RESEARCH REPORT

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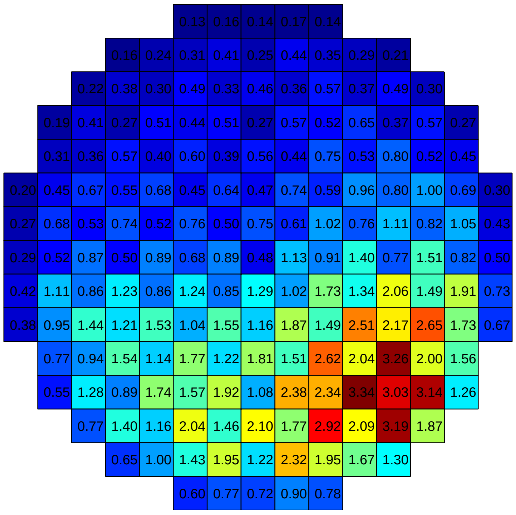

SAFIR2010/TRICOT

TRAB-3D Validation through comparison calculations with TRACE/PARCS

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Confidentiality: Public

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Summary

This report describes the work done in the TRAB-3D validation subtask of the SAFIR2010/TRICOT project. The work consists of three international benchmark excercises that were recalculated with VTT's own TRAB-3D reactor dynamics code and US NRC's TRACE/PARCS coupled neutronics/thermal hydraulics code.

The results show good agreement, and as expected, there seems to be no significant source of uncertainty rising from the 3D neutronics solution in transient calculations.

A second motivation to this work was to gain some experience in the use of the TRACE/PARCS code at VTT, as it can be a major tool for independent analyses for the regulator in future.

Confidentiality	Public

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Contents

1 Introduction

The 3D reactor dynamics code TRAB-3D[1] has been developed at VTT during the FINNUS, SAFIR, and SAFIR2010 public research programmes. The validation history has included calculating international benchmark exercises, as well as real plant transients at Finnish nuclear power plants[2].

Normally, when calculating international benchmark exercises, each participant uses only their own computer code and input decks that they have made according to the benchmark specifications. This leaves always some room for interpretation and even misunderstandings. An individual participant can never know the exact details of the calculation performed by another participant.

Through the CAMP agreement with the United States Nuclear Regulatory Commission (NRC), VTT has the possibility to use the thermal hydraulics and system simulating computer code TRACE[3], which is presently the main tool endorsed by the NRC for nuclear reactor analysis, replacing the older codes RELAP and TRAC. Concerning 3D neutronics calculations, TRACE now includes the Purdue Advanced Reactor Core Simulator (PARCS[4]) as an integral part (a static library) of the TRACE package. Coupled TRACE/PARCS calculations are relatively easy to perform, at least compared to the earlier RELAP-5/PARCS coupling realized using the parallel virtual machine (PVM) method, in which two codes had to be executed simultaneously with online data exchange. Standalone PARCS code with its own simple thermal hydraulics models is available for CAMP members as well.

PARCS is a three-dimensional reactor core simulator, developed at Purdue University, which solves steady-state and time-dependent multi-gorup neutron diffusion and SP3 equations. PARCS can be used for orthogonal and hexagonal core geometries. Normally, for reactor transient calculations, two-group neutron diffusion equations are solved using a two-level hybrid technique, which alternates between an advanced nodal solution and a finite difference solution during the iteration process. This is not unlike the HEXBU method used in TRAB-3D[5].

The availability of TRACE/PARCS opens new possibilities for TRAB-3D validation. Exactly the same problems can now be calculated with two computer codes by a single user, and input files directly compared by the same user, in order to minimize the modeling differences. Fortunately, the developers of both codes have participated in the same OECD NEA benchmark activities, and ready input data exists for some cases.

Besides TRAB-3D validation, this work is motivated by getting familiar with and gaining some experience on TRACE/PARCS 3D transient calculations. TRACE has probably a significant role as an independent analysis tool for the regulator STUK in future.

The work described here has been done in the TRICOT project of the SAFIR2010 research programme, and concentrates on the core neutronics module PARCS. The system and thermal hydraulics features of TRACE are being studied e.g. in the THEA project.

The first part of the work was to identify the possible comparison cases for TRAB-3D and TRACE/PARCS, and get the already existing input files for TRACE/PARCS. This was done by contacting prof. Thomas Downar at Purdue University, who together with his colleagues helped the work greatly by providing the PARCS files for the benchmark cases, as well as the standalone PARCS code.

Three cases were calculated in 2007. Two were OECD NEA core transient cases (NEACRP A1 and C1), the third being the OECD NEA PWR MSLB exercise 2 separate core calculation. At this point the work was concentrated on separate core transients, because analysing the differences in plant models is a much more difficult task than comparing core models. As observed before, core calculations should give quite similar results, the real uncertainties and deviations between analyses are caused by the enormous amount of details relevant to the modeling of the rest of the plant.[6]

2 Possible cases for TRAB-3D vs. TRACE/PARCS comparison

Preparing input data and getting all the needed information correct for a reactor that has previously not been calculated with a given computer code, can be a difficult and time-consuming task. Also, questions of confidential information can rise. In order to avoid this, the TRAB-3D/PARCS comparison work performed in the TRICOT project is based on public, well-defined international benchmark exercises. Since these exercises have already been calculated with both codes, the input decks already exist, and should be ready to use.

With the help of prof. Thomas Downar from Purdue University, several TRACE/PARCS input data decks were obtained by VTT, and the possible cases for comparison were identified as follows (i.e. input data files available at VTT for both TRAB-3D and PARCS):

1. OECD NEA LWR Core transient benchmarks (PWR cases calculated with standalone PARCS)
    a. A1, PWR central control rod ejection from zero power
    b. A2, PWR central control rod ejection from full power
    c. C1, PWR peripheral control rod ejection from zero power
    d. D1, BWR cold water injection transient (RELAP-5/PARCS)
2. OECD NEA PWR Main Steam Line Break benchmark
    a. Exercise 2, 3D core calculation
    b. Exercise 3, full plant simulation

In addition, there are cases that could be calculated with both codes with some additional effort:

1. OECD NEA BWR Turbine Trip benchmark
   a. Exercise 2, 3D core calculation; Exercise calculated with TRAB-3D, but PARCS input not at VTT
   b. Exercise 3, full plant simulation; PARCS input at VTT, but exercise not calculated with TRAB-3D
2. AER dynamic benchmarks 1 and 3, calculated at VTT with HEXTRAN, PARCS coupled to RELAP-5

Of the above NEA CRP cases A1, and C1, as well as PWR MSLB exercise 2 were chosen for the calculated cases in 2007. These are all separate 3D PWR core cases, where the differences in thermal hydraulics and plant modeling should have minimal influence. The main difference between the cases is that CRP A1 and C1 are calculated with standalone PARCS, while PWR MSLB exercise 2 is calculated with PARCS coupled to TRACE.

As PARCS is now integrated to TRACE, calculations with TRACE/PARCS are relatively straightworward, only executing TRACE with both TRACE (for thermal hydraulics) and PARCS (for neutronics) input files in the same folder is needed. For the cases where PARCS is coupled to RELAP-5, the situation is much more complicated, as these cannot be directly calculated by executing TRACE. The procedure for RELAP-5/PARCS runs involves executing PARCS and RELAP-5 simultaneously. However, this execution mode has not been tested at VTT.

3 NEA PWR Core transient benchmarks

3.1 Benchmark overview

OECD NEA CRP benchmark series is a set of 3D core calculational benchmarks defined in the early 1990's[7]. The series consists of eight cases, six of which are control rod ejection (CRE) transients for PWR. The remaining two are BWR cold water inection and core pressurization transients. Table 1 lists the NEACRP benchmark cases. All the cases have, earlier, been calculated with TRAB-3D as the very first dynamic validation cases.

Table 1. NEACRP benchmark cases.

Case	Reactor type	Description
A1	PWR	Central CRE from zero power (quarter core symmetry)
A2	PWR	Central CRE from full power (quarter core symmetry)
B1	PWR	Peripheral CRE from zero power (quarter core symmetry)
B2	PWR	Peripheral CRE from full power (quarter core symmetry)
C1	PWR	Peripheral CRE from zero power (half core symmetry)
C2	PWR	Peripheral CRE from full power (half core symmetry)
D1	BWR	Cold water injection
E1	BWR	Core pressurization

The benchmark definitions include the neutronic cross section data and fuel and cladding thermodynamic properties, as well as core thermal hydraulic boundary conditions, which remain constant during the transient. The calculation of the dynamic thermal hydraulic conditions inside the core is left to the individual code, making the benchmark not a pure neutronics benchmark, but an exercise for coupled dynamics codes.

Cases A1 and C1 were chosen for calculation. There are two differences between the cases: 1) A1 is calculated in quarter core symmetry, whereas C1 is calculated in half core symmetry; and 2) A1 has the central control rod ejected, while in C1 the ejected control rod is situated in the core periphery. It should be noted that calculating one quarter of the core is a symmetry option considered as "obsolete" in TRAB-3D, and has not been used for at least for a decade.

The PARCS input files for the NEACRP cases were made for standalone PARCS, so no TRACE thermal hydraulics calculation was necessary in these cases. On the other hand, the PARCS thermal hydraulics solver is extremly simple consisting of only one FORTRAN subroutine, and cannot be relied on in the case of more complicated transients. For control rod ejections, where the coolant has little time to react, it may be sufficient.

3.2 NEACRP PWR A1

The transient is a control rod ejection from hot zero power, which is calculated with a quarter core symmetry using reflective boundary conditions in the symmetry axes. As noted earlier, the use of quarter core is considered "obsolete" for TRAB-3D, and it may be that not all of the code improvements have been made from the point of view of using this symmetry option. The ejected rod is situated in the center fuel assembly in a core consisting of 157 fuel assemblies. The nominal power of the reactor is 2775 MWth. There is no decay heat, nor xenon taken into account.

There where some minor differences in how the specified fuel thermodynamic properties were implemented in the original input files, but these did not have significant impact on the results.

The control rod ejection speed was actually slightly wrong in the original TRAB-3D input file that was used in the earlier validation work. The total time for the ejection was specified as 0.1 seconds, but this includes some movement in the top reflector after the control rod has left the active core region, thus the actual ejection time, if only active core height is considered is shorter, about 0.098 seconds. This 2 % deviation in the ejection speed does not change the results very much, but serves to demonstrate, how easy it is to misinterpret the specifications. Working with two input files side-by-side it is easy to identify such discrepancies that most probably woud go unnoticed, if just results from two separate calculations were compared.

