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Multi-Scale Coupling of TRACE and SUBCHANFLOW based on ECI for the Analysis of 3D Phenomena inside the PWR RPV

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ABSTRACT

The paper describes the multi-scale coupling of a system code and a sub-channel code in order to better simulate the 3D thermal-hydraulics inside the RPV of Light Water Reactors. For this purpose, the TRACE code which is an advanced, best-estimate reactor system code developed by USA NRC and the sub-channel code SUBCHANFLOW (SCF) which is developed by KIT were selected. The coupling was implemented using the Exterior Communications Interface (ECI) which is originally designed to couple TRACE and other codes, TRACE and TRACE itself by forming a multi-task parallel system. ECI is already a highly integrated module in TRACE and a new specific ECI was designed for SCF. The coupling is composed of two elements: spatial and numerical coupling. The spatial coupling could be further divided into computational domain coupling and geometry coupling. A non-overlapping strategy was implemented to the domain coupling and a factor weighted method was adopted by the geometry coupling. The numerical coupling is classified to Steady State (SS) and Transient coupling. For both modes, data transfers perform between time steps, which are more or less an explicit way. For SS, SCF always runs SS steps and it could be activated or suppressed by TRACE according to the transferred data perturbation checking result. For Transient, two modes are available: step to step calculation and SCF step skipped calculation. TRACE and SCF run their steps sequentially under the step to step mode. While several SCF steps could be skipped by TRACE during the latter mode. Data from a VVER1000 coolant mixing benchmark were employed to verify the coupling system. The results obtained by TRACE standalone and the coupled system TRACE/SCF were compared with the experimental data which show that TRACE/SCF made considerable improvements in the prediction of the coolant temperature at the hot legs. Further tests on the special techniques for numerical coupling show that the computation resource cost could be significantly reduced while at the same time no impact on the numerical results were introduced.

KEYWORDS

MULTI-SCALE COUPLING, TRACE, SUBCHANFLOW, ECI

1. INTRODUCTION

Thermal hydraulic simulation tools are increasingly crucial in today's nuclear industry and researc h. Normally, they could be classified into three types based on the precision of their prediction o n specific physical problems: system code, sub-channel code and CFD code which corresponds to the simulation scale dimensions: macro scale, component scale and micro scale, respectively. Th e macro scale - system code runs very coarse meshes thus can catch the dynamic of the whole N uclear Power Plant (NPP) with acceptable computation resource cost. The component scale - sub-channel code is specially designed to predict flow phenomenon in reactor cores. Its grid density i s larger than that of system code thus can produce result with higher spatial resolution. On the ot her hand, it consumes more computation resources. The micro scale - CFD code is able to descri be the flow details locally with much better resolution. However, when simulations of large dimension are desired, numerous computational resources will be occupied due to its huge grid quantity.

In an attempt to balance the result precision and computational cost, the method of multi-scale thermal hydraulic simulation was put forward, which aims to concentrate on thermal-hydraulic details for specific parts of the Nuclear Power Plant (NPP) while at the same time to catch dynamics of the entire system. Lots of multi-scale simulation systems were developed over the last few decades. Such as MARS [1], RELAP-3D/COBRA-TF [2], TRACE/FLUENT [3], ATHLET/CFX [4] and ATHLET/COBRA-TF [5]. This paper describes a multi-scale system which is able to simulate thermal hydraulic phenomenon on both macro and component scales by coupling the system code - TRACE and the sub-channel code – SUBCHANFLOW (SCF) by the Exterior Coupling Interface (ECI).

2. CODES FOR THE MULTI-SCALE COUPLING

2.1. The System Code – TRACE [6]

TRACE is the abbreviation of TRAC/RELAP Advanced Computational Engine which is formerly called TRAC-M. It is the latest in a series of advanced, best-estimate reactor systems codes developed by USA NRC for analyzing neutronic thermal-hydraulic behavior in light water reactors. TRACE takes a component-based approach to modeling a reactor system. Each physical piece of equipment in a flow loop can be represented as some type of component. VESSEL is the special 3D component which can model the Reactor Pressure Vessel and other components in which 3D phenomena take place. The basic governing equation set of TRACE includes six equations which can simulate a full two-fluid hydrodynamic like the gas-liquid flow. In addition, two more equations are applied to describe the non-condensable gas field and to track dissolved solute. TRACE is able to run both SS and Transient calculations. Usually, TRACE runs in a typical serial mode. Nevertheless, TRACE could run in parallel by dividing the model into several sub-models and each of them will be simulated by one TRACE executable. This is a so called “multi-task” system. All the tasks run at the same time and communicate with each other through a specially designed Exterior Communication Interface (ECI).

