2. Therefore, a very detailed model of the active core region with a total of 740 hydraulic cells for the TRACE-3D and TRACE-3D/SCF models has been built. Finally, the bottom/top nozzle axial levels of the fuel assemblies along with the lower/upper core plates have been explicitly modeled in the TRACE models. Finally, the bypass flow is modelled separately using PIPE components (one for the TRACE-1D model and four for the TRACE-3D and TRACE-3D/SCF models).
- Regarding the modeling of the crossflows within the core, two different modeling approaches have been applied in the TRACE-3D and TRACE-3D/SCF cases. In the former case, the crossflows

among fuel assemblies are restricted by means of the reduction of the transversal flow area due to the presence of the latest row of fuel rods and no additional friction is considered in the crossflow direction. But in the latter case, an estimated crossflow resistance coefficient is included in the SCF model based on summing up the pressure loss coefficients of the rod rows inside the fuel assembly, as it is recommended in (Imke, 2020).

- Another relevant region to be modelled with care is the one in which the HCSG tube bundles are allocated. As commented, the primary side is modelled using the dedicated option of PIPE (1D) and VESSEL (3D) in TRACE (‘Tube bank crossflow’) switching on the adequate heat transfer and friction correlations to simulate this kind of special geometry. Similarly, the dedicated kind of PIPE, ‘Curved pipe’, in TRACE in combination with a fine nodalization of the HCSGs tubes with 39 hydraulic cells has been implemented in the models of the secondary side representing the inner flow through the HCSGs tubes, as it is recommended in (Mascari et al., 2023). Finally, for the four different HCSG tube bundles to be explicitly modelled, four PIPE components were implemented in the models.
- The modeling of the PZR region is also performed using the dedicated kind of 1D PIPE component, ‘Pressurizer’, in TRACE allowing to consider the actuation of the PZR heaters and PZR spray to control the RCS pressure along with its trip in a very simple manner.
- The CVCS makeup and letdown lines have been implemented in the models as boundary conditions (mass-flow rate, injection temperature and boron concentration are controlled), as can be seen in Fig. 2, Fig. 3, and Fig. 4. At this point, it is worth to mention that the injection and discharge of CVCS makeup and letdown lines in NuScale is performed in only one point of the RCS respectively, see (NuScale Company LLC, 2020e, 2016b). In the TRACE-3D and TRACE-3D/SCF TH models, the assumption that the injected and discharged mass-flow rate by the CVCS lines are distributed among the four azimuthal sectors uniformly is made.
- Regarding the secondary side and the safety systems implemented in the models, it should be noted that the secondary side is modelled up to the turbine stop valve along with the DHRS actuation valves, DHRS piping, DHRS ICs and the reactor pool using 1D components.
- The instrumentation and control signals of the plant, paying special attention to the SCRAM signals logic along with the control rods worth, have been implemented in the TH models to simulate the plant behaviour during the selected transient.

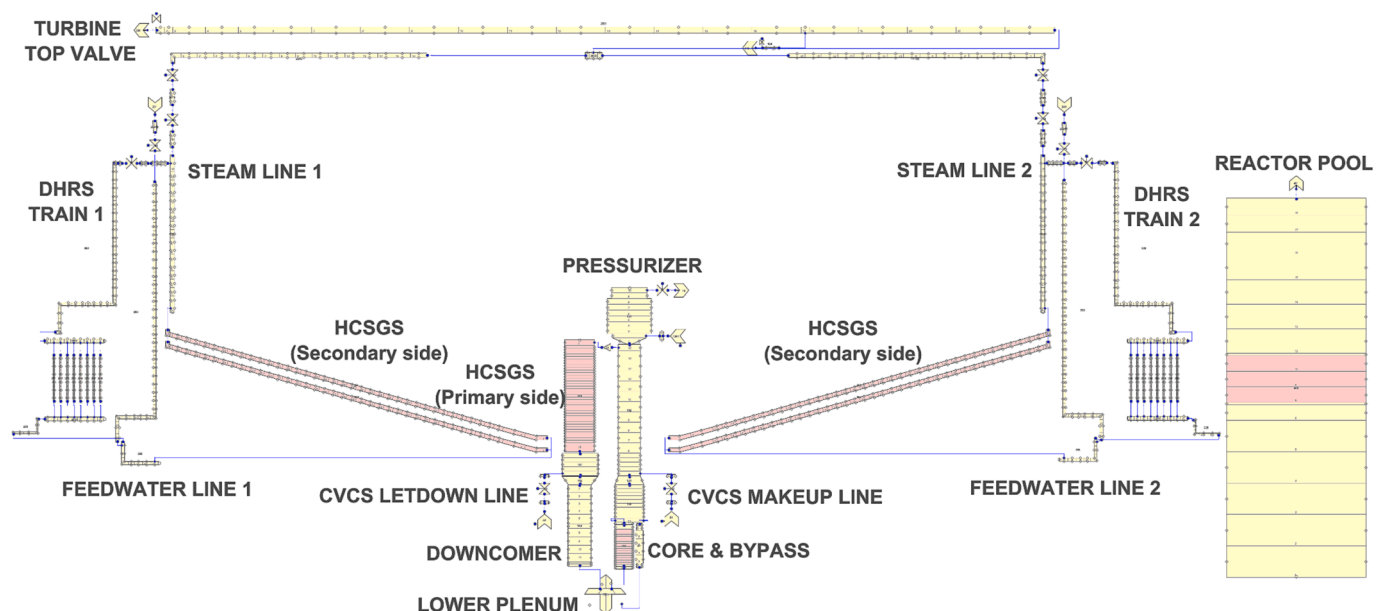


Fig. 2. Nodalization scheme of the full-plant TRACE-1D model.