The initial state critical boron is 561 ppm for PARCS and 563 ppm for TRAB-3D, and the ejected rod worth ($\Delta k/k$) is 0.8277% and 0.84208% for PARCS and TRAB-3D, respectively. Also the power distributions for steady state agree well

(Figure 1). The calculated quarter core distribution has been expanded to full core in all figures.

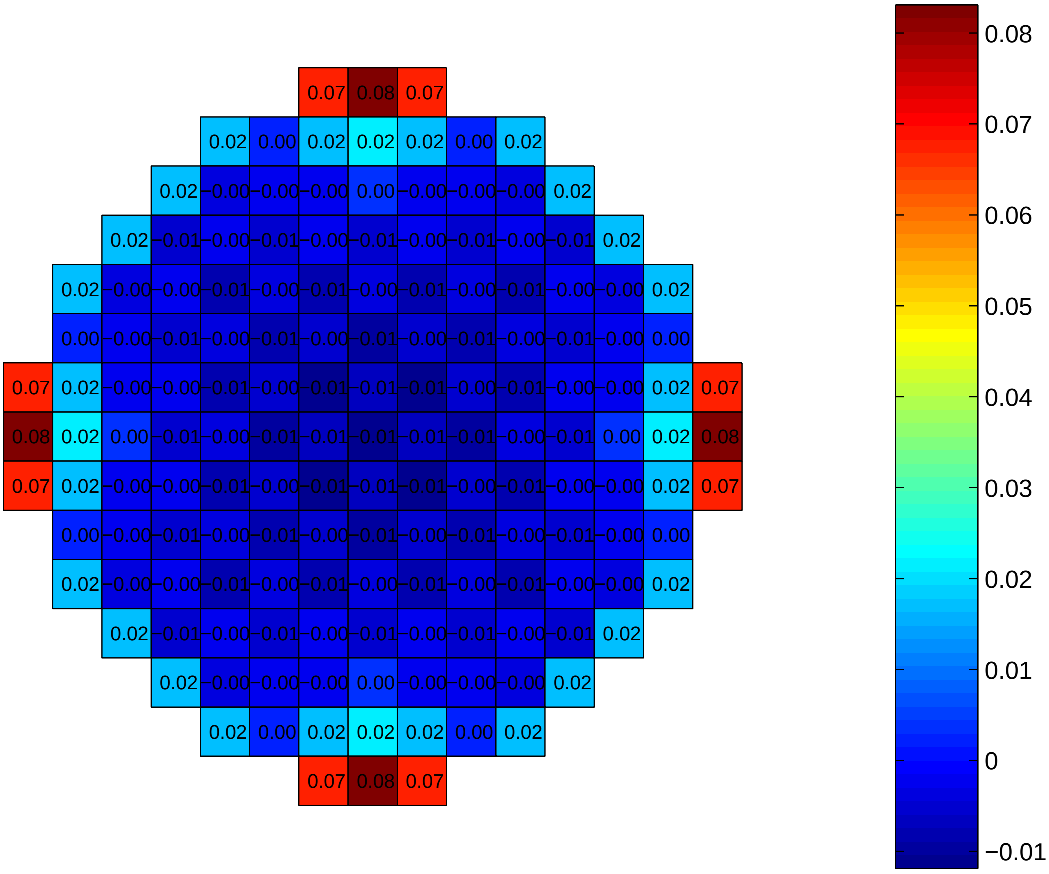

Figure 1. Deviation in initial power distribution TRAB-3D vs. PARCS (NEACRP A1)

Figure 2 shows the power behaviour during the transient calculated by TRAB-3D and PARCS. The agreement is surprisingly poor, both the timing and the height of the power peak differ with TRAB-3D calculating a later and smaller power increase. The specifications and given cross section files leave very little room for modeling interpretation. A special effort was made to search the cause for such a deviation, checking the sensitivity of the results to time step size, time integration methods, delayed neutrons, control rod ejection speed etc. but none of these had an effect even close to the deviation in the results. Thus the result remains unexplained. The deviation is naturally also refelected in other global parameters, e.g. core average fuel temperature (see Figure 3).

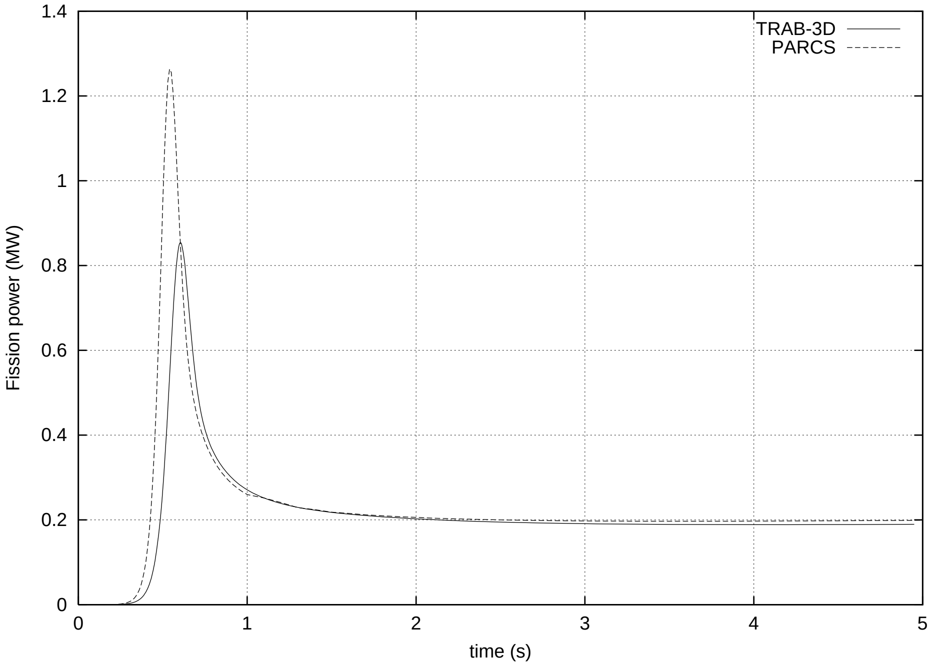

Figure 2. Power vs. time (NEACRP A1)

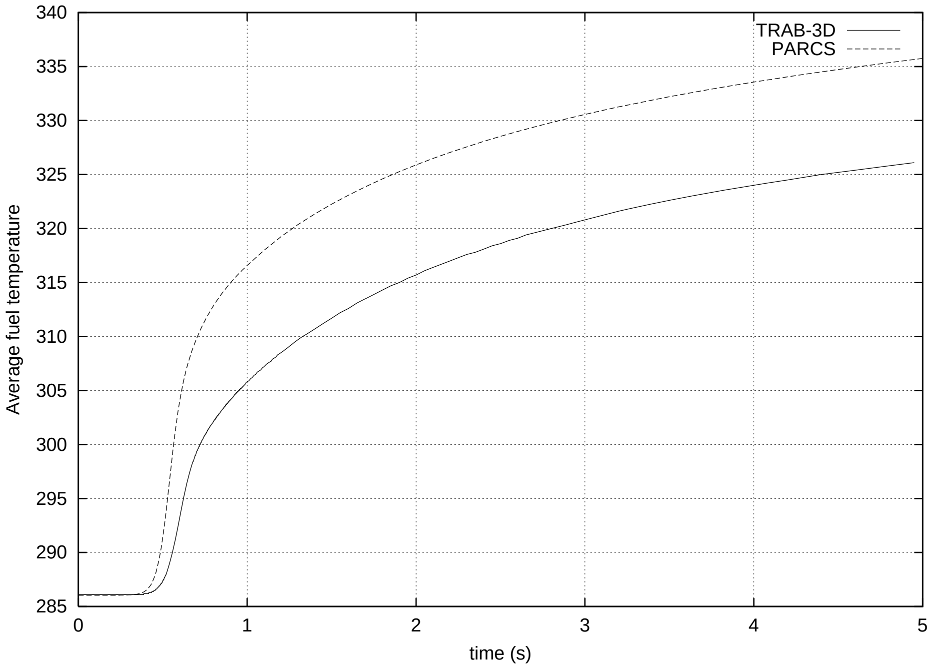

Figure 3. Core average fuel temperature vs. time (NEACRP A1)

After seeing the poor agreement with the global core parameters, it is another surprise that for the power distribution, the TRAB-3D and PARCS results agree well, as can be seen by the behaviour of assemblywise fission power peaking during the transient (Figure 4) and snapshot of power distribution at the time of power maximum (Figure 5 and Figure 6). Similarly as in steady state, only the low power assemblies in the outer ring have significant deviation.

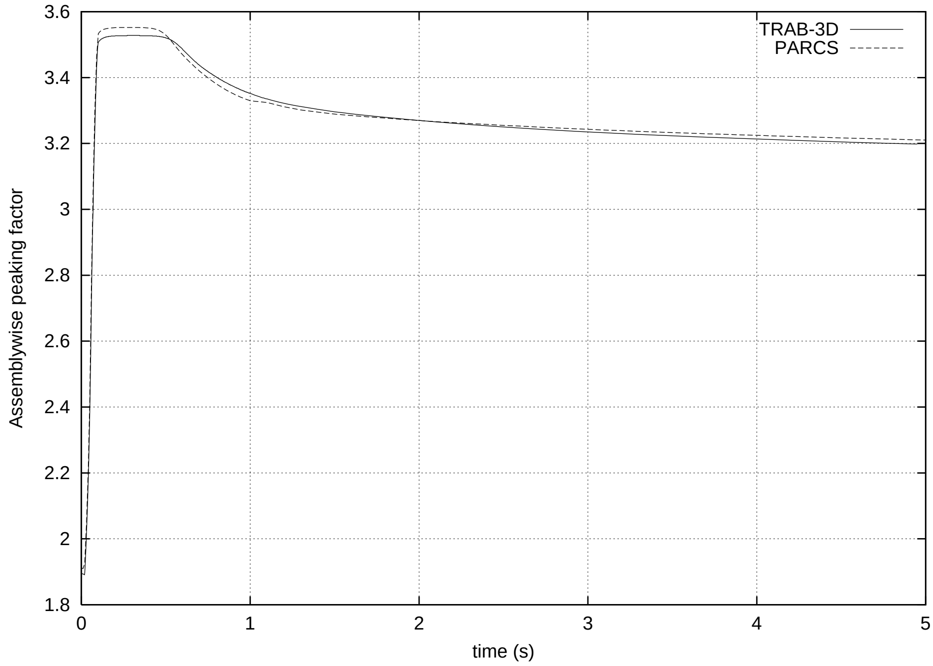

Figure 4. Assemblywise power peaking factor vs. time (NEACRP A1)

