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APPLICATION OF THE COUPLED CODE ATHLET-QUABOX/CUBBOX FOR THE EXTREME SCENARIOS OF THE OECD/NRC BWR TURBINE TRIP BENCHMARK AND ITS PERFORMANCE ON MULTI-PROCESSOR COMPUTERS

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Abstract

The OECD/NRC BWR Turbine Trip (TT) Benchmark [1] is investigated to perform code-to-code comparison of coupled codes including a comparison to measured data which are available from turbine trip experiments at Peach Bottom 2. This Benchmark problem for a BWR over-pressure transient represents a challenging application of coupled codes which integrate 3D neutron kinetics into thermal-hydraulic system codes for best-estimate simulation of plant transients. This transient represents a typical application of coupled codes which are usually performed on powerful workstations using a single CPU. Nowadays, the availability of multi-CPUs is much easier. Indeed, powerful workstations already provide 4 to 8 CPU, computer centers give access to multi-processor systems with numbers of CPUs in the order of 16 up to several 100. Therefore, the performance of the coupled code ATHLET-QUABOX/CUBBOX on multi-processor systems is studied. Different cases of application lead to changing requirements of the code efficiency, because the amount of computer time spent in different parts of the code is varying. This paper presents main results of the coupled code ATHLET-QUABOX/CUBBOX for the extreme scenarios of the BWR TT Benchmark together with evaluations of the code performance on multi-processor computers.

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Introduction

The main goal of the OECD/NRC BWR Turbine Trip (TT) Benchmark [1] is to validate best estimate coupled code systems with integrated 3D neutron kinetics by comparing solutions with measured plant data. As an extension of the BWR turbine trip transient additional hypothetical extreme scenarios were defined for the purpose of code-to-code comparison. GRS results for the BWR TT Benchmark obtained with the coupled code system ATHLET-QUABOX/CUBBOX [2,3] of the Exercises 1 and 2 are presented in [4] and the results for Exercise 3 in [5].

The specification of the BWR TT Benchmark provides the geometric data and the operational conditions of the Peach Bottom 2 nuclear power plant. Complementary to the Exercises of the BWR TT Benchmark analyzing in three steps the reactor core and the plant behaviour, a set of hypothetical extreme cases is formulated. The first extreme case is the postulated TT transient without bypass system relief opening; the second one is TT without reactor scram initiation (ATWS) and the third is the combined scenario – turbine trip with bypass system relief failure and without reactor scram. The extreme case 4 with postulated failure of relief valves was already presented in [5]. All the extreme cases are calculated by coupled code systems with integrated 3D neutron kinetics for testing the code coupling and feedback modelling under extreme conditions.

These extreme scenarios of Exercise 3 and for comparison two calculations for Exercise 2 of the BWR TT Benchmark are used to discuss the performance of the coupled code ATHLET-QUABOX/CUBBOX on multi-CPU computers and to evaluate the capability of code parallelization. For this purpose the software standards of parallel programming are briefly reviewed. As starting point for the stepwise code parallelization a detailed analysis of code performance of ATHLET-QUABOX/CUBBOX is performed for the Benchmark calculations to identify those sections of code which are most effectively executed in parallel mode.