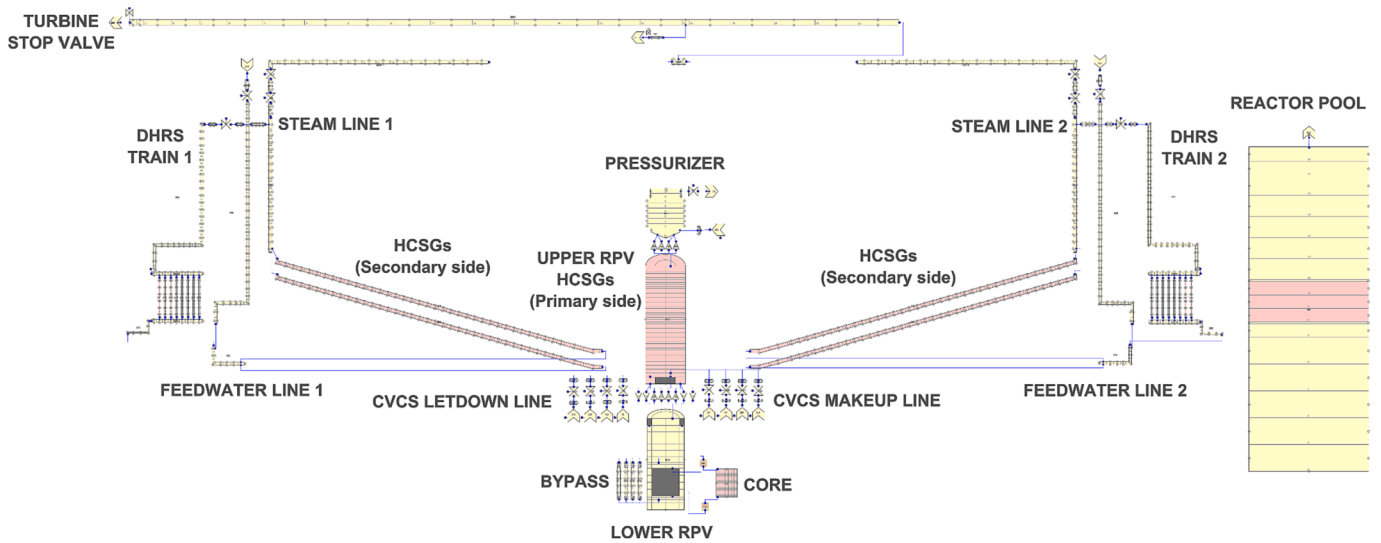


Fig. 3. Nodalization scheme of the full-plant TRACE-3D model.

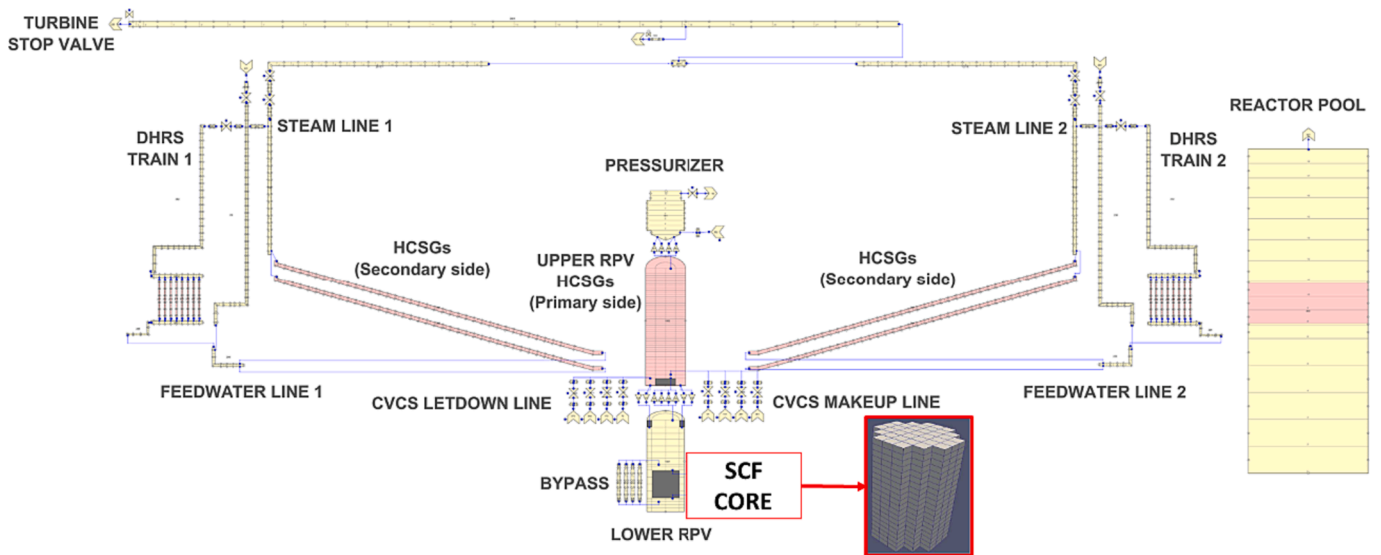


Fig. 4. Nodalization scheme of the full-plant TRACE-3D/SCF model.

- Finally, for the transport of boron within the RCS to be properly modelled, the semi-implicit method has been implemented in the TRACE models for doing the time integration along with the high-order numerical technique, Van Leer with flux limiters, for the spatial differences allowing to reduce the amount of numerical diffusion. On the SCF side, an explicit solver for the time integration is used in combination with a second-order technique for the spatial differences.

The main hypotheses assumed to perform the steady-state and the correspondent transient calculations are in line with the ones described in (NuScale Company LLC, 2020g) and listed below:

- The reactor is initially working at Hot Full Power (100 %) Beginning-of-Cycle (BOC) condition. This condition determines the axial power profile included in the models, see Fig. 5. The Decay Heat is increased up to a value of 120 %.
- Normal AC power is assumed to be available.
- The plant control systems and safety features perform as designed.
- No human actions are credited to mitigate the effects of the transient.
- The regulating CRA bank is not credited to mitigate the reactivity insertion associated with a boron dilution of the RCS.
- Nominal values are assumed for the RCS except for the mass-flow rate (535.24 kg/s).
- The letdown mass-flow rate is equal to the makeup mass-flow rate (3.15 kg/s).
- The initial Boron concentration is fixed at 1600 ppm.
- Reactivity feedbacks are not credited in the steady state calculation. However, in the best-estimate calculation of the boron dilution sequence, the following values (conservative) for the reactivity coefficients have been selected, see (NuScale Company LLC, 2020g):
 - Coolant temperature reactivity coefficient: 0.00 pcm/K
 - Fuel temperature (Doppler) reactivity coefficient: 2.52 pcm/K
 - Boron reactivity coefficient: 10.00 pcm/ppm
- A deviation of around $\pm 5\%$ from the nominal value (33.535) of the feedwater mass flow is implemented in each Feed Water (FW) line to evaluate the HCSG performance under asymmetrical conditions.
 - FW line 1 mass-flow rate: 35.22 kg/s
 - FW line 2 mass-flow rate: 31.85 kg/s
- The FW injection temperature is fixed on 421.875 K.