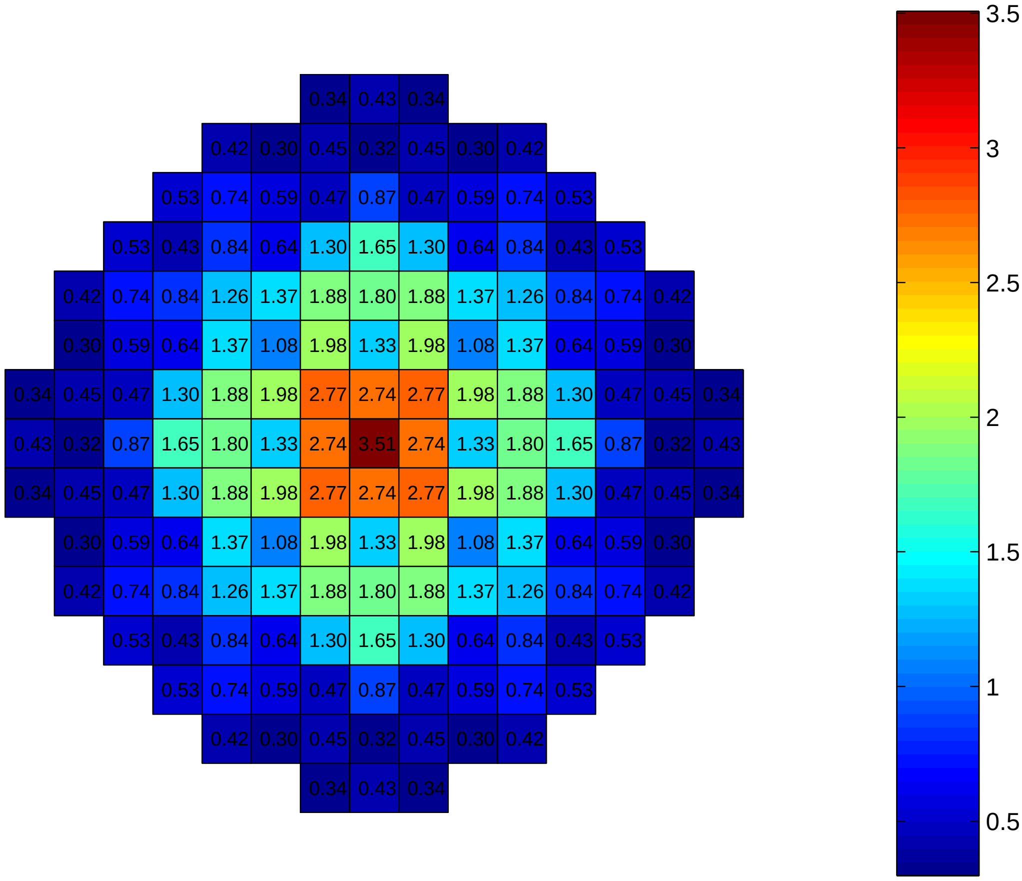

Figure 5. Power distribution at power maximum calculated by TRAB-3D (NEACRP A1)

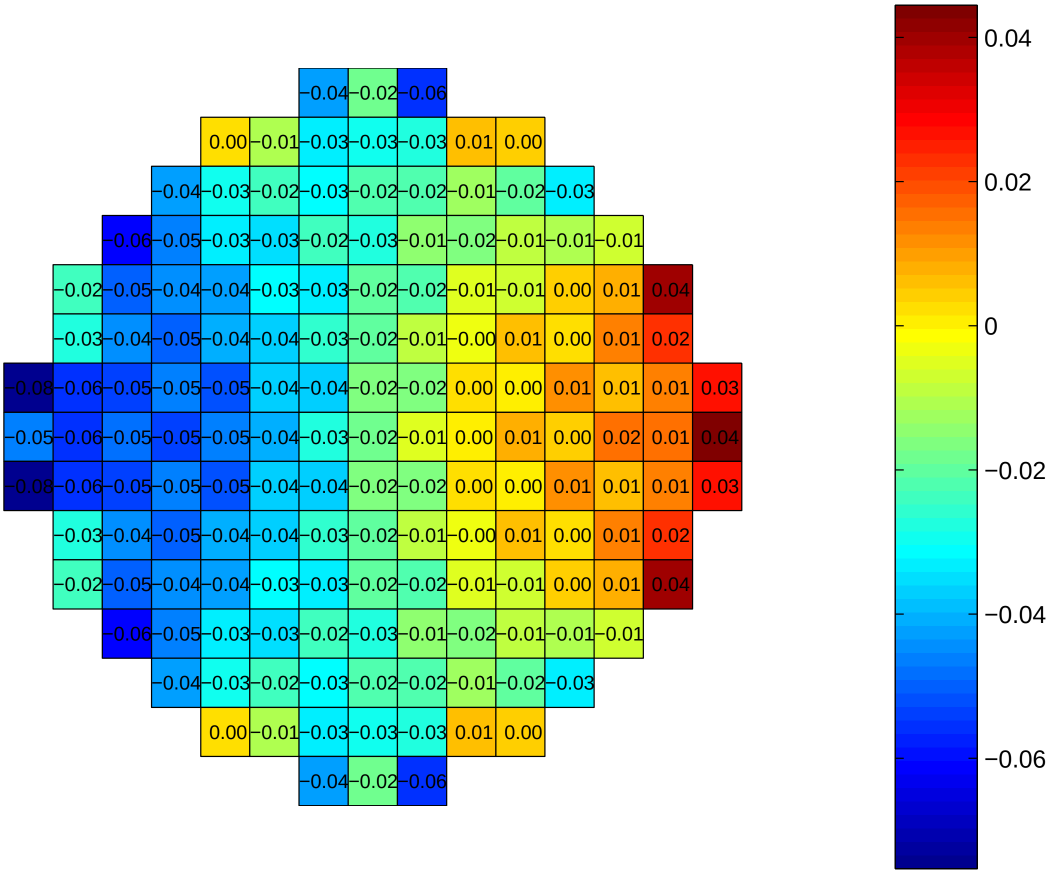

Figure 6. Deviation in power distribution at power maximum TRAB-3D vs. PARCS (NEACRP A1).

3.3 NEACRP PWR C1

Case C1 is a similar to case A1, except for the half core symmetry and that the ejected rod is situated in the core periphery. The results are, however, quite different. The initial state critical boron concentrations agree, again, well. TRAB-3D calculates 1128 ppm and PARCS 1129 ppm for criticality. Steady state power distribution is, again, almost identical except for the few peripheral channels with low power (Figure 7).

For this case, TRAB-3D and PARCS agree extremely well on the timing of the power maximum. As can be seen in Figure 8, TRAB-3D still gives a lower peak power, but the overall agreement looks good for power and other global parameters. Even usually difficult local parameters, such as maximum fuel centerline temperature are calculated almost the same (see Figure 9), although the temperature increase in TRAB-3D is somewhat slower.

Also for the C1 case the power distribution behaviour during the transient is in extremely good agreement, as shown by assemblywise peaking factor (Figure 10), and power distribution at the time of power maximum (Figure 11 and Figure 12).

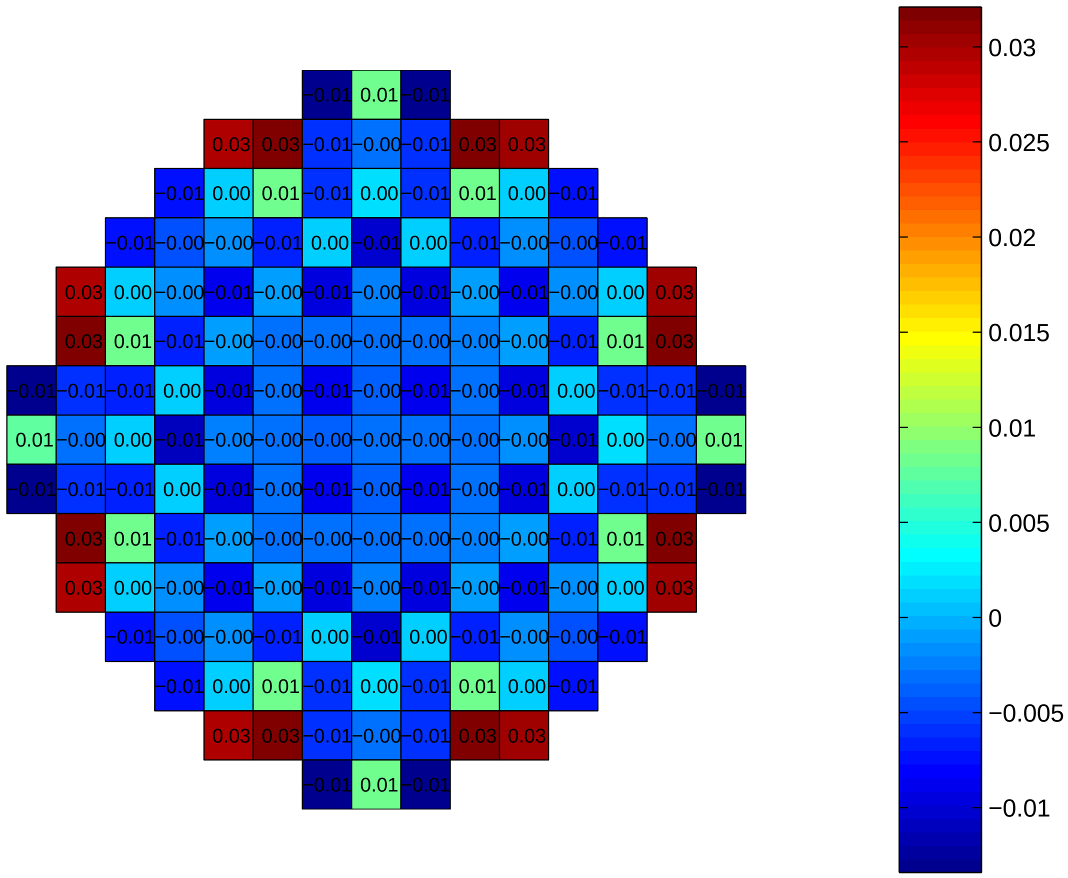

Figure 7. Deviation in initial power distribution TRAB-3D vs. TRACE (NEACRP C1).