Plant configuration and scenarios for the extreme cases

The ATHLET model of Peach Bottom 2 NPP (Fig.1) consists of a nodalisation describing the primary circuit with two external symmetrical recirculation loops, the reactor vessel with a lower plenum, a core region with the specified 33 thermal-hydraulic channels (THC), one core bypass channel, an upper plenum, stand pipes, a separator and a steam dome. The downward flow path in the reactor vessel is modelled by an upper down comer section, where the feed water is supplied, the jet pumps and a lower down comer section with the diffusors. The flow path of the steam to the turbine is modelled by the main steam line pipe with the turbine stop valve (TSV) at the end and the connected bypass line with the turbine bypass valve (TBV). As the transient is initiated by a sudden closure of the turbine stop valve pressure wave oscillations appear on the steam line that requires a detailed description. The total length of the main steam line is 133 m. The bypass line of 74.8 m length is connected to the steam line 9 m before the TSV. The location of the three groups of relief valves (RV) and the safety relief valve (SRV) is chosen to be 10 m downstream from the reactor vessel on the main steam line. A linear discharge characteristic of the RV and SRV has been defined, for example for RV number 1 at P=7.95 MPa (103% of set pressure) a mass flow rate of G=103.19 kg/s is assumed. The core model represents the coolant flow by parallel flow channels without cross-flow. A fuel rod model, solving the heat-conduction equations with 5 radial zones for the fuel pellet, a gap heat resistance and a single zone for the cladding, is attached to each THC. Three types of THCs are defined corresponding to 7x7 fuel assemblies and 8x8 fuel assemblies with and without flow restriction. The values of flow area, fuel rod diameter and flow resistances are determined according to the specification. In the ATHLET code the 5-equation model is used solving the fluid dynamic conservation equations. The 3D neutron kinetics code QUABOX/CUBBOX solves the neutron diffusion equations for two energy

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groups by a coarse mesh method based on neutron flux expansion by local polynomials. Each fuel assembly of the BWR core is represented by a single node in the X-Y plane, totally 764. The core loading of the fuel assemblies and the position of control rods correspond to the specification. In axial direction, the active core region is described by 24 nodes with one additional node for each of the top and bottom reflector. The nuclear cross-sections are calculated from the specified tables dependent on fuel temperature and coolant density. The effect of the fuel assembly bypass flow is considered using an effective coolant density correction when calculating nuclear data. The effect of the Xenon concentration on the cross-sections is taken into account as specified. No ADF corrections are considered, in consistency with the solution method of QUABOX/CUBBOX based on local neutron flux expansion. Each THC and the corresponding fuel rod is mapped to a group of fuel assemblies of the core loading as specified (Fig.2).

The hypothetical transients being analyzed is a turbine trip at 62% power with additionally postulated failures. The transient is determined by the following sequence of events. It begins at t=0 s with the sudden closure of the turbine stop valve, which is fully closed after 0.096 s. In extreme cases 1 and 3 the steam bypass valve remains closed, for case 2 it begins to open at 0.060 s reaching the final fully open position at 0.846 s. Reactor scram is considered only for case 1, and it takes place at the specified time of 0.75 s.

Results of the three extreme scenarios

For the extreme case 1 the ATHLET-QUABOX/CUBBOX calculation reaches the power maximum of 620 % at 0.722 s (Fig.3) before power reduction due to the scram initiation at 0.750 s. The sudden closure of the turbine stop valve causes a reduction of the steam flow, which results in a pressure increase. In addition, it initiates a pressure wave travelling along the steam line which is superposed to the pressure increase. The pressure increase is limited by the steam release through the RVs (Fig.4). The RV 1 opens at 2.8 s and remains open till 6.98 s while RV 2 and 3 open with 1 s delay after the RV 1 and stay open less than 1.4 s. After the scram the reactor remains sub-critical.

For the second extreme case (Fig.3) the power maximum (420 %) is reached at 0.718 s (like by the best estimate scenario [5]) and due to the strong negative void reactivity the power is reduced to the initial level. Due to the absence of a scram and due to the pressure increase, the power continues to oscillate at a level of 180% and decreases after depressurization at 4.5 s because of reaching the opening pressure set point of relief valves. Like in the first case, the RV 1 opens first and afterwards RV 2 opens for about 2.3 s (Fig.5). RV 3 remains closed. After 7 s the reactor power stabilises at a power level of 140 % and the reactor has still an excess reactivity of 0.0003 dk/k.

For the extreme case 3 the amplitude of the first power peak is the same as for case 1, but the absence of a scram and also the failure of opening of the bypass valves cause higher second and third power peaks compared to case 2 (Fig.3). Within a shorter time the opening pressure set points for all three relief valves are reached. RV 1, 2 and 3 remain open during the 10 s transient (Fig.6) and the power is stabilized again at a level of about 140 %.