BOC		0.895	0.911	0.888		
	1.033	1.137	0.957	1.135	1.033	
0.888	1.135	1.054	0.967	1.054	1.136	0.895
0.911	0.957	0.967	1.091	0.967	0.957	0.911
0.895	1.136	1.054	0.967	1.054	1.135	0.888
	1.033	1.135	0.957	1.137	1.033	
		0.888	0.911	0.895		

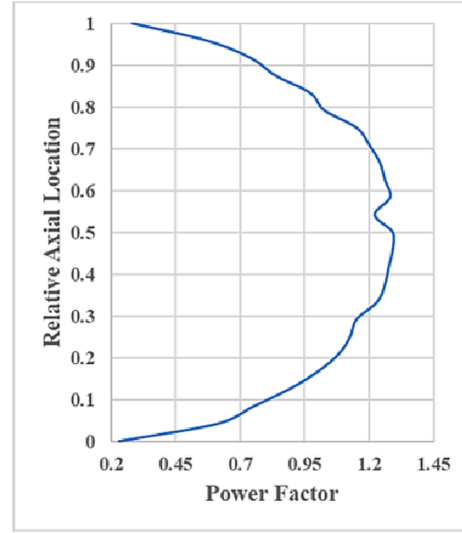


Fig. 5. BOC Radial (left) and Axial(right) power profile implemented in the core models (NuScale Company LLC, 2020a).

5.1. Steady-State calculation

A steady-state calculation has been performed using the described models for NuScale obtaining a very good agreement with the reference data included in the DCA of NuScale (NuScale Company LLC, 2020g), see Table 2. The 3D distributions of the main parameters of the core (power, pressure, temperature and mass-flow rate) obtained using the TRACE-3D/SCF model during the steady-state calculation are presented in Fig. 6 and Fig. 7. More in detail, Fig. 8 and Fig. 9 present the radial distributions channel-by-channel for the core mass-flow rate and for the core outlet temperature obtained using the TRACE-3D and TRACE-3D/SCF models.

6. Boron dilution transient calculation with constant power

Regarding the boron dilution transient, the acceptance criterion is based on the fact that the available time for the operator to perform the human action required to terminate the boron dilution transient should be greater than 15 min under normal operation conditions (NRC, 2007). It means that the time to loss the shutdown margin (SDM) should be greater than 15 min. According to the results of the analysis performed in the DCA report of NuScale, that time is 30.5 min (NuScale Company LLC, 2020g). It should be highlighted that the analysis of the time to loss of SDM can be performed by analytical methods or utilizing numerical simulations introducing the boron dilution rate in the CVCS interface with the RCS (through the CVCS make-up mass-flow rate) and maintaining the power as constant so that the boron concentration evolution within the RCS can be evaluated up to reaching the value corresponding to the loss of SDM. In addition, it is important to keep in mind that no human actions are credited in the calculations of the time to loss the SDM presented below.

In the DCA report of NuScale, (NuScale Company LLC, 2020g), the time to loss of shutdown margin analysis under a boron dilution scenario is evaluated employing two simplified models: the Perfect mixing and the Boron Dilution Slug models:

- The **perfect mixing model** assumes that the unborated water injected in the RCS by the CVCS is mixed instantaneously with the whole RCS volume in a homogenous way resulting in a continuous and decreasingly monotonic variation in the Boron concentration of the RCS. The formula used is shown below:

$$\frac{dC}{dt} = \frac{Q_{in}}{M_{RCS}} \cdot C(t) \quad (1)$$

Table 2

Comparison of results of the steady-state calculations.

Plant parameter (SI Units)	Reference	TRACE-1D (Error, %)	TRACE-3D (Error, %)	TRACE-3D/ SCF (Error, %)
RCS Pressure [MPa]	12.755	12.768 (0.10)	12.772 (0.13)	12.754 (-0.00)
RCS Inventory (No PZR) [kg]	-	40009.51	39920.26	39856.82
Avg. RCS Mass-flow rate [kg/s]	535.24	533.81 (-0.27)	532.38 (-0.55)	535.35 (0.02)
RCS Mass-flow rate S1 [kg/s]	-	-	133.05	133.79
RCS Mass-flow rate S2 [kg/s]	-	-	133.14	133.89
RCS Mass-flow rate S3 [kg/s]	-	-	133.05	133.78
RCS Mass-flow rate S4 [kg/s]	-	-	133.14	133.89
Avg. Core Mass-flow rate [kg/s]	496.17	495.59 (-0.12)	496.34 (-0.03)	497.27 (0.22)
Core Mass-flow rate S1 [kg/s]	-	-	123.81	123.95
Core Mass-flow rate S2 [kg/s]	-	-	124.36	124.69
Core Mass-flow rate S3 [kg/s]	-	-	123.81	123.94
Core Mass-flow rate S4 [kg/s]	-	-	124.36	124.69
Avg. Core Inlet Temperature [K]	531.48	531.13 (-0.06)	531.12 (-0.07)	532.72 (0.23)
Core Inlet Temperature S1 [K]	-	-	530.99	532.61
Core Inlet Temperature S2 [K]	-	-	531.24	532.84
Core Inlet Temperature S3 [K]	-	-	530.99	532.60
Core Inlet Temperature S4 [K]	-	-	531.24	532.84
Core Inlet [B] [ppm]	1600.00	1600.00 (0.00)	1600.00 (0.00)	1600.00 (0.00)
PZR level [%]	60.00	59.998 (-0.00)	59.995 (-0.01)	60.03 (0.05)
Avg. Steam Temperature [K]	580.04	585.50 (0.94)	585.01 (0.86)	582.37 (0.40)
Avg. SG Outlet Pressure [MPa]	3.447	3.464 (0.48)	3.451 (0.12)	3.447 (0.00)