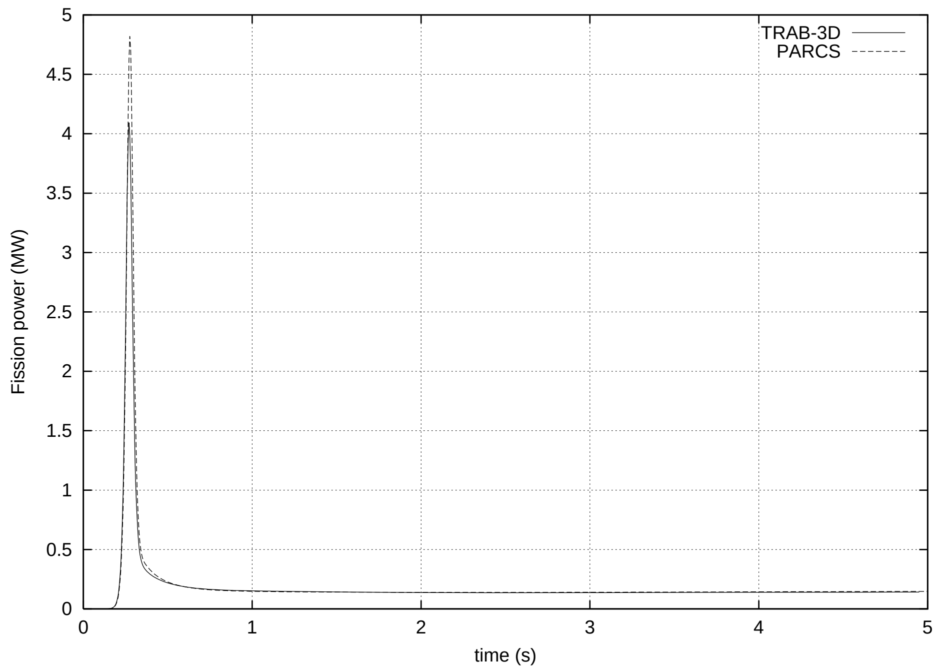

Figure 8. Power vs. time (NEACRP C1)

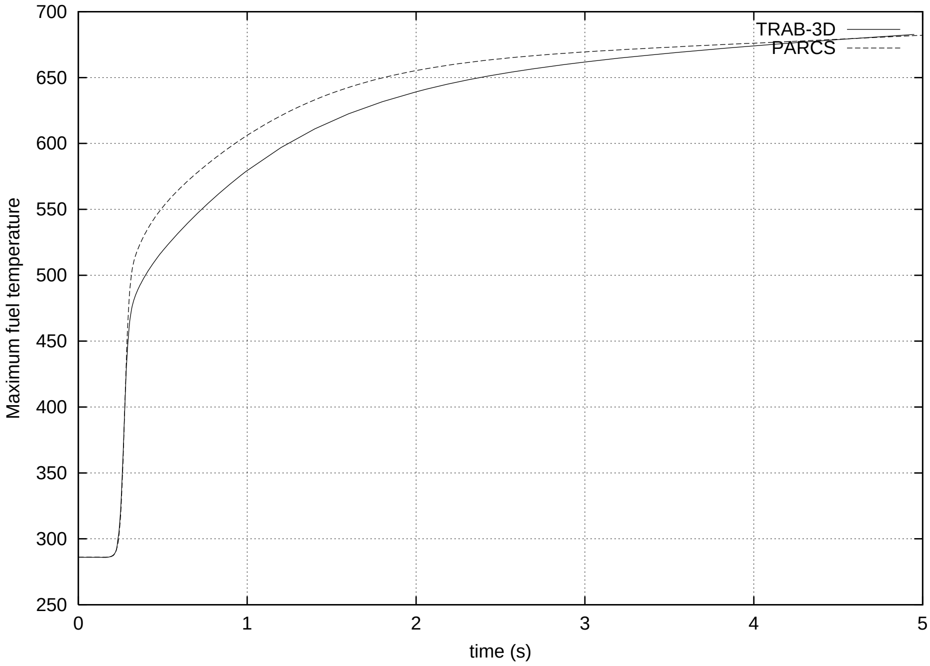

Figure 9. Maximum fuel centerline temperature vs. time (NEACRP C1)

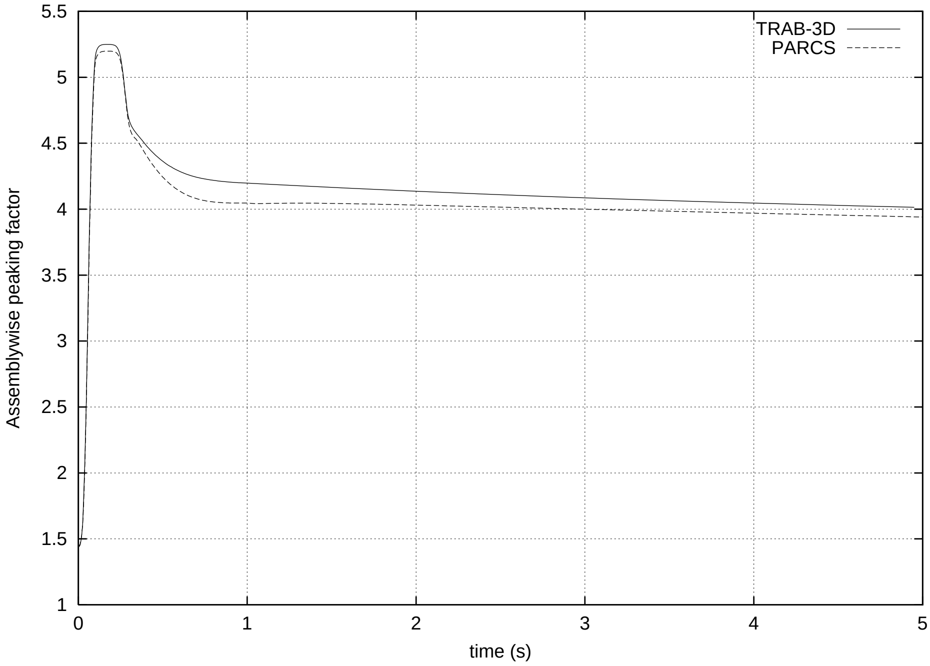

Figure 10. Assemblywise power peaking factor vs. time (NEACRP C1)

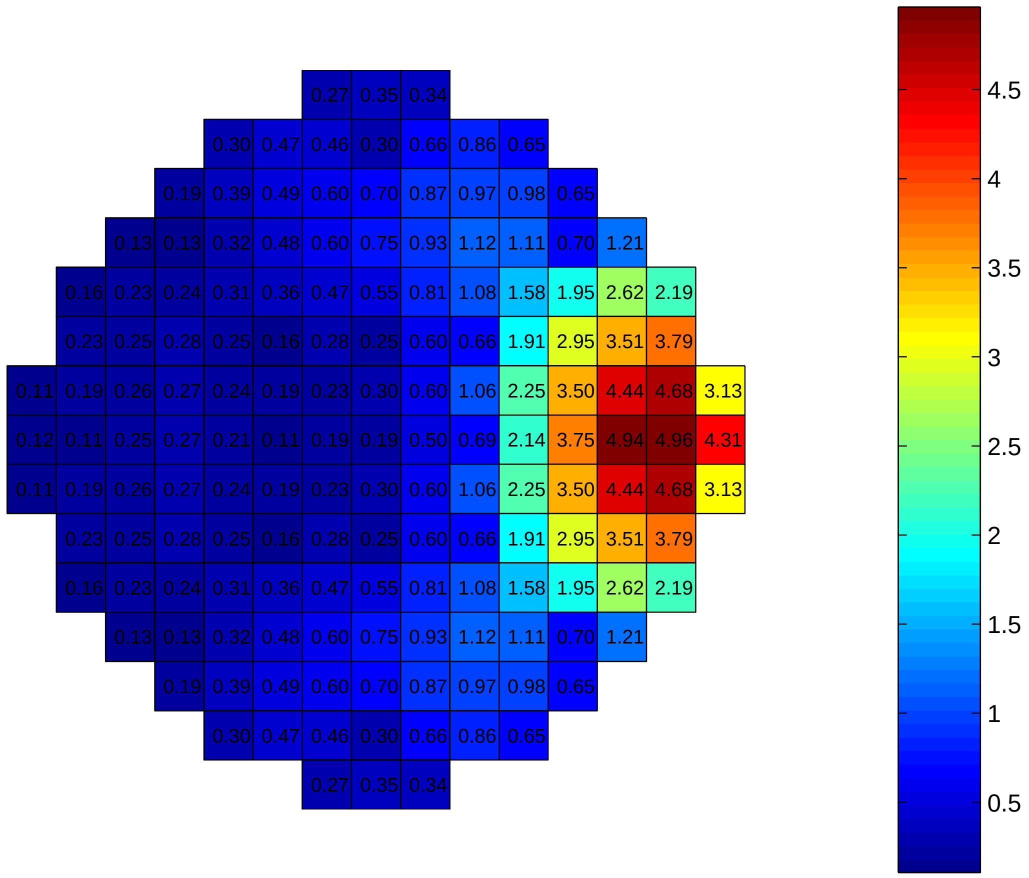

Figure 11. Power distribution at power maximum calculated by TRAB-3D (C1).

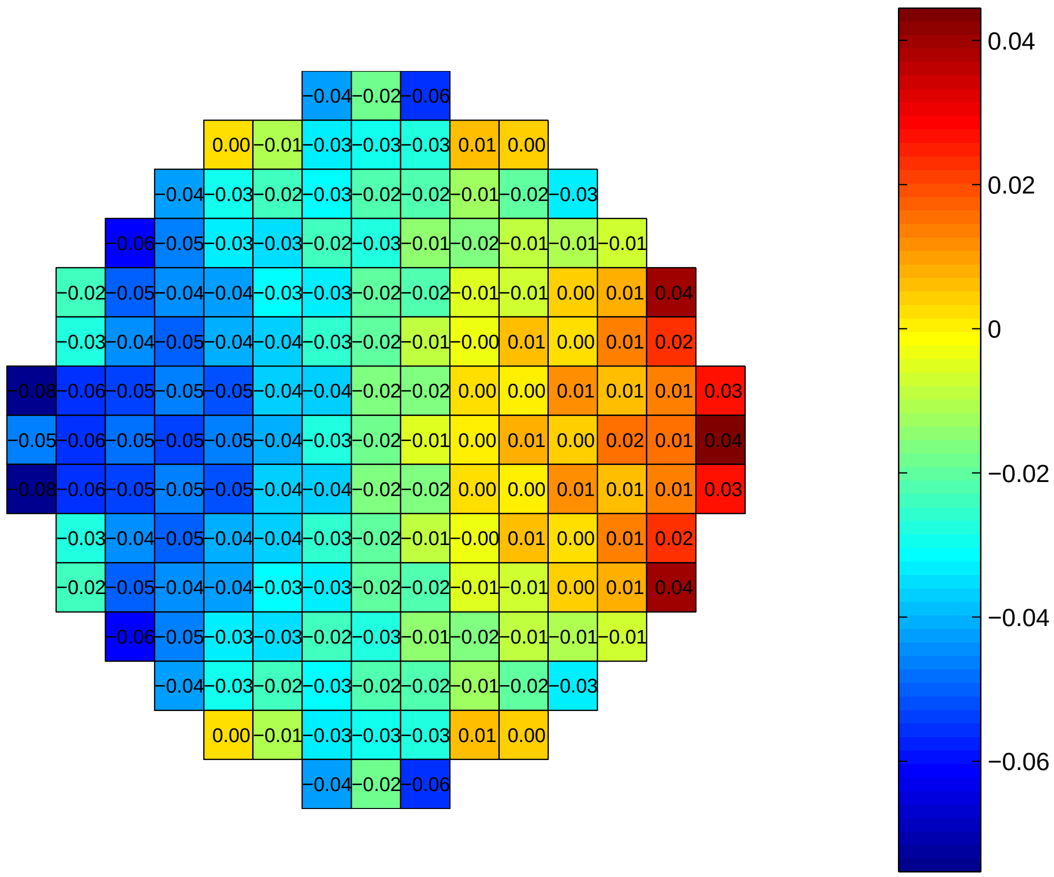

Figure 12. Power distribution at power maximum TRAB-3D vs. PARCS (C1).