2.2. ECI and the Concept of Multi-Task System

ECI was originally designed to disperse a single serial TRACE process to form a multi-task parallel system. It was also developed for the coupling of TRACE and other simulation codes, in a parallel way. Two different message passing mechanisms are available in ECI. One is shared memory (OpenMP is a typical shared memory model.), the other one is socket. Socket is normally the bottom level of all message passing mechanisms through network. The most famous MPI and PVM are all socket-based models. Socket endows the coupling system with quite flexible expansibility especially on distributed computational systems. Hence, the ECI Socket capability was selected. ECI is a highly integrated module in TRACE and is closely related to TRACE’s data flow and file structure. In order to implement the coupling, a new ECI was developed for SCF to reflect its data flow and file structure.

ECI couples codes together by implementing a multi-task system. As the name implies, it is a system composed of several tasks. The tasks communicate with each other through their ECIs. And each two of those tasks can directly exchange data with each other which indicates this is a server-less system (Figure 1). This is an unusual model from normal network communication models which usually include one server and several clients. Moreover, the coupled codes’ number is not limited and additional tasks could be conveniently merged into the system, which benefits from the socket model properties (In Figure 1, there are three TRACEs, more TRACEs and other codes could be easily included in the system on condition that their specific ECI has been well developed). Generally speaking, the generation of the multi-task system along with its coordination, synchronization and the inter-task communication, are all in the charge of ECI. In another words, the multi-task system is actually a concept, while ECI is the exact tool implementing the concept.

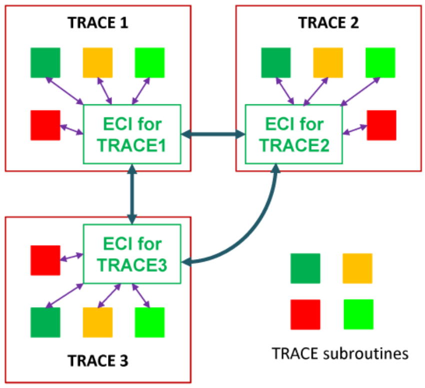


Figure 1 – Multi-task system

2.3. The Sub-Channel Code SUBCHANFLOW (SCF)

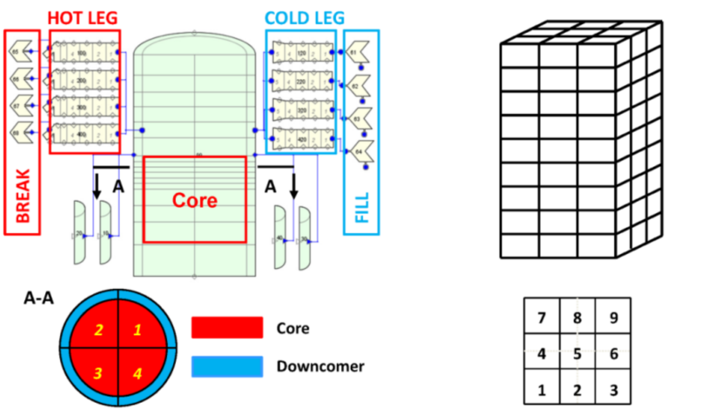
SCF is a thermal hydraulic sub-channel code which was developed at KIT-INR for the simulation of fuel rod bundles and cores of light water and innovative reactor systems. It is based on the COBRA-family, while the obsolete programming style was updated and refined with a modular Fortran-95 style. SCF can handle both rectangular and hexagonal fuel bundles and core geometries. Both SS and Transient calculations are available in SCF. It could utilize the OpenMP capability to perform calculations in parallel. What's more, SCF has already been successfully coupled to SALOME which is an open-source software providing a generic platform for pre- and post-processing for numerical simulation. SCF is able to simulate various coolant systems, including water (IAPWS 97), lead, lead-bismuth, sodium, helium and air. It has been validated against a wide range of test cases or benchmarks [7, 8].