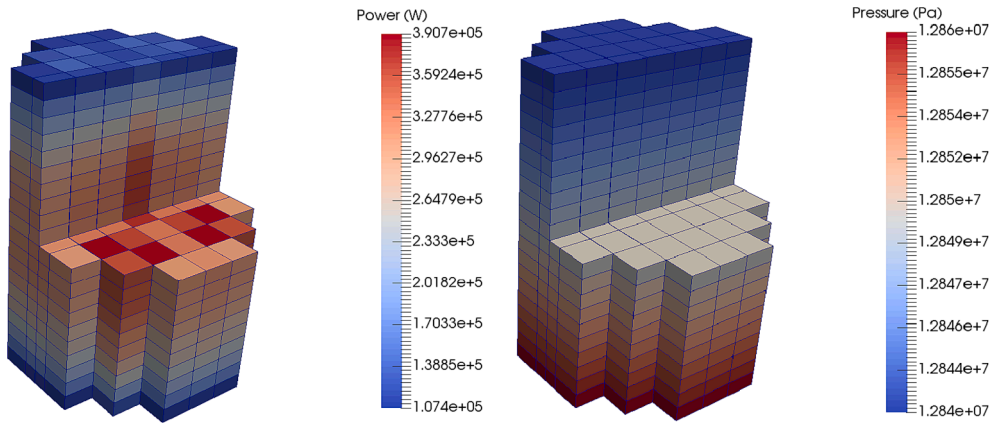


Fig. 6. Core power (left) and pressure (right) in the steady state calculation (TRACE-3D/SCF).

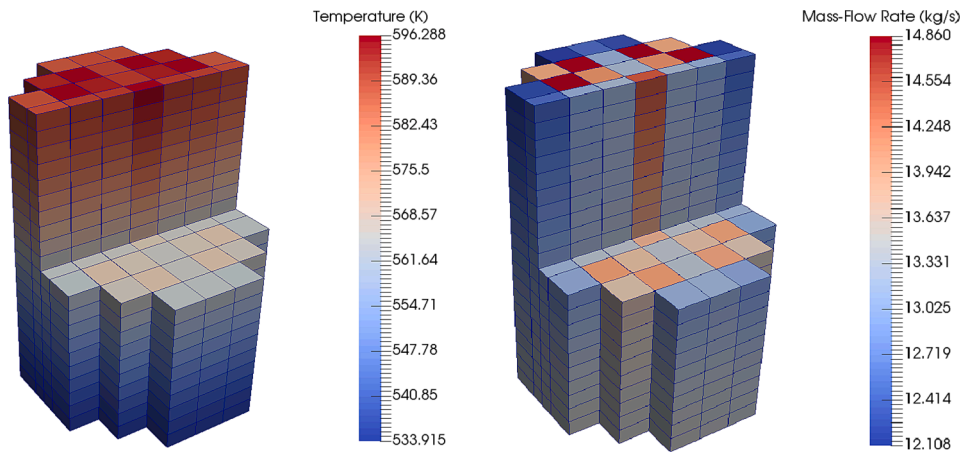


Fig. 7. Core temperature (left) and mass-flow rate (right) in the steady state calculation (TRACE-3D/SCF).

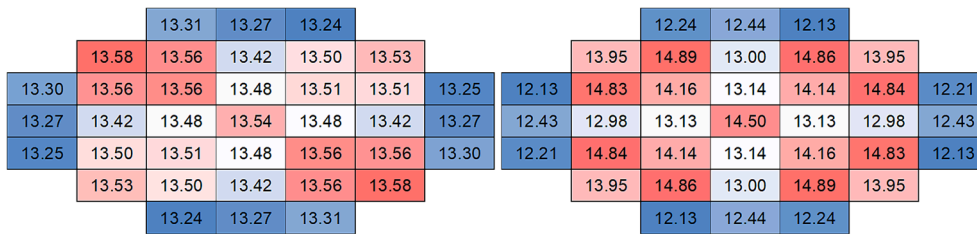


Fig. 8. Radial distribution of the core mass-flow rate (TRACE-3D (left) | TRACE-3D/SCF (right)).

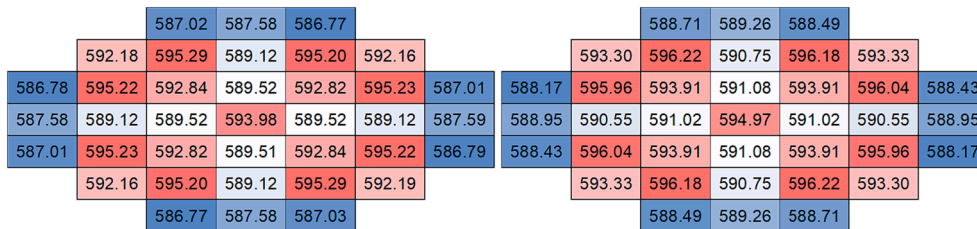


Fig. 9. Radial distribution of the core outlet temperature (TRACE-3D (left) | TRACE-3D/SCF (right)).

where,

C = boron concentration [ppm]

Q_{in} = CVCS makeup mass-flow rate [kg/s]

M_{RCS} = RCS mass without considering the PZR [kg]

Integrating (1):

$$C(t) = C(0) \cdot e^{-\frac{Q_{in}}{M_{RCS}} t}$$

(2)

- On the other hand, the boron dilution front or **slug flow model** is based on the movement of the dilution front along the RCS. Therefore, the Boron concentration variation within the core is a function of the transit time, the number of times that the dilution front had passed through the core and the dilution front Boron concentration itself. In addition, the slug flow model is a discrete one and the formulas used are presented below:

$$C(N) = C(0) \cdot \left[\frac{W_{NC}}{W_D + W_{NC}} \right]^N \quad (3)$$

$$t(N) = \frac{M_{RCSI} + (N - 1) \cdot M_{RCS}}{W_D + W_{NC}} \quad (4)$$

where,

$C(N)$ = the Nth front boron concentration passing through the core region [ppm]