4 OECD PWR MSLB benchmark

4.1 Benchmark overview

The OECD/NEA PWR Main Steam Line Benchmark (MSLB)[8] was organized starting from 1997 in order to compare coupled 3D neutronics/thermal hydraulics reactor dynamics codes. The benchmark acitivity lasted for several years and consisted of three separate excercises: 1) Plant transient with point kinetics, 2) 3D Core kinetics with given TH boundary conditions, and 3) Plant transient with 3D core model. VTT participated in all of the exercises with the TRAB-3D and SMABRE codes, which were parallelly coupled for the first time in order to calculate the third exercise[6].

The benchmark reference core design was derived from the Three Mile Island 1 nuclear power plant, a PWR with 177 fuel assemblies, and a nominal power level of 2772 MWth.

The benchmark transient was a main steam line break in one of the two steam generator loops. This event is characterized by significant space-time effects in the core caused by asymmetric cooling and the normal assumption of one stuck control rod in the most reactive position during the reactor scram. One of the main concerns is the possibility of return to power and criticality as the reactor cooling continues with the transient progress. To get meaningful code-to-code comparisons, the neutronic cross sections were modified in order to ensure the return to criticality. This was not achieved with a realistic set of cross sections.

The neutronic cross sections were provided by the benchmark organizers. Thus, the deviation in results is not caused by uncertainties and differencies in the cross section data.

4.2 Excercise 2: 3D core calculation

The second exercise was recalculated with TRAB-3D and TRACE/PARCS for this project. The thermal hydraulic core inlet and outlet boundary conditions were provided with the benchmark specifications as time-dependent inlet temperature, inlet mass flow, and outlet pressure for 18 core channels each consisting of several fuel bundles. The core thermal hydraulics was calculated with TRACE, not with the PARCS thermal hydraulics subroutine as in the NEACRP benchmarks. Thus, in this calculation the coupled code TRACE/PARCS was used at VTT for the first time.

In the original results submission, the TRAB-3D calculation was performed with 177 core TH channels, one channel for each fuel bundle. The TRACE input was made with 18 channels, corresponding to the boundary condition data. To investigate how large an effect this modeling feature has on the results, a second TRAB-3D model with 18 channels was made specifically for this project.

Figure 13 shows the calculated fission power behaviour vs. time. All results agree well with the TRAB-3D result calculated with 18 channels being a little closer to the TRACE/PARCS calculation as would be expected. Global parameters, such as core average coolant density are extremely close together (see Figure 14).

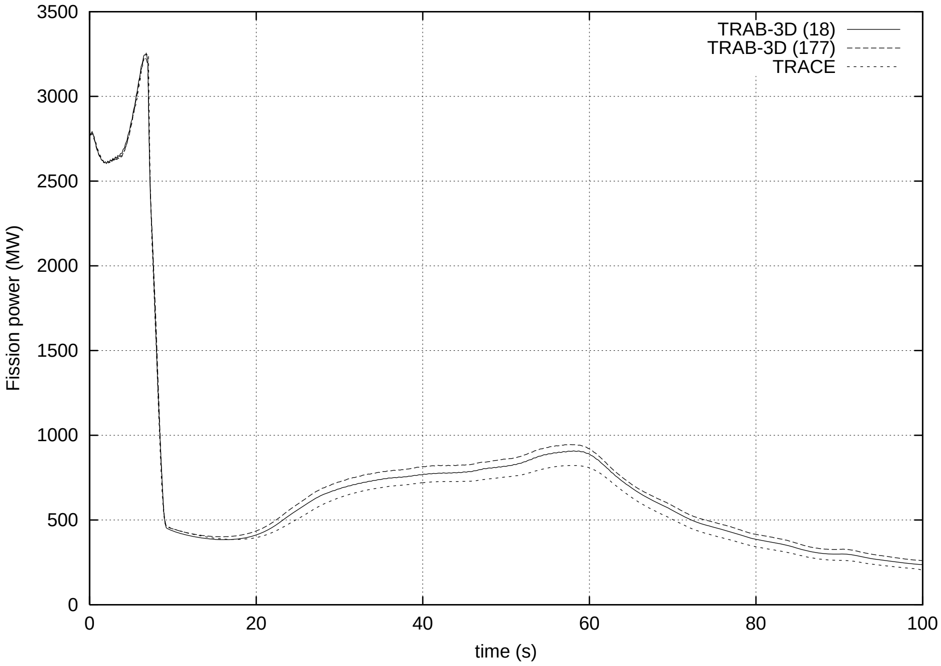

Figure 13. Fission power vs. time (MSLB)

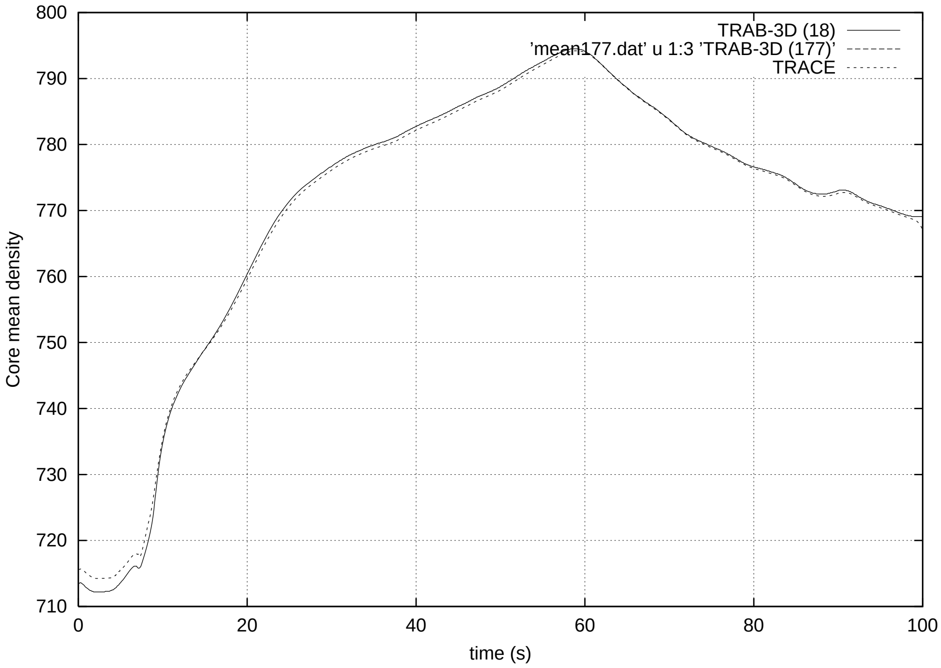

Figure 14. Core average coolant density vs. time (MSLB).

In the initial state, the radial power distributions look satisfactory (see Figure 15, Figure 16, and Figure 17). The asymmetry in the lower right quadrant is caused by the stuck rod being in fully withdrawn position, while the rest of the same control rod group is slightly inserted. The maximum deviation is 3% using similar thermal hydraulic channel grouping, and 5% using 177 TRAB-3D core channels.

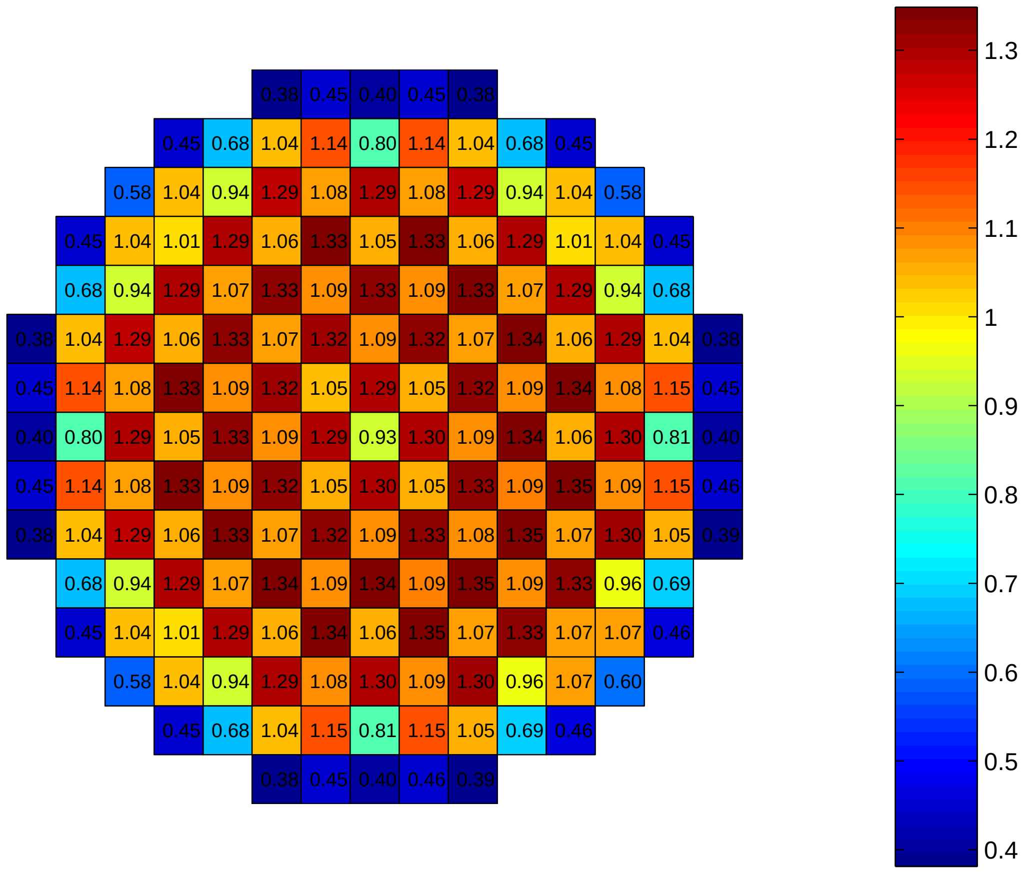

Figure 15. Initial power distribution, TRAB-3D with 177 channels. (MSLB)

