Application of FFTBM to Severe Accidents

Andrej Prošek, Matjaž Leskovar
Jožef Stefan Institute
Jamova 39, SI-1000 Ljubljana, Slovenia
Andrej.Prosek@ijs.si, Matjaz.Leskovar@ijs.si

ABSTRACT

In Europe an initiative for the reduction of uncertainties in severe accident safety issues was initiated. Generally, the error made in predicting plant behaviour is called uncertainty, while the discrepancies between measured and calculated trends related to experimental facilities are called the accuracy of the prediction. The purpose of the work is to assess the accuracy of the calculations of the severe accident International Standard Problem ISP-46 (Phebus FPT1), performed with two versions of MELCOR 1.8.5 for validation purposes. For the quantitative assessment of calculations the improved fast Fourier transform based method (FFTBM) was used with the capability to calculate time dependent code accuracy. In addition, a new measure for the indication of the time shift between the experimental and the calculated signal was proposed. The quantitative results obtained with FFTBM confirm the qualitative conclusions made during the Jožef Stefan Institute participation in ISP-46. In general good agreement of thermal-hydraulic variables and satisfactory agreement of total releases for most radionuclide classes was obtained. The quantitative FFTBM results showed that for the Phebus FPT1 severe accident experiment the accuracy of thermal-hydraulic variables calculated with the MELCOR severe accident code is close to the accuracy of thermal-hydraulic variables for design basis accident experiments calculated with best-estimate system codes.

1 INTRODUCTION

Recently an initiative for the reduction of uncertainties in severe accident safety issues was initiated. However, the extension and application of uncertainty methods to severe accidents is more difficult than for design basis accidents because the availability of experimental data and the level of development and validation of computer codes are quite different. Generally, the error made in predicting plant behaviour is called uncertainty, while the discrepancies between measured and calculated trends related to experimental facilities are called the accuracy of the prediction. In the present work the accuracy of the MELCOR 1.8.5 calculations of the International Standard Problem ISP-46 (Phebus FPT1) were quantified. The calculations of the experiment were performed in 2002 by the Jožef Stefan Institute (JSI), with the MELCOR 1.8.5 QZ and the MELCOR 1.8.5 RE version. With the severe accident code the main thermal-hydraulic, fuel degradation and aerosol phenomena, which occurred in the bundle and circuit of the Phebus facility during the first 18660 s of the experiment, were simulated. The MELCOR input model was developed strictly following the recommendations on noding for the reference case simulation provided in the ISP-46 Specification Report [1].

For the quantitative assessment the improved fast Fourier transform based method (FFTBM) was used with the capability to calculate time dependent code accuracy [2]. The qualitative analysis revealed that the shape of the trends and the parameters used in the severe accident analysis differ significantly from design basis accidents. In this study it is shown that FFTBM with some improvements is applicable to severe accidents. Also is should be clear, that quantitative assessment is not replacement of qualitative analysis rather a complement information giving possibility to compare quantitative results of different calculations of the selected experiment or even comparison of calculations performed for different experiments. Namely, the accuracy information is not given only for single parameter but also calculation as a whole.

2 METHOD DESCRIPTION

As the basis for the quantitative assessment the FFTBM method was used. For more detailed information on the method and its applications the reader is referred to [3] and [4]. In this paper the original FFTBM method is briefly described first. Then it is described how the method was further adapted for the use in the severe accident area. Namely, in the past a few applications of FFTBM to severe accidents were done, quantitatively assessing only thermal-hydraulic parameters. In some other cases large uncertainties caused large values of accuracy measures requiring special weighting factors, not physically based. This makes difficulties in making consistent statements with respect to applications done in design bases area. Therefore method improvement was needed.

2.1 Original FFTBM

For calculation of measurement-prediction discrepancies the experimental signal $F_{\mathrm{exp}}(t)$ and error function $\Delta F(t)$ are needed. The error function in the time domain is defined as $\Delta F(t) = F_{\mathrm{cal}}(t) - \tilde{F}_{\mathrm{exp}}(t)$, where $\tilde{F}_{\mathrm{cal}}(t)$ is the calculated signal. The code accuracy quantification for an individual calculated variable is based on the amplitudes of the discrete experimental and error signal obtained by fast Fourier transform (frequency domain) at frequencies f_{n}, where n=0,1,...,2^m and m is the exponent defining the number of points N=2^{m+1}. The average amplitude AA is defined:

$$\mathrm{AA} = \sum_{n=0}^{2^m} \left|\tilde{\Delta} F(f_n)\right| \Big/ \sum_{n=0}^{2^m} \left|\tilde{F}_{\mathrm{exp}}(f_n)\right|, \tag{1}$$

where $\tilde{\Delta} F(f_n)$ is the error function amplitude at frequency f_{n} and $\tilde{F}_{\mathrm{exp}}(f_n)$ is the experimental signal amplitude at frequency f_{n}. The AA (in the following called D'Auria AA) factor can be considered a sort of average fractional error and the closer AA value is to zero the more accurate is the result.