$C(0)$ = initial boron concentration (1600 ppm)

$t(N)$ = time when the Nth front boron concentration passes through the core region [s]

N = number of times that the boron dilution front has passed through the core region [-]

W_{NC} = RCS mass-flow rate (535.24 kg/s)

W_D = CVCS mass-flow rate (3.155 kg/s)

M_{RCSI} = mass between the CVCS injection point and the core inlet level [kg]

M_{RCS} = total RCS inventory without considering the PZR volume [kg]

It is important to notice that these simplified analytical models are conservative. On one hand, the perfect mixing assumption does not consider the transit time of the boron dilution front through the RCS and mixes the boron instantaneously with the rest of the RCS inventory. On the other hand, the slug model takes into account the transit time and, consequently, the flow path within the RCS but not the effect of the CVCS letdown mass-flow rate. Finally, in both models the PZR mass is removed from the calculation of the total mass inventory within the RCS which is a conservative assumption (NuScale Company LLC, 2020g).

In this study, a comparison between the results computed using the simplified analytical models presented in (NuScale Company LLC, 2020g) explained above and the results obtained from the simulations with the TH models presented in Section 5 is made. To do so, it is important to remember that only the transport of the boron concentration through the RCS should be computed in the simulations without any change in the reactor power or plant conditions since the Figure of Merit of the analyses is the time to reach a specific core boron concentration. By doing so, it will be possible to compare the time, at which the boron concentration causing the loss of the SDM is reached, obtained in the simulations with the results presented in the DCA of NuScale.

As can be seen in Table 2, the values of the RCS inventory computed in the steady-state calculation using the three modeling tools are very similar. In that sense, the TRACE-1D model data will be used to obtain the time to loss the SDM using the explained analytical methods. To do so, it should be noted that according to the results presented in the DCA of NuScale, the time to loss the SDM is 30.5 min (NuScale Company LLC, 2020g). Therefore, introducing that value in (2) and considering that the value of the mass between the CVCS injection and the core inlet calculated using the TRACE-1D model is 33566.52 kg along with the parameters presented in Section 5 and Table II, a value of 1384.99 ppm is obtained for the boron concentration causing the loss of the SDM the TRACE-1D model. A summarizing table with the results obtained using the commented analytical methods and the simulations using the TH models described is included, see Table 3.

Finally, it should be noted that a very good agreement has been achieved among the results obtained using the commented methods and the reference value (30.5 min) for the time to loss the SDM. Therefore, it can be concluded that the obtained results are within a reasonable range in comparison to the reference value and that the developed TH models

Table 3

Comparison of the time to loss of the SDM computed by the analytical methods (Perfect mixing and boron dilution slug models) and the numerical simulations.

Plant parameter	Time to loss the SDM [min]
Perfect mixing model	30.50
Boron dilution front or slug model	30.76
TRACE-1D	30.96
TRACE-3D	31.08
TRACE-3D/SCF	30.98

of the RCS for the different cases are simulating properly the physics of the problem, see Fig. 10, despite the appearance of a certain amount of numerical diffusion at the very endings of the simulations, see Fig. 11.

Last but not least, it has been also demonstrated that the acceptance criterion associated with the time to loss the SDM is met no matter which calculation approach is applied and that the presented analytical methods provide with more conservative values to this analysis than the numerical calculations, see Table 3 and Fig. 10, as it was expected.

7. Boron dilution transient analysis with point kinetics

In this section, the plant response to the boron dilution sequence is simulated and the results obtained using the modeling approaches presented previously are analyzed. It must be noted that the core power evolution predicted by the Point Kinetics model of the TRACE-3D case is transferred to the SCF model so that the SCRAM actuation can be considered in the boron dilution simulations. Therefore, in the TRACE-3D/SCF case, the boron dilution front transport is computed but without any boron reactivity feedback since the core power is input through a time-dependent table. A brief description of the sequence of events occurring during the simulation of the accidental sequence is included below:

The transient begins with the injection of unborated water in the RCS due to the CVCS malfunction. Firstly, a boron dilution front is formed immediately after the CVCS injection point and begins to travel following the RCS flow path up to reaching the core inlet region, see Fig. 12. Therefore, when the boron dilution front passes through the core region, the reduction in the boron concentration causes a positive insertion of reactivity, see Fig. 13, and, consequently, an important increase in the core power, see Fig. 14. For that reason, the pressure in the primary circuit begins to rise, the 'High PZR Pressure' setpoint is eventually reached, see Fig. 15, and the associated SCRAM signal is triggered. After a signal delay of 2 s, the control rod insertion starts, the reactor emergency shutdown takes place and the turbine is tripped, as it is shown in Fig. 14 by a very sharp reduction of the core power. The commented SCRAM signal activation also demands the CVCS isolation so that the injection of unborated water can be stopped, the NPM isolation from the secondary side by the closure of the MSIVs and FWIVs, and the DHRS actuation.

On one hand and as NuScale relies on natural circulation, the reactor trip causes a mass-flow rate transient with a strong reduction of the core and RCS mass-flow rate in which very low values can be reached, see Fig. 16. At this point, it should be noted the mass-flow rate presents certain oscillations rapidly dumped in a similar behaviour to the one described in the manometer problem in (Hoon Kim et al., 2014). Additionally, the reactor trip along with the DHRS actuation allows to control and to eventually reduce the RCS pressure, see Fig. 15. Finally, it should be noted that the PZR level follows the same trend as the RCS pressure, as can be seen in Fig. 17.

On the other hand, the turbine trip and the rapid secondary side isolation accomplished 5 s after the reactor trip cause a sharply increase in the secondary pressure, see Fig. 18. However, the opening of the DHRS actuation valves creates a new flow path establishing an approximately steady mass-flow rate driven by natural circulation through the DHRS piping for the long term cooling, as shown in Fig. 19.