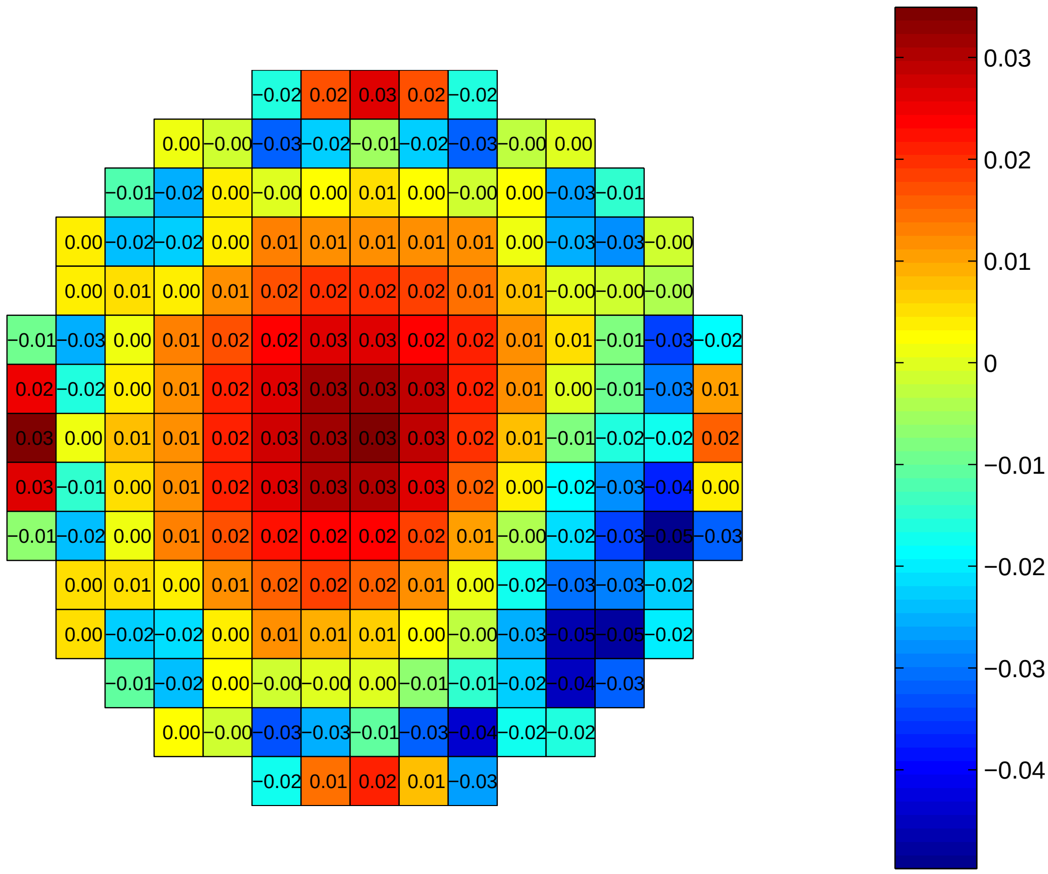

Figure 16. Initial power TRAB-3D 177 channels versus TRACE (MSLB)

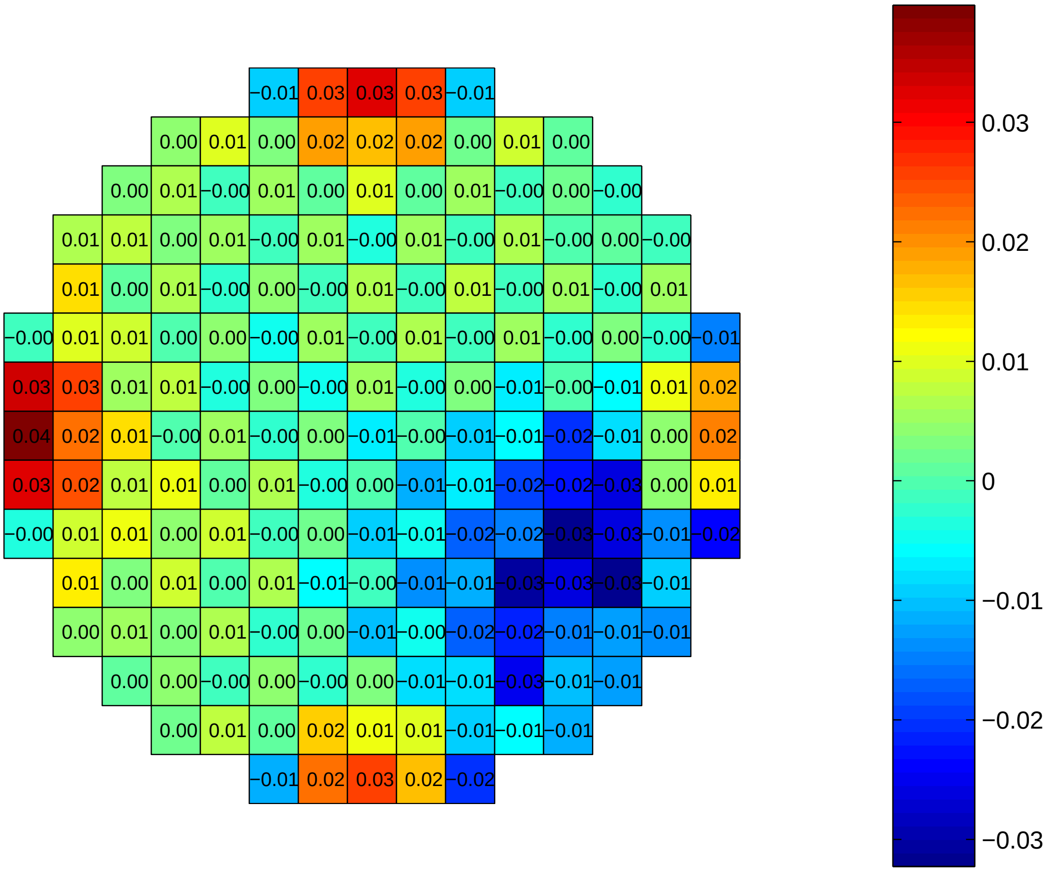

Figure 17. Initial power TRAB-3D 18 channels versus TRACE (MSLB)

However, during the transient the power distributions start to deviate strongly. This can be seen in the time behaviour of the assemblywise power peaking factor (Figure 18) and comparison of the power distributions at the time of return to power (Figure 19, Figure 20, and Figure 21). The stuck rod position can be seen in Figure 19 as the location of the power maximum in the lower right core quadrant. For some reason, the TRAB-3D calculation with 177 channels, which should be further away from the TRACE result, has almost exactly the same power peaking at the time of the power maximum (57.7 seconds after transient beginning). Accordingly the agreement in Figure 20 looks surprisingly good near the stuck rod position.

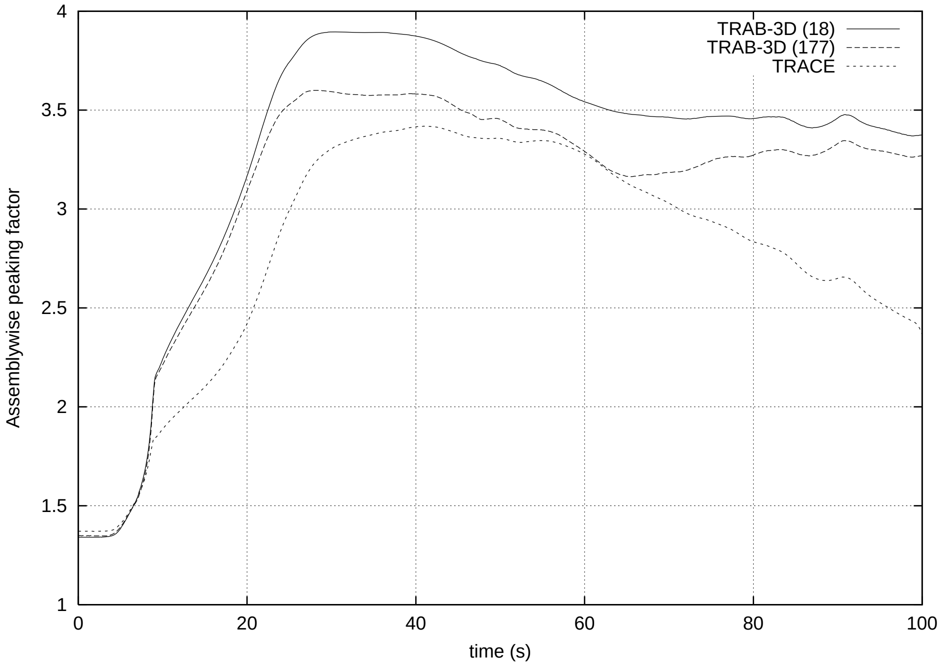

Figure 18. Assemblywise power peaking factor vs. time (MSLB).