Status of parallel programming

The approach to make simulation codes more efficient by using multi-CPU computers or parallel programming has a long history. It is accompanied by a continuous speed-up of single CPU efficiency, which made workstations and also PCs from year to year faster, contributing in this way to the speed-up of simulation codes without any programming effort. In the initial or pioneering phase of parallel programming, it was obligatory to apply dedicated software libraries to organize the initialization, the data exchange and the synchronization of multi-CPUs. In addition, the software was related to particular hardware configurations excluding the portability of codes. These conditions constituted a strong disadvantage for efficient software development.

Nowadays, the situation has changed, because the software tools for parallel programming are much mature. New standards like OpenMP and MPI have been established which support parallel programming for languages like FORTRAN90 and C, C++. The support of FORTRAN is important, because main simulation codes in the nuclear field as in other fields have been developed using this language. Both codes, the system code ATHLET as well as the 3D neutron kinetics model QUABOX/CUBBOX are written in FORTAN. Due to regular up-dates they can be compiled by current FORTRAN90 compiler versions. The new parallel programming model is using directives in the source code which give the compiler the necessary information about the code structure and the code sections where the compiler can generate parallel processes or threads to distribute the calculation tasks on multi-CPUs. These directives support the fork and join of the program control flow as well as the definition of the private and the global data variables.

It is well known that the greatest success of parallel programming can be achieved for simulation codes fulfilling particular requirements. In general, most of the computing time should be spent in a few subroutines of the numerical solution algorithms. If these subroutines or the corresponding task is well suited for parallel execution, the computing time can be strongly reduced and a high gain factor of computing time is achieved. An example of parallelization of a discrete ordinate method is presented in [6]. The structure of coupled codes doesn't fulfil this requirement. Nevertheless, it is worth to study carefully the performance of such type of codes on multi-CPU computers, because their use will be made easier and more practical if the computing time can be further reduced.

Profiling of the coupled code system ATHLET-QUABOX/CUBBOX

Before analyzing the code performance, the approach of the code coupling is briefly described. Detailed information about coupling considerations and the definition of the interface between both codes is documented in [2]. The coupling of the fluid dynamic system code ATHLET and the 3D neutron kinetics code QUABOX/CUBBOX is based on the principle that the coolant flow in the primary circuit including the core region as well as all components like main coolant pumps and valves are modelled by ATHLET objects, and the power generation in the reactor core is calculated by QUABOX/CUBBOX solving the time-dependent neutron diffusion equations. Generally, the time-dependent solution is generated by solving the fluid dynamic conservation equations, the heat-conduction equations and the equations of ATHLET components for a time-step using the power density distribution from the begin of the time-step. After terminating the integration of ATHLET model equations, the new power density distribution for the end of the time-step is determined by solving neutron diffusion equations taking into account the coolant conditions, i.e. coolant temperature, coolant density and boron concentration, and the fuel rod temperatures as calculated by ATHLET. So both codes are coupled in a serial manner. The size of the time-step is controlled such, that the delay between thermo fluid dynamic parameters and neutron kinetics parameters is acceptable. In this coupling approach both codes remain independent as far as possible, the necessary data exchange is performed by specific interface subroutines.

The analysis of the coupled code ATHLET-QUABOX/CUBBOX in view of the computing times is performed for three examples which represent typical cases of coupled code applications. The

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example 1 and 2 are models of the BWR-TT core calculations of Exercise 2, modelling the thermal hydraulic feedback with 33 THCs as proposed in the specification and for comparison with 764 THCs using a 1:1 mapping between fuel assemblies of the core loading and the THCs describing the feedback. The example 3 corresponds to example 1 with 33 THCs in the core region including the whole plant model as it was applied for the extreme cases.

For these examples the relative fraction of total computing time of each subroutine is determined by profiling options of the compiler and tools evaluating the simulation run. The main results of this analysis are summarized in Table 1.