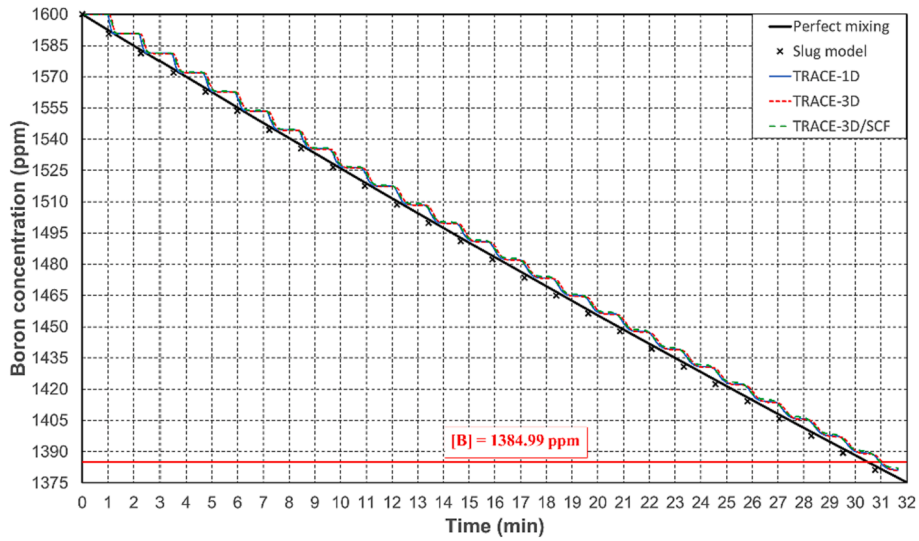


Fig. 10. Boron concentration evolution in the constant power analysis.

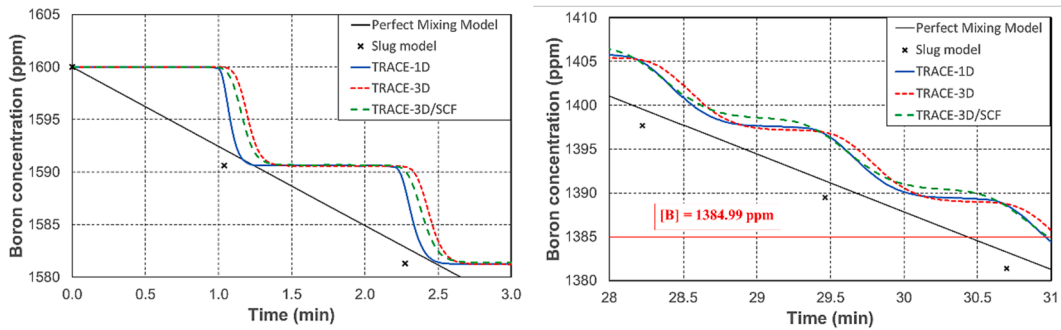


Fig. 11. Boron concentration detail at the beginning (left) and the ending (right) of the transient.

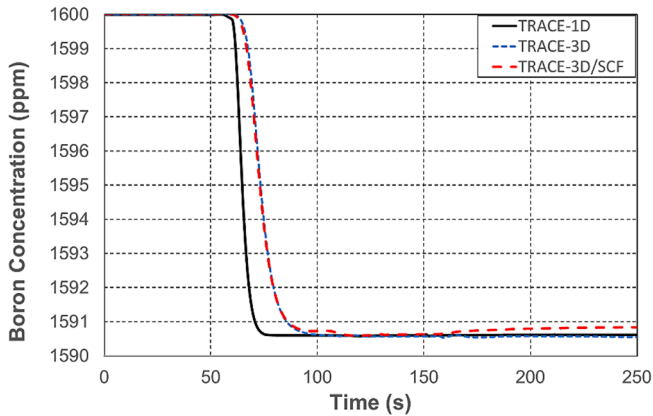


Fig. 12. Averaged core inlet boron concentration.

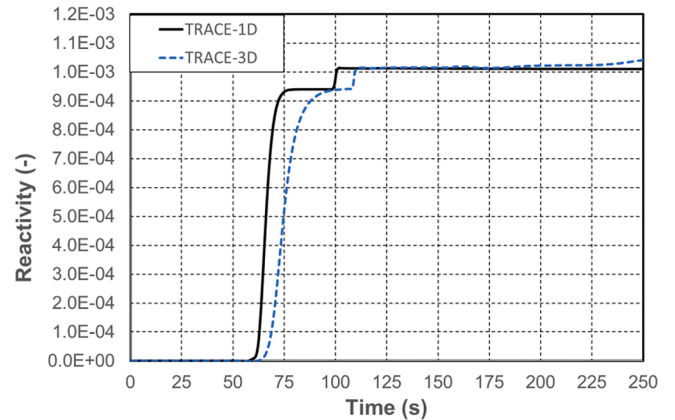


Fig. 13. Boron reactivity.

In that sense, the secondary pressure and temperature begin to decrease due to the DHRS performance, see Fig. 18 and Fig. 20, and the reactor pool becomes the new ultimate heat sink of the system. Finally, the temperature, the mass-flow rate and the boron concentration at the core inlet region are depicted in Fig. 21 and Fig. 22, respectively, to demonstrate that no relevant asymmetrical consequences appear in the transient simulation results.

To put all the above in a nutshell, the computed sequence of events during the boron dilution calculations using the previously described modeling approaches (see section 5) is included in Table 4.

8. Conclusions

The main conclusions drawn from these analyses are the following:

- The boron dilution sequence has been successfully simulated using different modeling approaches. The usage of high-order numerical techniques with flux limiters for solving the spatial differences allows the physics involved in the transport calculation of the boron concentration through the NuScale RCS to be captured properly.

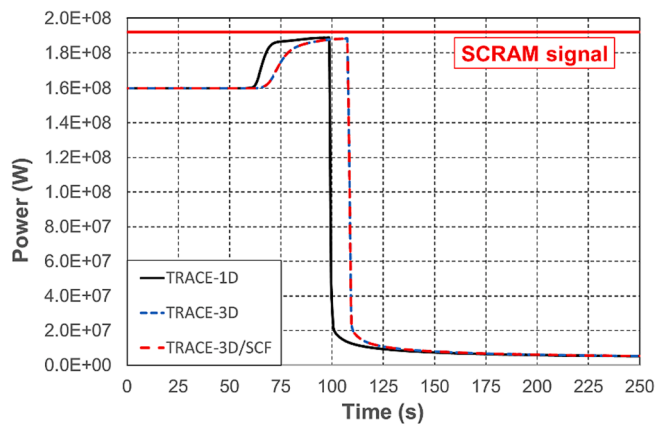


Fig. 14. Core power evolution.