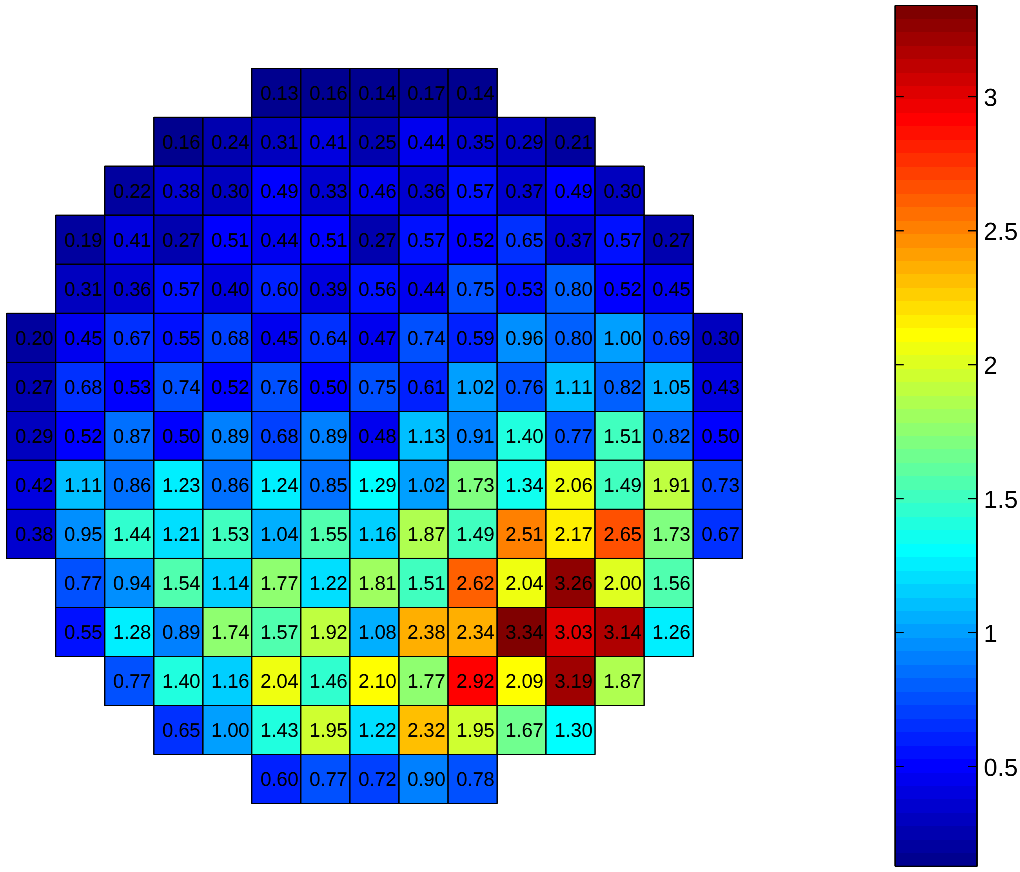

Figure 19. Power distribution at the time of power maximum after reactor scram with one stuck control rod calculated by TRAB-3D 177 channels

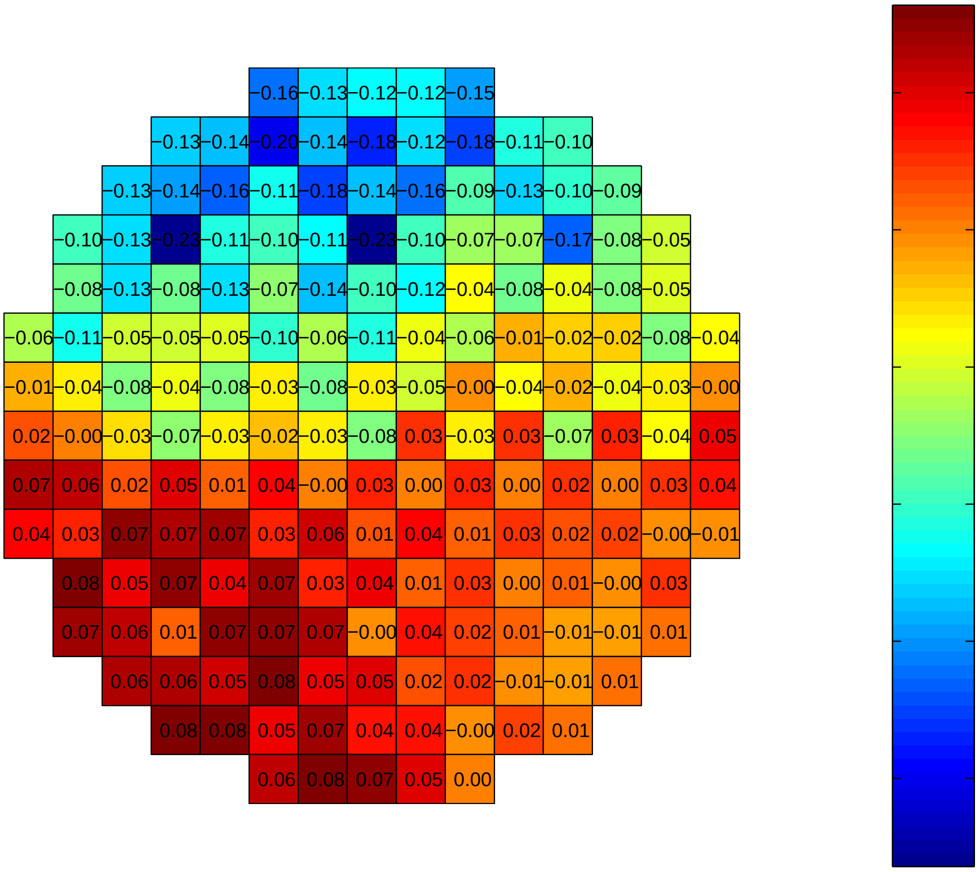

Figure 20. Power at maximum after scram, TRAB-3D 177 channels vs. TRACE

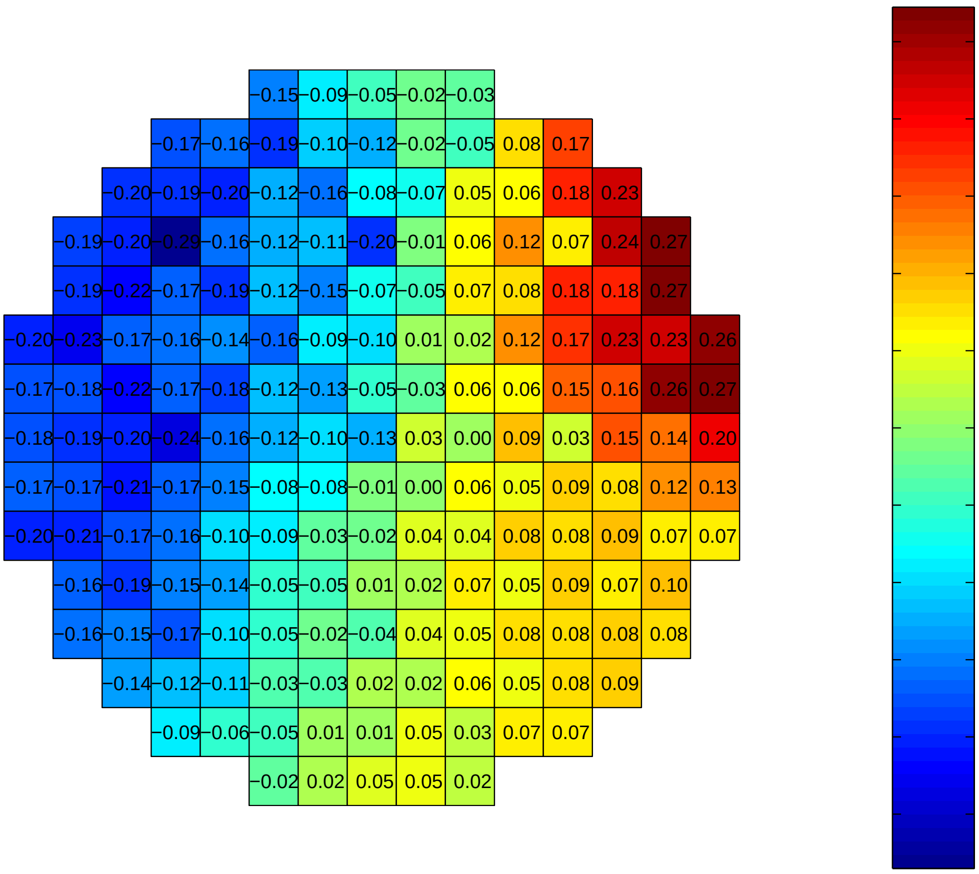

Figure 21. Power at maximum after scram, TRAB-3D 18 channels vs. TRACE

The answer to the poor agreement in transient power distributions was found to be the difference in the definition of power distribution between the codes. In TRAB-3D, power distribution is calculated based on the sum of instantaneous neutron fluxes weighted by the fission absorption cross section and the power per fission in each neutron group. In other words, power here means the power produced (immediately and after any delay up to infinity) from the fissions taking place at the time. In TRACE/PARCS power distribution is the actual power distribution at the time, i.e. the sum of immediate fission power and decay power originating from the preceding history of fissions.

While the TRACE/PARCS definition gives the correct *power distribution* at any time point, the TRAB-3D definition has the advantage of describing power measurements more accurately, and thus, enabling more sensible comparisons against measured data. Power distribution measurements are based on neutron detectors, and measure therefore more correctly *fission distribution*. In the initial state the distributions of fission power and decay power are identical, assuming infinite operation on that power, so this does not have any effect. But especially after reactor scram, as in the later phases of the MSLB transient, the decay power distribution remains according to the initial full power state, while the fission power distribution changes drastically, and is heavily concentrated in the vicinity of the stuck control rod.

To show the effect described above, a second set of calculations was performed with decay power calculation switched off in both codes. This does not greatly change the behaviour of global parameters, but has a significant effect on the distributions, as can be seen in Figure 22, Figure 23, and Figure 24. The assemblywise peaking factor behaviour is almost identical, when both codes use the same thermal hydraulic channel model, with the TRAB-3D calculation using 177 channels having somewhat lesser peaking during the transient.

The TRAB-3D result with 177 channels seems to deviate more from the TRACE result near the stuck rod position than in the case where decay heat calculation was included, but the good agreement with decay heat was possibly caused by chance as the time behaviour of power peaking deviates much more.

For TRAB-3D with 18 channels the agreement is now very good, as can be expected from the nearly identical power peaking time behaviour. Only some peripheral channels with low power have larger deviations (6-7%). It can be concluded that decay heat distribution was the source of deviation between the TRAB-3D and TRACE results.

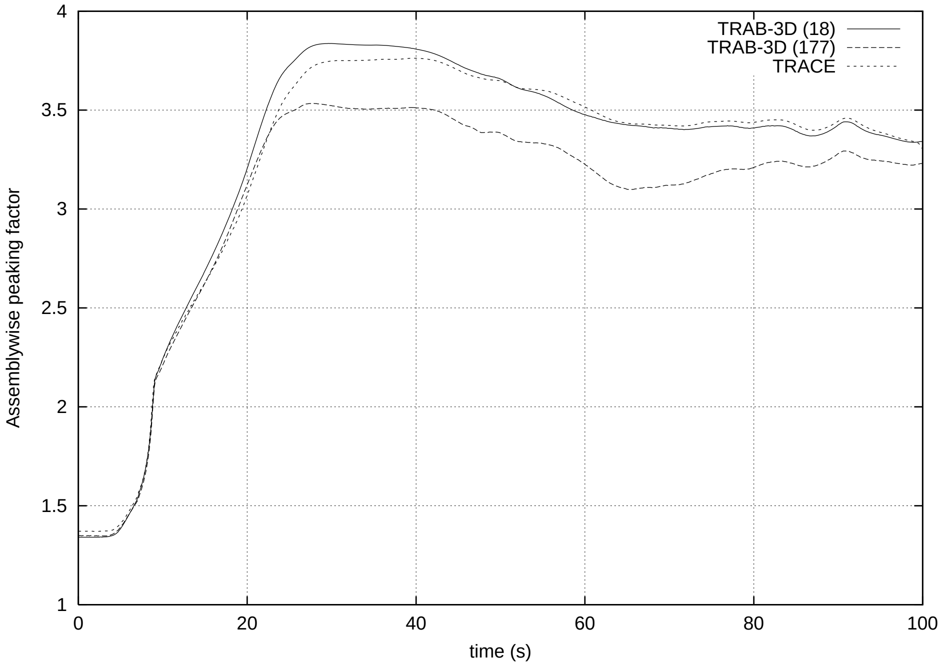

Figure 22. Assemblywise power peaking factor vs. time with no decay heat (MSLB).