3. DESCRIPTION OF THE COUPLING

The coupling involves two elements: spatial coupling and numerical coupling. The former solves the data translation between different meshes of TRACE and SCF. The latter manages the data passage between different data flow of TRACE and SCF.

3.1. Spatial coupling

In order to illustrate the spatial coupling vividly, a TRACE model which has four loops (Figure 2a) and a SCF model which has nine channels (Figure 2b) are proposed. Both of them are originally standalone models which are also the base models for the full section.



a. TRACE standalone model b. SCF standalone model

Figure 2 – TRACE standalone model and SCF standalone model

The spatial coupling is also composed of two elements: domain coupling and geometry coupling. The non-overlapping approach was adopted by domain coupling, in which, SCF simulates the core area in the vessel and TRACE is in charge of the rest (Figure 3). This is a much convenient and efficient way since TRACE can directly introduce the accurate influence from SCF to its domains. In order to implement the non-overlapping coupling, the original TRACE model should be properly modified (Figure 4). The core area in TRACE should be blocked and additional FILL and BREAK components should be added and connected to the core upper and lower boundary.

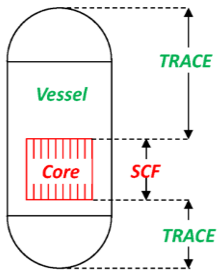


Figure 3 – Non-overlapping domain coupling

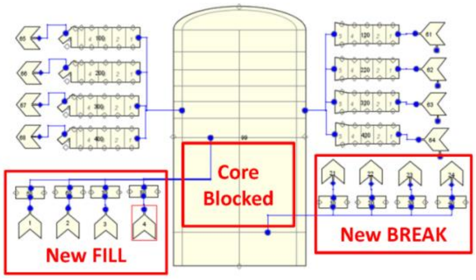


Figure 4 – TRACE model for coupling

Compared with TRACE model, there is nothing to change for SCF model. Nevertheless, new subroutines and logics should be merged into the source of both the two codes in order to get and put appropriate data from and to their data structure. Now the domain coupling was established (Figure 5). Two algorithms which relates to the interface-components were developed in order to enhance the flexibility and simplicity of the re-modeling process. First, the new BREAKs and FILLs could be flexibly attached to the VESSEL component with various combinations. Thus various flow scenarios at the two codes' junctions could be simulated. The second point is, TRACE could recognize those interface-components from normal ones automatically.

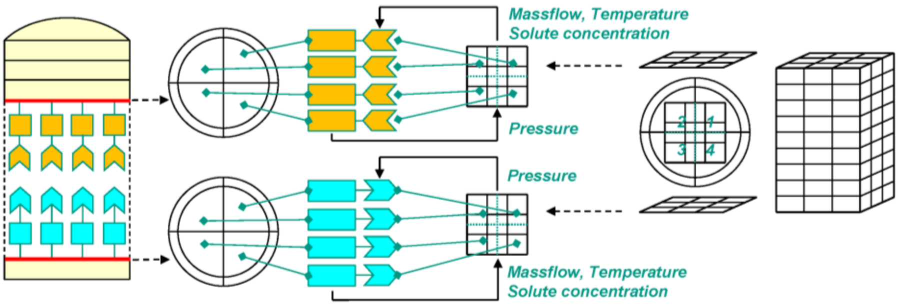


Figure 5 – Non-overlapping domain coupling of TRACE and SCF

Figure 5 also presents the positional correspondence of the TRACE sections and SCF channels. The complicated issue is that several channels may contribute to one section and several sections may also contribute to one channel in turn, according to their overlapping area proportions. It will become even more complicated when the cases include hundreds of channels or sections which could even have irregular areas, shapes and arrangement. A special algorithm and subroutine was developed to solve this problem. Take the model shown in Figure 6 for instance, SCF has 163 channels and TRACE has 16 core area sections. For the red-line marked channel, its data comes from four TRACE sections: 2, 3, 10 and 11, multiplied by their contribution proportions. The channel itself, in turn, contributes to the four TRACE sections as well. The contribution ratios from each SCF channel to each TRACE section are calculated based on their overlapping area and vice versa. All the data are automatically calculated and stored in two specially-designed arrays. This is an overlapping-area-weighted algorithm which could ensure the mapping process as accurate and handy as possible. This subroutine could also be employed by other applications.