Table 1 Relative fraction of total computing time of the coupled code ATHLET-QUABOX/CUBBOX for three cases of applications

	Exercise 2 3D core model		*Exercise 3* 3D core model and plant model
Number of THC in the core model	33 THC	764 THC	33 THC
Number of subroutines for 90% fraction of computing time	12 subroutines, only from QUABOX-CUBBOX	50 subroutines, both QUABOX-CUBBOX and ATHLET subroutines	16 subroutines, mainly QUABOX-CUBBOX subroutines, only one subroutine from ATHLET contributing less than 2%
QUABOX/CUBBOX calculation of nuclear cross-sections	70.2%	29.4%	65.1%
QUABOX/CUBBOX solving neutron diffusion equations	17.6%	7.7%	16.0 %
Matrix decomposition	9.6%	4.0%	8.6%
Coefficients of neutron flux approximation	8.0%	3.7%	7.4%

As integral information, it is indicated how many subroutines contribute to the 90 % fraction of the total computing time. It can be seen that for both cases with 33 THCs of the feedback model, the computing time is mostly spent in QUABOX/CUBBOX subroutines solving the neutron kinetics problem. This is only slightly affected when the whole plant model is included, whereby only one ATHLET subroutine contributes more than 2% of the total computing time. In case of example 2, the core model using 764 THCs, about 50 subroutines contribute to the 90% fraction of total computing time. This great number of subroutines can be further classified: only 16 subroutines contribute more than 1%, from these, only three ATHLET subroutines have a relevant contribution in the order of 2% to 5%. The other subroutines contribute less than 1% each, mostly less than 0.6%.

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It is concluded that a more detailed subdivision is only needed for the 3D neutron kinetics model QUABOX/CUBBOX. The relative fraction of computing time is determined for two main solution steps, namely 1) the calculation of nuclear cross-section values for each node from cross-section libraries which describe the dependence on feedback parameters, 2) the solution of neutron diffusion equations. This second task is further divided into steps solving neutron diffusion equations by matrix decomposition and calculating coefficients of neutron flux approximation for each node. The evaluation shows: The relative fraction of time for cross-section calculation is in the order of 70% to 65% for the core models using 33 THCs, this relative fraction is reduced to about 30% for the core model using 764 THCs. The effort for solving neutron diffusion equations corresponds to 17.6% and 16% for the core model using 33 THCs, but only about 8% for the core model using 764 THCs. The analysis of computing times shows that the relative fraction of various tasks strongly varies with the application. A clearly identified task with a high contribution under all conditions is found only in the task calculating the nuclear cross-section values.

The corresponding two subroutines calculating the nuclear cross-section values in QUABOX/CUBBOX were adjusted by OpenMP directives for parallel execution. A speed-up for this part of the code by a factor of 2.5 was achieved using 4 CPUs. The advantage of the available software standards for using multi-CPUs is seen that they can be applied in a step by step approach. On the other side, the analysis performed shows the restriction by the code structure, which limit the gain of efficiency to relatively low values.

Conclusions

The presentation describes the results of the coupled code system ATHLET - QUABOX/CUBBOX for three hypothetical extreme cases of the BWR TT Benchmark. The results allow a consistent comparison of codes in view of physical effects and modelling features under severe conditions. The 3D neutron kinetics integrated in coupled codes give the possibility to calculate precisely the reactivity changes and the local parameters relevant for safety evaluations. The BWR TT Benchmark is an important contribution to the validation of coupled code systems. These typical applications were used to evaluate the code performance of ATHLET-QUABOX/CUBBOX on multi-CPU computers. The analysis demonstrated that the code performance is strongly dependent on the application problem, because the ratio of computing time for the fluid dynamic part and neutron kinetics part is varying. In most cases, the solution of neutron diffusion equations needs up to 90% of total computing time. A reduction for this neutron kinetics part is observed only for cases using a very high number of thermal hydraulic channels modelling the feedback effects in the reactor core. Therefore, the parallel programming is most effective for the neutron kinetics part. The solution steps for this part were evaluated in detail. The task of calculating the nuclear cross-sections was identified as the task requiring the highest fraction of total computing time for all examples studied. The gain factor of computing time by parallising the cross section calculation is estimated in the order of 2 to 3. Generally, the analysis shows that coupled codes like ATHLET-QUABOX/CUBBOX are not very well suited for parallel programming. Nevertheless, the new software standards allow the use of multi-CPU computers for these simulation codes with a minimum effort of programming and the gain in computing time makes the use of such coupled codes easier and more practical for safety analysis.