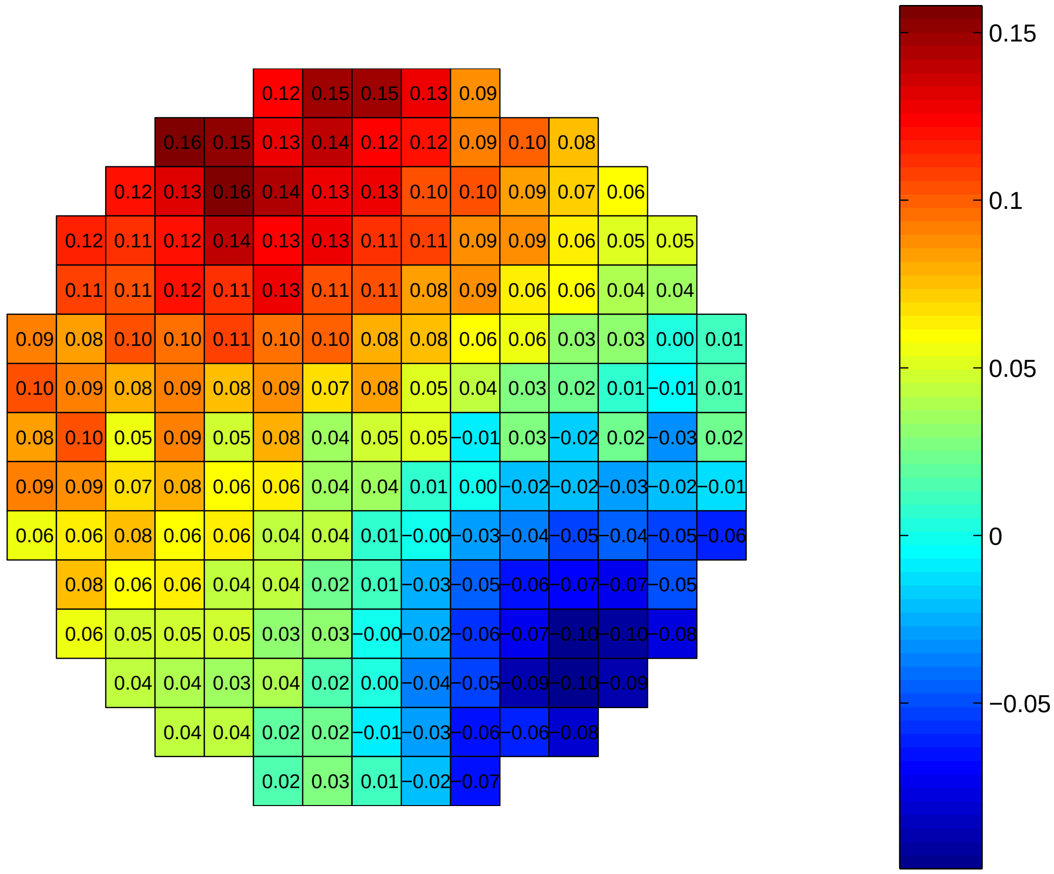

Figure 23. Power at the maximum after scram, TRAB-3D 177 channels vs. TRACE with no decay heat (MSLB).

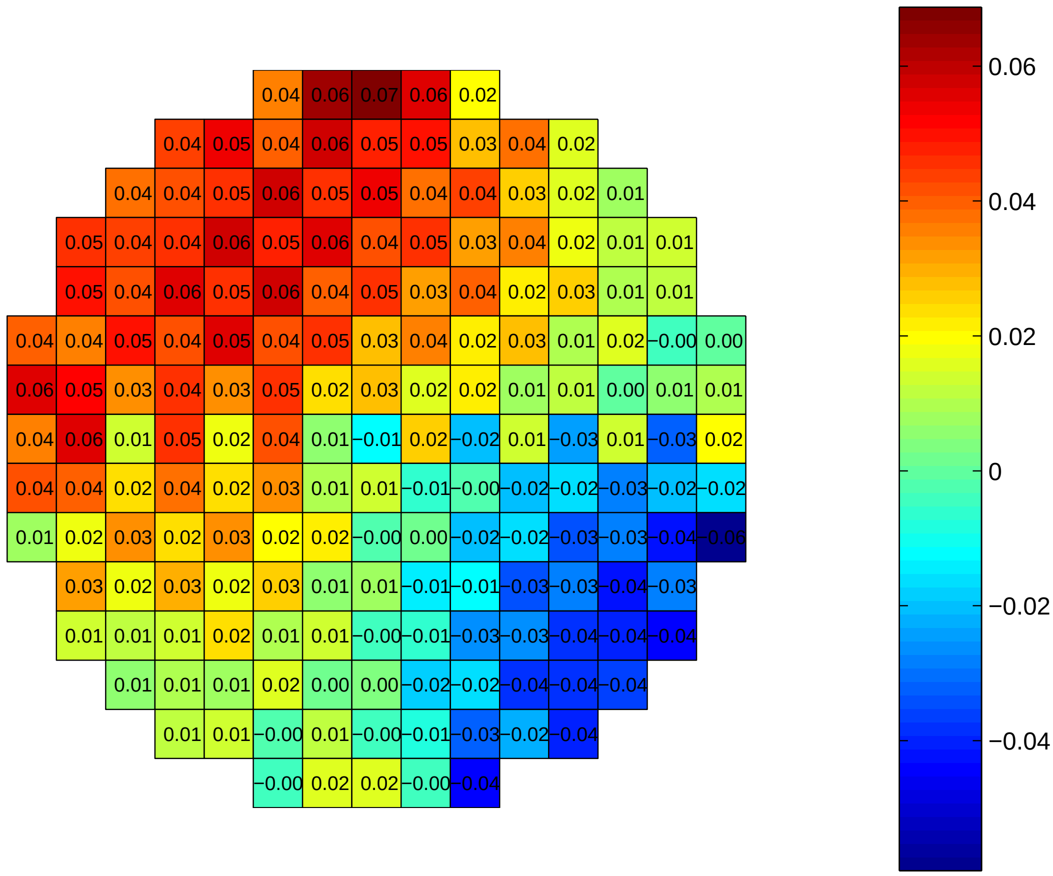

Figure 24. Power at the maximum after scram, TRAB-3D 18 channels vs. TRACE with no decay heat (MSLB).

5 General remarks on the use of TRACE/PARCS

The use of TRACE is presently based on the graphical user interface SNAP, which should make the modeling of complicated plant systems easier. However, PARCS cannot be used this way. The only possibility is to use the traditional input file. This is not a problem, as preparing the reactor core input is quite straight forward, and fairly similar to other core simulators (e.g. SIMULATE). Some undocumented features were found even with these relatively few calculations, e.g. control rod groups with negative numbers do not participate in scram. This could be only found by reading the source code, which fortunately is included in the TRACE/PARCS distribution. The PARCS user’s manual exists only in a draft version, and some work on it is still needed.

It is possible to name the PARCS input file through SNAP, and make the thermal hydraulics model graphically. But using TRACE this way appeared to be difficult in practice, and in the end, normal comand line execution seemed to be the most convenient way. Actually, the PARCS developers at Purdue University also use this method of execution. SNAP is useful for making the thermal hydraulics network of channels and checking that every pipe is connected to the right place, however.

There are persons much more experienced with TRACE thermal hydraulics at VTT, but making simple networks of pipes and valves seemed not to be very cumbersome. On the other hand, full plant models, such as the TMI-1 model for MSLB benchmark exercise 3, are quite complicated. Even the use of a ready model is not easy. An effort was made to calculate exercise 3 also, but it was not successful. Apparently the input from Purdue was for some different TRACE version than the version received through the official channels of the CAMP agreement. For a successful calculation of exercise 3, support from experienced TRACE user’s would be essential. Interestingly, the core thermal hydraulics model for exercise 2 did not cause any problems. Of course the amount of geometric and other data is very limited in the core model compared to the full plant.

6 Conclusions

In 2007, work was started in SAFIR2010 research programme TRICOT project task on TRAB-3D validation by taking into use at VTT the US NRC coupled neutronics/thermal hydraulics code TRACE/PARCS and identifying the possible comparison cases that could be calculated with both TRAB-3D and TRACE/PARCS.

Three pressurized water reactor core benchmark excercises were recalculated, and results of the two codes were compared. The agreement between the results of the codes is extreemly good, even if the cases deal with dramatic changes in the fission power distribution caused by an ejected control rod (NEA CRP A1 and C1) or by a stuck control rod during reactor scram (NEA PWR MSLB).

Biggest deviations were found in the overall dynamics behaviour in case A1, which is an ejection of a central control rod and should be the simplest of the three cases. The explanation remains unclear, but it could be that the use of quarter core symmetry conditions is dealt differently in the codes. Also, the quarter core symmetry is considered an “obsolete” feature in the TRAB-3D User’ Manual, and there could be some recent developments that have not been considered from this point of view. Even for this case, the power distributions looked surprisingly good, nevertheless.

As an overall conclusion, it could be said that the 3D nodal neutronic model is not a significant source of uncertainty in transient analysis. The uncertainties and modeling options of thermal hydraulic details cause much larger deviations. For boiling water reactors thermal hydraulics play an essential role already in the reactor core, but the real differences come largely from plant modeling. This was the conclusion already during the international meetings related to the NEA PWR MSLB benchmark, where it was relatively easy to come into agreement on core model, but several unsettled issued remained for especially the secondary circuit of the plant[6].

In the following years of the TRICOT project, this work will be continued with more challenging boiling water reactor cases, and PWR MSLB exercise 3 including the plant model. Based on the preliminary attempts, it is clear that, in order to calculate these cases, support from experienced TRACE/PARCS users will be essential. Towards this end, a contact was established with Tomasz Kozlowski at KTH in Sweden, who is one of the original PARCS developers at

Purdue. One possibility is a common NKS project application for code comparisons.

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