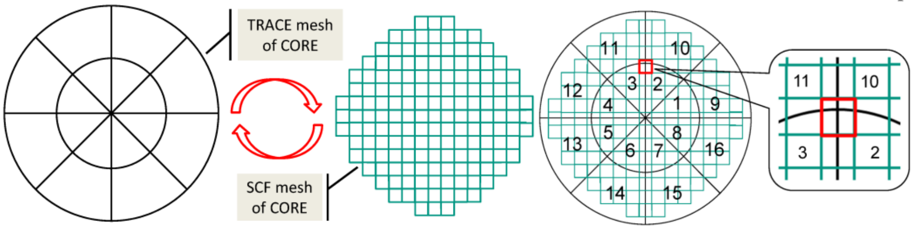


Figure 6 – Data translation between different mesh of TRACE and SCF

3.2. Numerical coupling

The coupling is some kind of an explicit way. Because data transfer is performed in unit of time-step. Two elements are included in this section: Steady-State (SS) and Transient (TS). For both of them, TRACE supervises the whole calculations. During SS, the SCF SS function will always be called at each time-step and the SCF TS function will be ignored. The entire SS calculation process is illustrated in Figure 7. First TRACE will run a SS iteration standalone and pass data to SCF once it converges. SCF then runs a SS step in sequence and pass data to TRACE. Next, TRACE moves a step forward and checks fluctuation of its data to SCF. If the fluctuation is over-criteria, TRACE will pass the data to SCF and permit SCF going on. Otherwise, TRACE will intercept the data transfer and suspend SCF until there is an over-criteria data fluctuation.

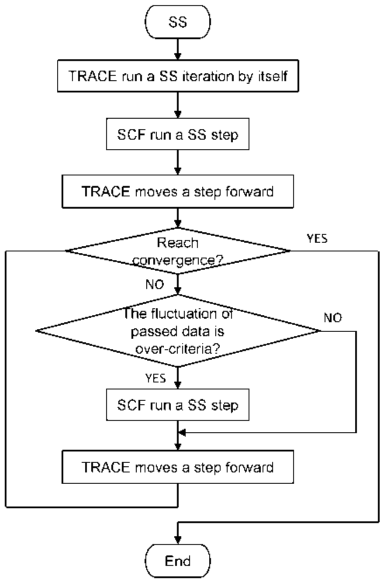


Figure 7 – SS calculation diagram of TRACE/SCF

As to TS calculation, there are two options available: step-to-step mode and step-skipped mode. TRACE and SCF will exchange data step by step in the former mode. Considering the fact that SCF normally take longer time for one time-step than TRACE and the latter may waste too much time on waiting. The step-skipped mode was proposed. Several SCF steps could be skipped by TRACE in this mode. The two schematics are shown in Figure 8. The two modes both run one TRACE and one SCF in sequence and reach point 2. Then, the step to step mode runs TRACE and SCF one by one while the SCF step skipped mode only runs TRACE. Up to point 3, Two SCF steps are skipped and the corresponding elapsed time is saved. Both of the two codes then run a SCF step reaching point 4. The process will be repeated until the calculation terminates.

The skipped steps number and length are automatically calculated by TRACE based on the two codes' current calculated time-step size. Normally, SCF could run with quite larger time-step size than TRACE. This is basically because SCF's equation set is implicitly solved while TRACE's is semi-implicitly solved. A large minimum time-step size could be pre-defined in SCF. When TRACE starts the step skipped trick, its time-steps' size will accumulate until the sum is equal or greater than the pre-defined SCF time-step size. Then SCF will adjust its time-step size to the TRACE sum and move one step forward. Accompanied with carefully selecting the data transfer point, a quite tight and precise synchronization scheme could be achieved for the coupling. Another point to note is that since there could be more than one TRACE involved in the coupling system, a special algorithm was developed to enable SCF automatically locate the VESSEL-occupied TRACE process and activate the duplex socket channel between SCF and the target TRACE, while keep other TRACE socket channels silent.