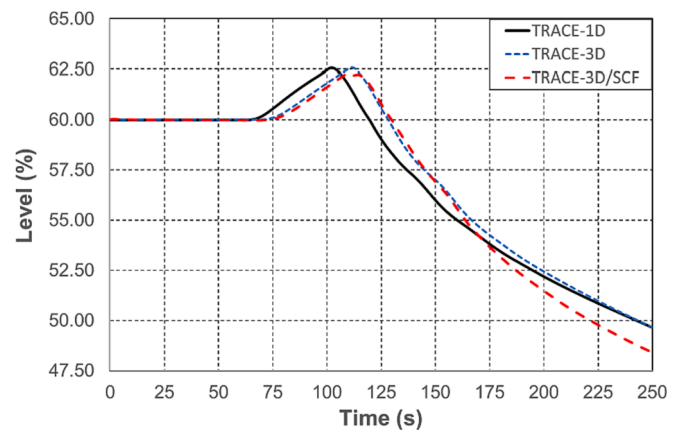


Fig. 17. PZR level.

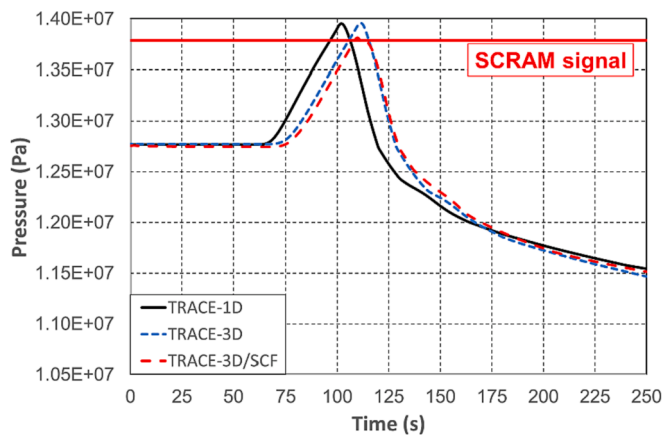


Fig. 15. Primary pressure evolution.

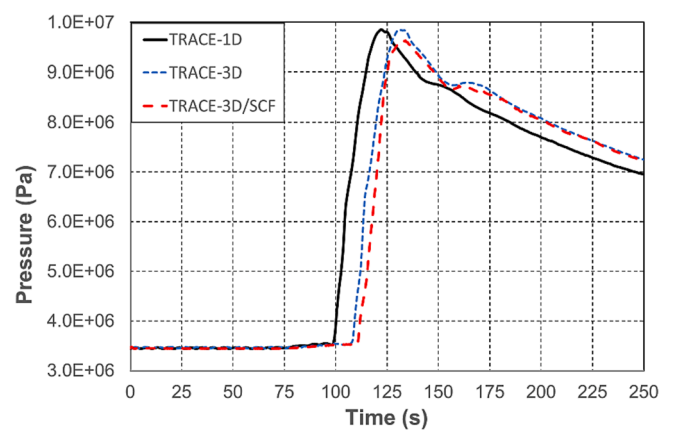


Fig. 18. Secondary pressure.

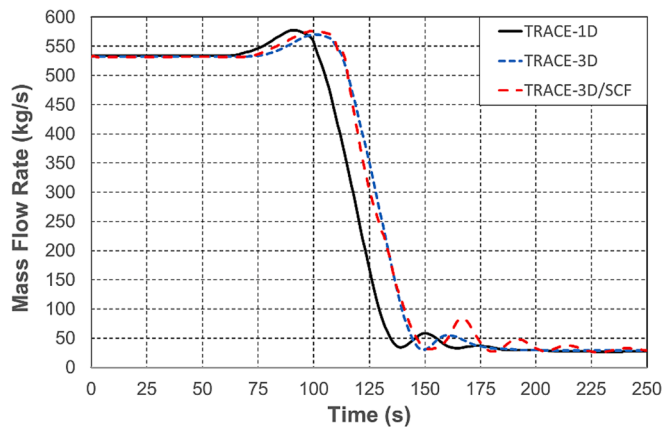


Fig. 16. RCS mass-flow rate.

- In this study, a very good agreement is obtained among the results of the boron dilution sequence in the NPM using TRACE-1D, TRACE-3D and the TRACE-3D/SCF models. Only a slight delay among several plant parameters among the results obtained using 1D and 3D modeling approaches that can be attributed to the redistribution of the boron in the 3D modelling cases.
- It has been demonstrated that the acceptance criterion based on the time to loss the SDM has been verified and according to the results of this study, the results of the analytical methods used in the DCA report of NuScale are conservative. Even further margin to the 15

min for the time to loss of SDM imposed by the acceptance criterion can be obtained with the application of the best estimate modeling approaches presented in this study.

- It has been demonstrated that the TRACE/SCF coupling tool developed at KIT can simulate the boron dilution and the exchange of data between both codes is performed properly.
- Considering the results of both one- and three-dimensional TH analyses of the NuScale behavior under boron dilution accident conditions, it can be stated that the applied tools have predicted only very small differences between the mass-flow and the temperature at the core inlet region, although an asymmetrical mass-flow rate in the feedwater lines was assumed. In addition, the design of the helically coiled heat exchanger in NuScale greatly prevents the development of asymmetrical TH conditions inside the RPV.
- Finally, the advantages of the use of three-dimensional TH codes to analyze the SMR-plant behavior under accident conditions compared to one-dimensional tools will become more apparent for other SMR-designs where non-symmetrical transients cannot be prevented as it is the case in the NuScale design.