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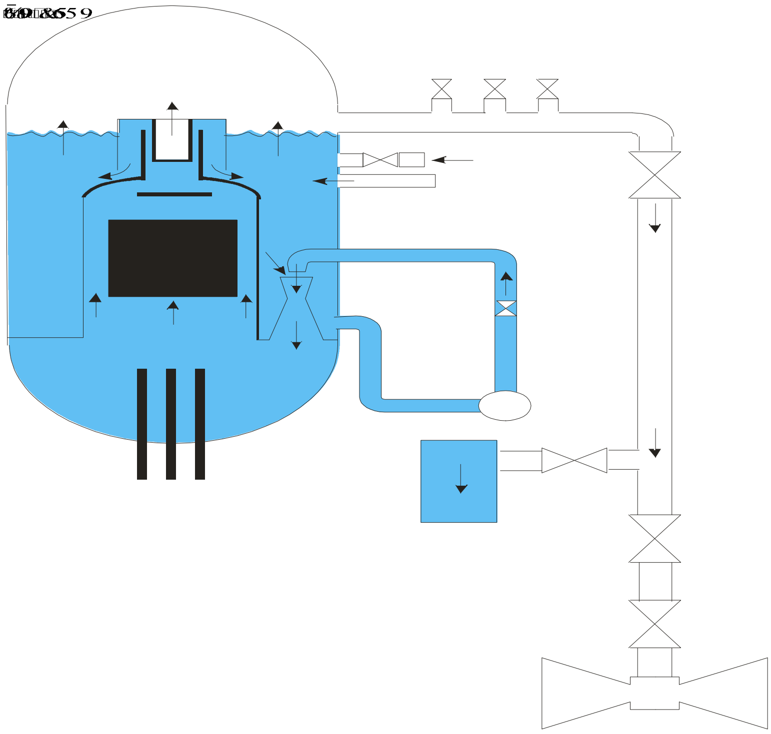