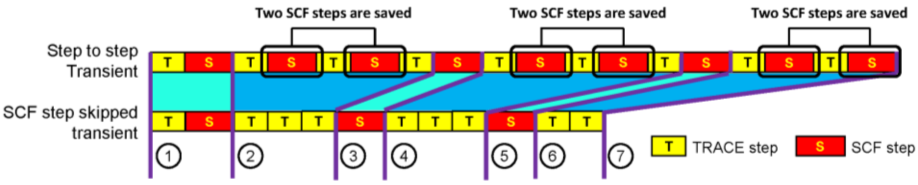


Figure 8 – Mechanism of the SCF step skipped trick in TRACE/SCF-IS transient

4. VERIFICATION OF THE MULTI-SCALE COUPLING SYSTEM

The data from a flow mixing experiment which was performed at Kozloduy NPP #6 in 2002 was selected to verify the multi-scale coupling system. The reactor is VVER-1000 whose sketch is shown in Figure 9. It has four loops and each loop is equipped with a steam generator and pump.

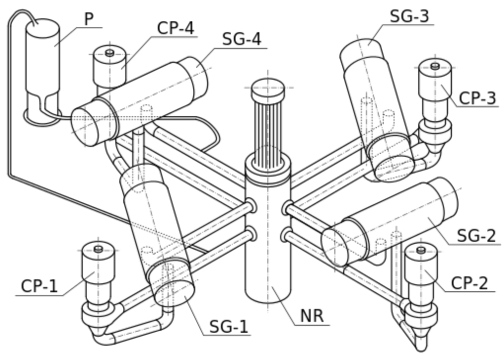


Figure 9 – Sketch of VVER-1000

4.1. Specification of the benchmark

The reactor core was at beginning of cycle conditions. All the equipment is under normal operation. Before the test, the total thermal power is 281 MW. Temperatures at the four hotlegs and coldlegs are around 541 K and 545 K respectively. During the test phase, the sequence of events is summarized in the following list.

1. Isolation of the steam generator (SG) of loop-1 and isolation of the SG from feed water.
2. Primary coolant temperature of loop-1 increase up to about 14 °C.
3. Coolant mixing first takes place in the downcomer region.
4. Coolant mixing in the lower plenum, core and upper plenum.
5. Temperature of the unaffected loops increased.
6. The test lasted for 1800s. At that time the power increased up to 286 MW.

4.2. Modeling

The VVER-1000 TRACE model for coupling is shown in Figure 10. There are four hotlegs and four coldlegs. Since TRACE doesn't simulate the core region, the core area in the vessel is blocked. A group of BREAK component and a group of FILL component are added and perform as the data transfer interface. Those FILL and BREAK components could be flexibly arranged and attached to the

VESSEL. TRACE can distinguish them from normal FILL and BREAK automatically. Figure 11 presents the sketch of TRACE model's profile.

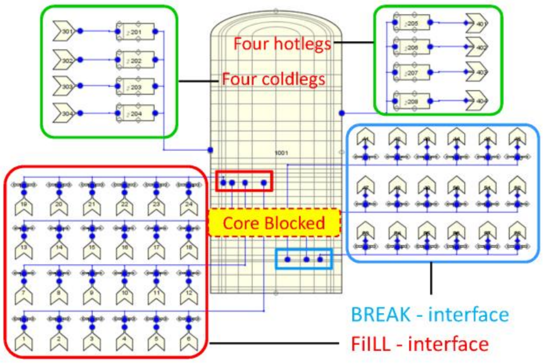


Figure 10 – VVER-1000 TRACE model for coupling

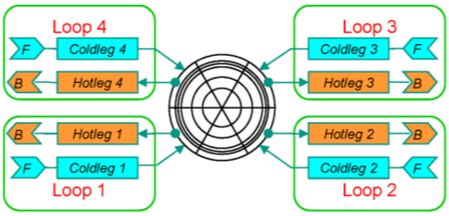


Figure 11 – Sketch of TRACE model's profile

The SCF model of VVER-1000 core is in unit of fuel assembly, which indicates one SCF channel represents one fuel assembly. The assemblies are hexagonal and hexagonally arranged in the core (Figure 12).