CRediT authorship contribution statement

Jorge Sanchez-Torrijos: Conceptualization, Methodology, Software, Investigation, Writing – original draft, Writing – review & editing, Visualization. **Kanglong Zhang:** Software, Investigation, Resources, Writing – review & editing. **Cesar Queral:** Conceptualization, Methodology, Resources, Writing – review & editing, Supervision. **Uwe Imke:** Software, Investigation, Writing – review & editing. **Victor Hugo Sanchez-Espinoza:** Methodology, Investigation, Writing – review &

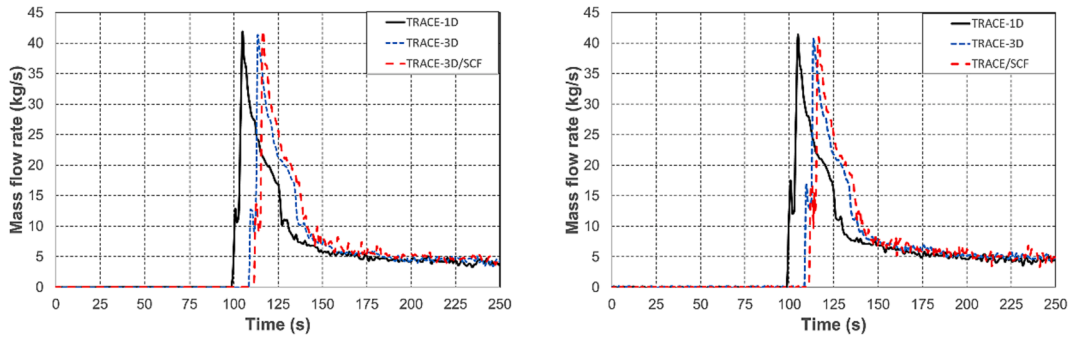


Fig. 19. DHRS1(left) and DHRS2(right) mass-flow rate.

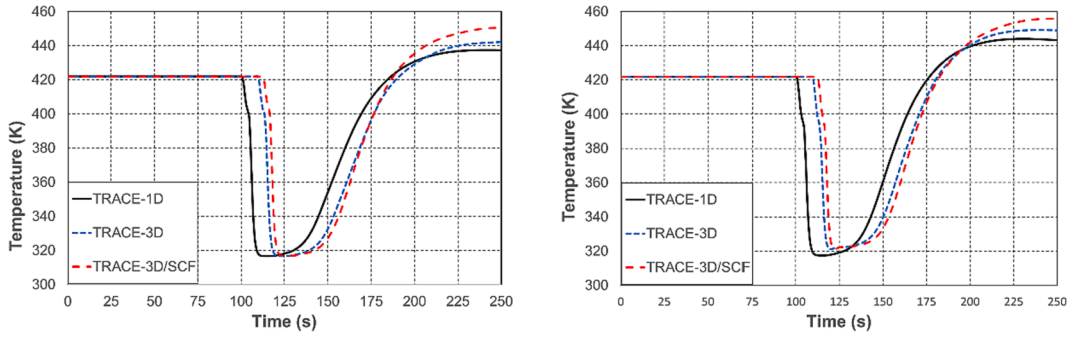


Fig. 20. SG1(left) and SG2(right) inlet temperature.

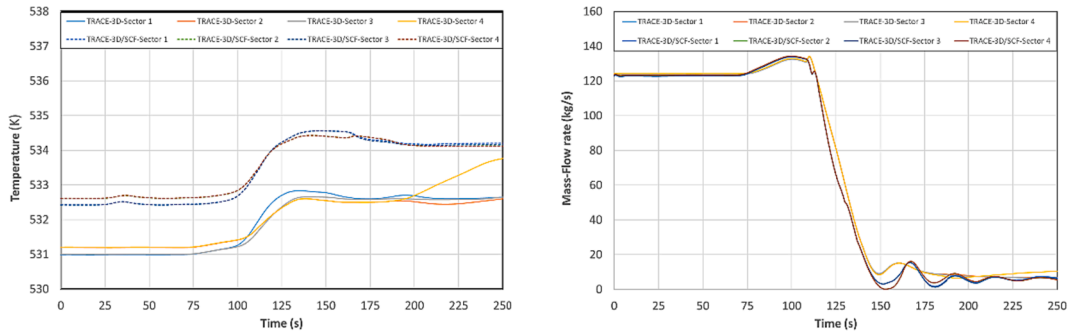


Fig. 21. Radial distribution of the temperature (left) and mass-flow rate (right) at the core inlet level during the transient.

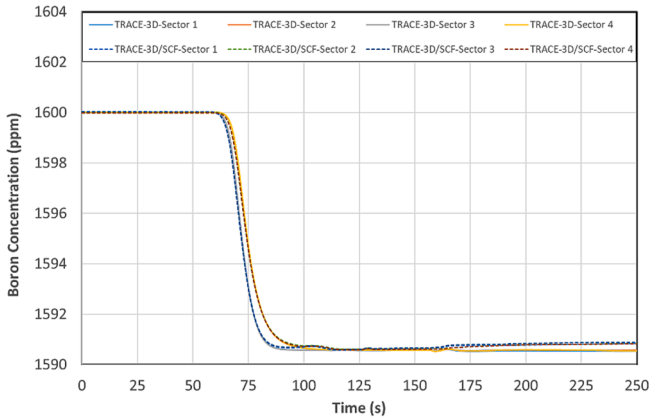


Fig. 22. Radial distribution of the core inlet boron concentration during the transient.

Table 4

Sequence of events in the simulation of the boron dilution transient.

Event	TRACE-1D	TRACE-3D	TRACE-3D/SCF
Boron Dilution begins	0	0	0
SCRAM set point	96.0	106.1	108.2
SCRAM (signal + 2 s delay):	98.0	108.1	110.2
Control rods begin to move			
Secondary side isolation:			
MSIVs/FWIVs begin to close			
DHRS actuation:			
DHRS actuation valves begin to open			
Max. pressure peak in primary side	101.7	111.4	110.0
MSIVs and FWIVs fully closed	103.0	113.1	115.2
CVCS isolation valves fully closed	105.0	115.1	117.2
Max. pressure peak in secondary side	122.0	131.7	132.5
DHRS valves fully open	128.0	138.1	140.2

editing, Visualization, Supervision.

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 authors do not have permission to share data.

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