Fig. 1 Scheme of BWR Peach Bottom 2 NPP

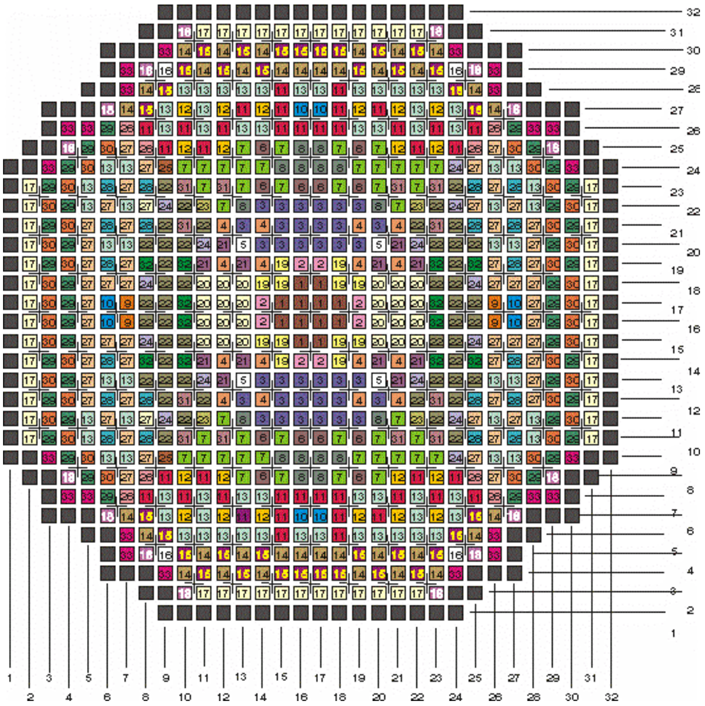

Fig. 2 Specified 33 thermal-hydraulic channel mapping scheme

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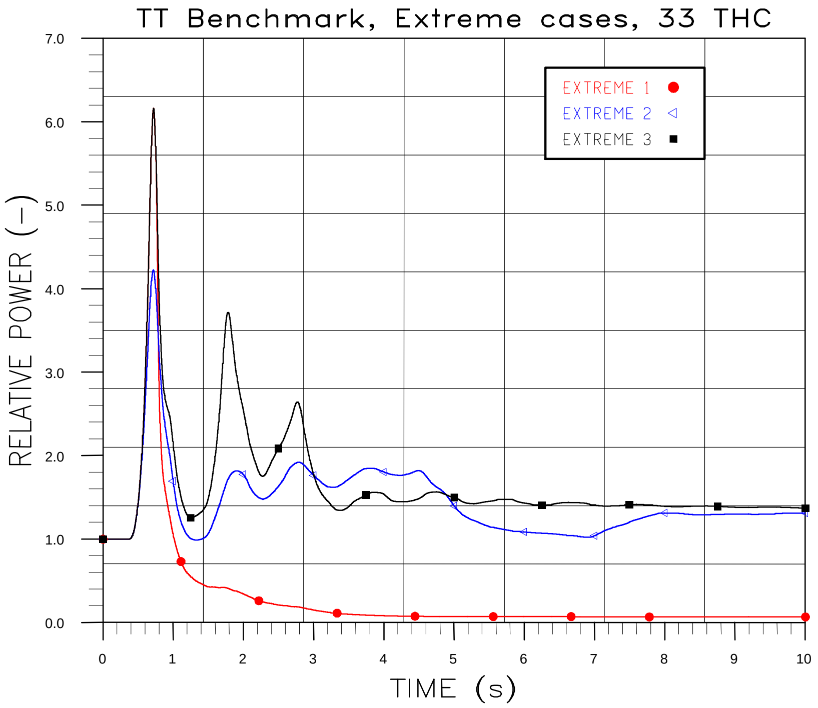