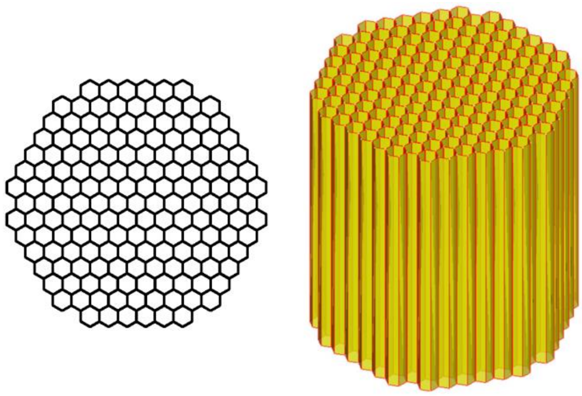


Figure 12 –VVER-1000 core

The boundary conditions of the coupling system were defined based on the experimental data of the benchmark. Moreover, only the TRACE boundary conditions need to be defined because SCF's boundary conditions come from TRACE directly.

4.3. Results and analysis

There are three data sets available: experimental data, result of TRACE standalone and result of the coupling codes. The coldlegs' temperatures of the three are basically identical because the numerical inlet boundary condition was just extracted from the experimental data. However, situation is quite different at hotlegs. Figure 13 – 16 present the temperature curves at the four hotlegs. It is obvious that the TRACE-SCF coupling codes make a remarkable improvement at the temperature prediction of hotleg 1 and 4, compared with TRACE standalone (the coupling code's curves locate more close to the experimental curves than that of TRACE standalone). The downside is that the coupling codes' result at hotleg 2 and 3 are still as poor as TRACE standalone. This could be due to the existence of additional TRACE sections between loop 2 - loop 3 and loop1 – loop4 (Figure 11). Nevertheless, the multi-scale system was already proved better than TRACE standalone.

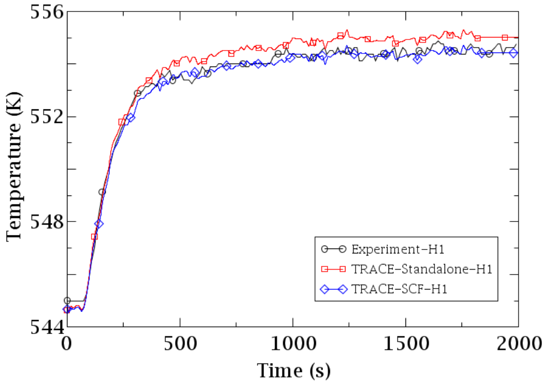


Figure 13 – Temperature at hotleg 1

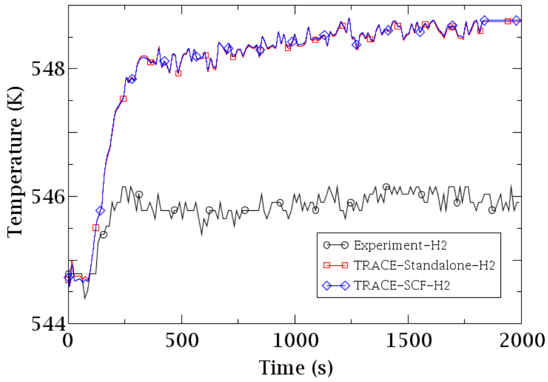


Figure 14 – Temperature at hotleg 2

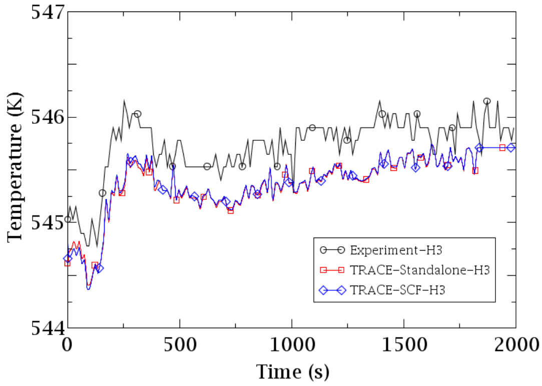


Figure 15 – Temperature at hotleg 3

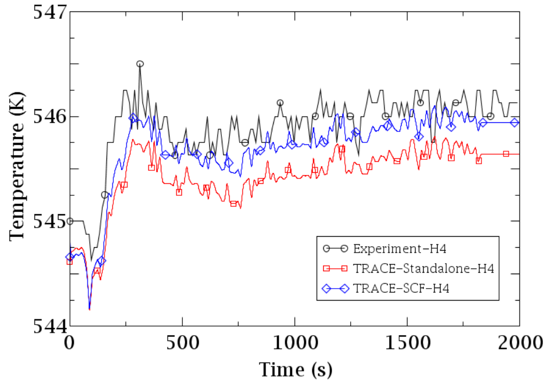


Figure 16 – Temperature at hotleg 4

In section 3.2 it has mentioned, several technics were developed aiming to save computation resource costs. Their validity and efficiency have to be tested. Above all, the validity is the key issue to be verified, which means the calculation with the technic must not produce significant bias from the normal calculation. In this premise, the technics should be proved efficient enough to cut computation resource cost. Here TS computation is the emphasis of the testing since SS don't have a reference substance. Figure 17 – 20 present the hotleg temperature curves obtained by different TS mode. One is the step to step mode. The second is SCF step skipped mode with a SCF pre-defined minimum time-step size of 0.5s. The last is SCF step skipped mode with a SCF pre-defined minimum time-step size of 1.0s. It can be observed that the three sets of data are almost the same which indicates the step skipped mode behaves as well as normal step to step mode. One more conclusion could be made is that The SCF time-step size has no significant effect on the final results. However, the criterion is, it could have large value but must be small enough to cover the real transient details.