Fig. 3 Power history for extreme cases 1,2 and 3

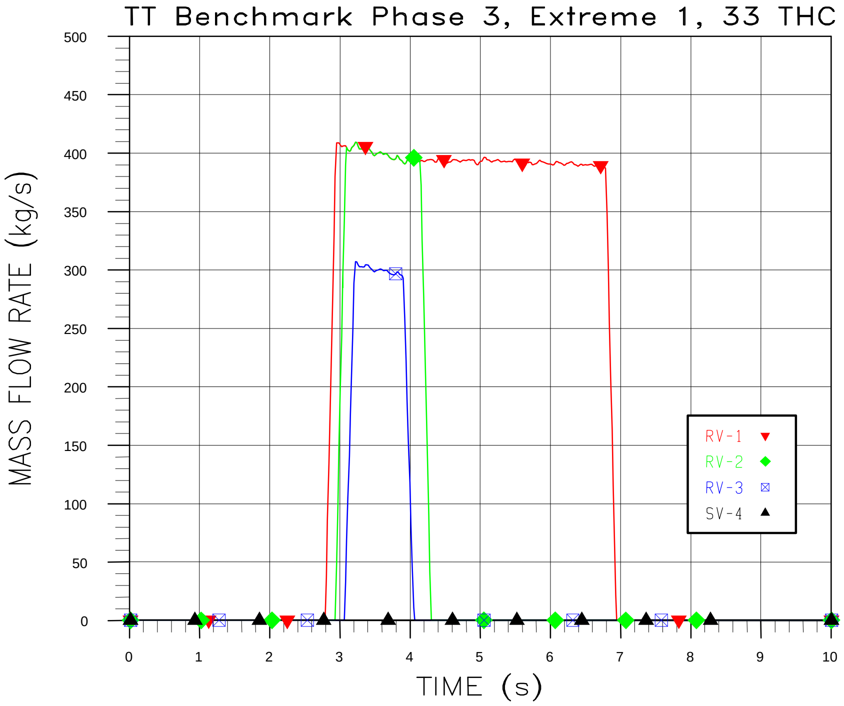

Fig. 4 RV and SRV mass flow rates for extreme case 1

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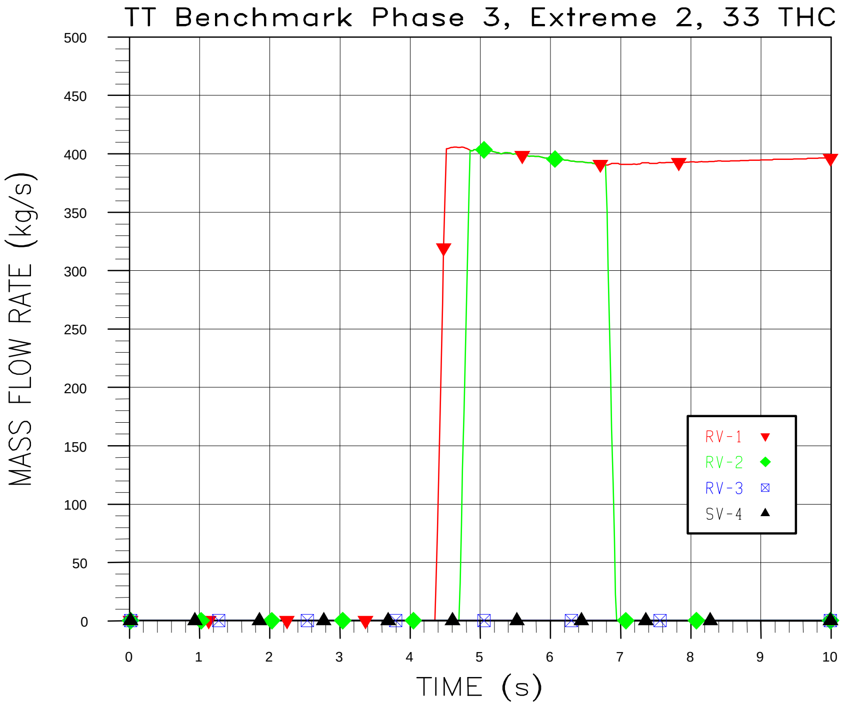

Fig. 5 RV mass flow rates for extreme case 2

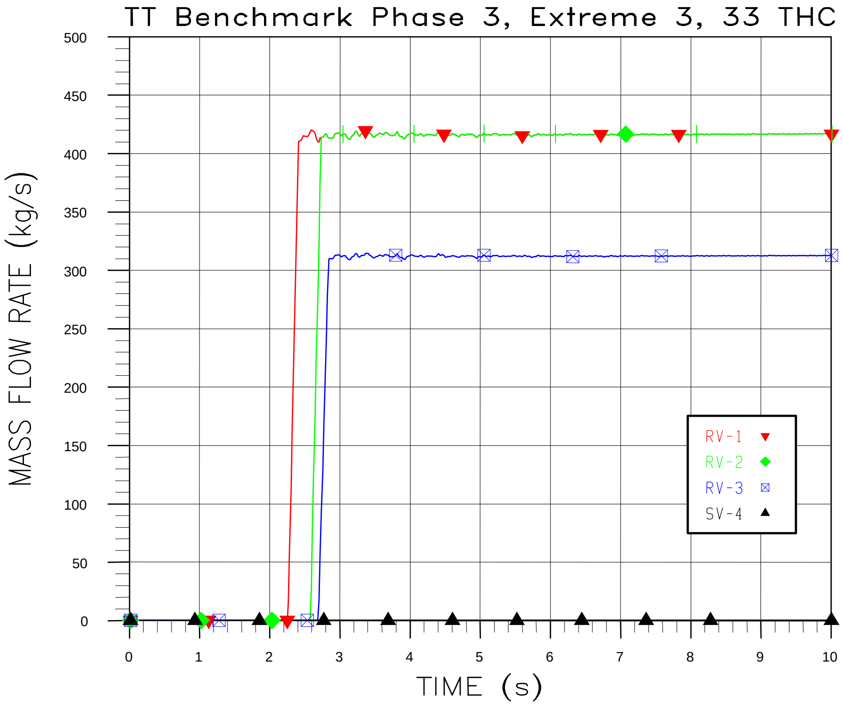

Fig. 6 RV mass flow rates for extreme case 3