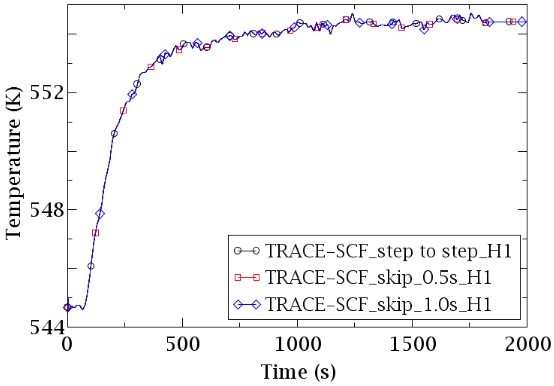


Figure 17 – Temperature at hotleg 1

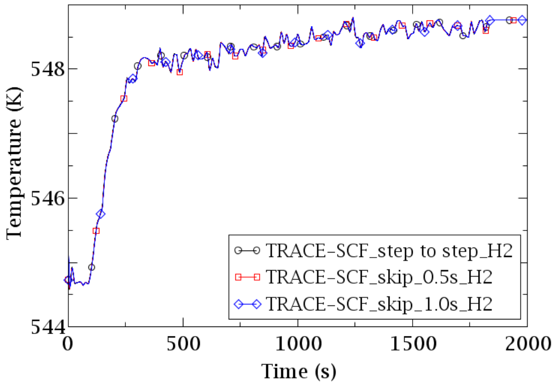


Figure 18 – Temperature at hotleg 2

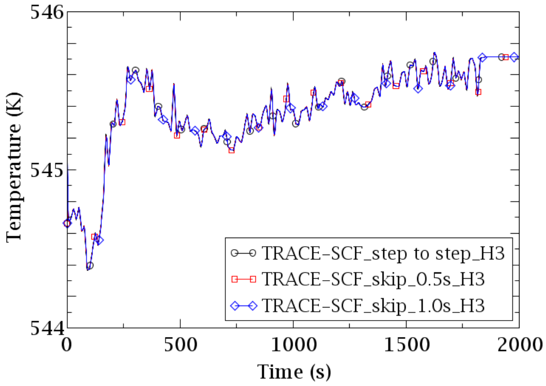


Figure 19 – Temperature at hotleg 3

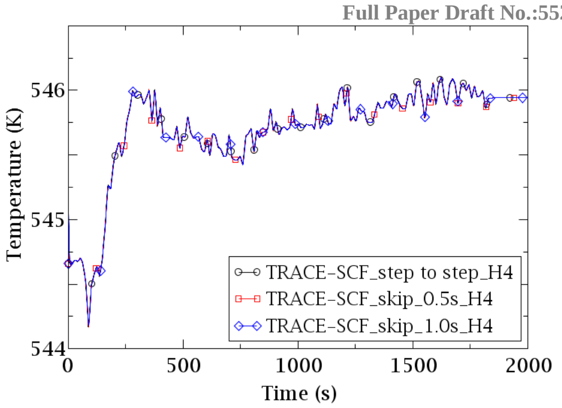


Figure 20 – Temperature at hotleg 4

Figure 21 presents the computation resource cost comparison of different modes. The definition of the bar titles are explained in Table 1. The information of hardware and software are:

1. Operating System and version: Debian GNU/Linux 8.
2. Software title and version: TRACE V5.1051 and Subchanflow 3.3.
3. Hardware information: Processor – 48 Intel(R) Xeon(R) CPU E5-2697 v2 @ 2.70GHz, installed memory (RAM) – 378 GB, System type – 64 bit.

TRACE standalone took around 1h15min to run the testing case. When coupled SCF to the system, the elapsed time increased dramatically to more than 12 hours, which implied SCF took up the majority of the cost. There would be a significantly elapsed time decrease down to 4h30min when SCF's OpenMP was activated and 8 cores were assigned to SCF. However, the cost is still high. The step-skipped mode gives out a better solution, whose elapsed time dramatically decreased to 2h3min and 1h45min when SCF time-step is pre-defined to 0.5s and 1.0s respectively. The efficiency of the time-step skipped technic was thus proved pretty good with 83% elapsed time cut, compared with step to step mode.

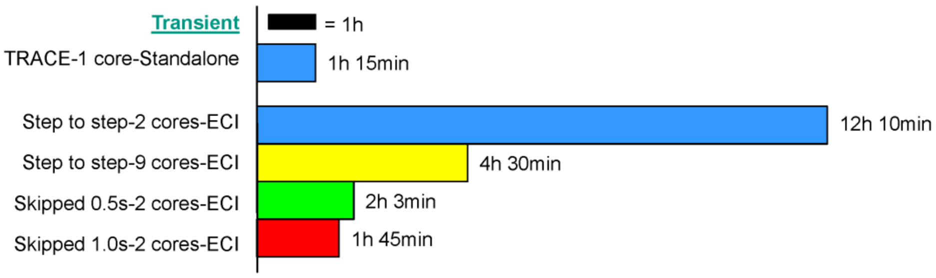


Figure 21 – Computation resource cost of different modes

Table 1 – Definition of the bar title of Figure 26

Bar title	Mode	Occupied cores	OpenMP?	Serial/Parallel
TRACE-1 core-Standalone	None	1	No	Serial
Step to step-2 cores-ECI	Step to step	2	No	Parallel
Step to step-9 cores-ECI	Step to step	9	Yes	Parallel
Skipped 0.5s-2 CORES-ECI	Step skipped	2	No	Parallel
Skipped 1.0s-2 CORES-ECI	Step skipped	2	No	Parallel

5. CONCLUSIONS

A multi-scale coupling system which involves TRACE and SCF and based on ECI was implemented and verified. The two elements of the coupling: spatial and numerical coupling were explained. For spatial coupling, the non-overlapping domain coupling and the factor weighted geometry coupling were illustrated with an example. For numerical coupling, the SS and TS modes were explained. The special technics which aim to save computation resource cost are also introduced. The coupling system was verified with data from a VVER1000 coolant mixing benchmark. The results show that the coupling is correctly implemented and perform better than TRACE standalone. The special technics were also well tested and proved pretty good validity and efficiency.

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