2.2 New proposed figure of merit

Please note that D'Auria AA figure of merit in Eq. (1) was not obtained by comparing the experimental and calculated magnitude spectrum, but by calculating the magnitude spectrum of the difference signal. Nevertheless due to the Fourier transform properties the magnitude spectrum of the error signal can also be obtained by adding (actually subtraction) the experimental and calculated signal magnitude spectra; they must be converted into rectangular notation, subtracted, and then reconverted back to polar form. The reason is, when spectra are in polar form (M, φ), they cannot be added by simply adding the magnitudes M and phases φ. The absolute value of Fourier transform $\left|\Delta\tilde{F}(f_n)\right|$ can be expressed as:

$$\begin{aligned}\left|\Delta\tilde{F}(f_n)\right| &= \left|\tilde{F}_{\mathrm{exp}}(f_n)-\tilde{F}_{\mathrm{cal}}(f_n)\right| = \sqrt{\left(\mathrm{Re}(\tilde{F}_{\mathrm{exp}}(f_n)-\tilde{F}_{\mathrm{cal}}(f_n))\right)^2+\left(\mathrm{Im}(\tilde{F}_{\mathrm{exp}}(f_n)-\tilde{F}_{\mathrm{cal}}(f_n))\right)^2} = \\ &= \sqrt{M_1^2+M_2^2-2M_1M_2\left(\cos\varphi_1\cos\varphi_2+\sin\varphi_1\sin\varphi_2\right)},\end{aligned} \tag{2}$$

where (rectangular form) $\tilde{F}_{\mathrm{exp}} = M_1\cos\varphi_1 + iM_1\sin\varphi_1$, $\tilde{F}_{\mathrm{cal}} = M_2\cos\varphi_2 + iM_2 sin\varphi_2$.

This general example shows that for the error magnitude spectrum calculation both, the magnitude and the phase of both, the experimental and the calculated spectra are needed. The information about the shape of the time domain signal is contained in the both, the magnitude and the phase. In other words, comparing the shapes of the time domain signals is done through calculating the error signal magnitude spectrum. At the time of the development of FFTBM it was mentioned that possible improvement of the method could involve “the development of the procedure taking into account the information represented by the phase spectrum of the Fast Fourier Transform in the evaluation of accuracy” [5]. As we can see from Eq. (2) the error signal magnitude inherently includes the magnitude and the phase of the experimental and calculated signal. The finding that both the magnitude and the phase of the experimental and calculated frequency spectra are contained in the D’Auria AA by making the Fourier transform of the difference signals is very important as this gives the possibility to compare the shapes of the signals. Therefore, the D’Auria is referred as $\mathrm{AA}^{M\varphi}$ since it contains the information of the magnitude M and phase φ. In addition, we agree with the authors that it is difficult to imagine which information is contained in the phase spectrum of the error signal. Please note that the experimental and calculated phase cannot be simply added. Therefore to the authors opinion the error signal phase information is not applicable for comparison of two signals.

In the FFTBM package there is an option of time shifting of the data trends to analyze separately the effects of delayed or anticipated code predictions concerning some particular phenomena or systems interventions. It is a Fourier transform property that a shift in the time domain corresponds to changing the phase. This property was used to identify the signals, which differ in time shift. Namely, the magnitudes of such signals are the same. Therefore the following expression was proposed:

$$\mathrm{AA}^M = \frac{\sum_{n=0}^{2^m}\left\|\tilde{F}_{\mathrm{exp}}(f_n)\right|-\left|\tilde{F}_{\mathrm{cal}}(f_n)\right\|}{\sum_{n=0}^{2^m}\left|\tilde{F}_{\mathrm{exp}}(f_n)\right|}, \tag{3}$$

where

$$\begin{aligned}\left\|\tilde{F}_{\mathrm{exp}}(f_n)\right|-\left|\tilde{F}_{\mathrm{cal}}(f_n)\right\| &= \left|\left(\left(\mathrm{Re}(\tilde{F}_{\mathrm{exp}}(f_n))\right)^2+\left(\mathrm{Im}(\tilde{F}_{\mathrm{exp}}(f_n))\right)^2\right)^{1/2}-\left(\left(\mathrm{Re}\tilde{F}_{\mathrm{cal}}(f_n)\right)^2+\left(\mathrm{Im}\tilde{F}_{\mathrm{cal}}(f_n)\right)^2\right)^{1/2}\right| = \\ &= \left|M_1-M_2\right| = \sqrt{\left(M_1-M_2\right)^2}.\end{aligned} \tag{4}$$

When $\varphi_1 = \varphi_2$ the Eq. (2) is equal to Eq. (4). This means that expression AA^M is a measure containing information from magnitudes *M* only. It is known that when two signals are only time shifted the magnitude spectra are the same. The value of AA^M is then zero. It is very unlikely to have the shape of the calculated signal, which is not shifted giving the same magnitudes as the experimental signal as predictions are required to be qualitatively correct. Therefore AA^M can be used when we are interested how the value of $\mathrm{AA}^{M\varphi}$ is increased due to the time shift contribution. In $\mathrm{AA}^{M\varphi}$ the information from both the shape of the time domain signal and the time shift is provided, while in AA^M only the time invariant information of the time domain signal is provided, what can be regarded to a certain degree as the shape of the time domain signal. Therefore making the difference $\mathrm{AA}^{\varphi} = \mathrm{AA}^{M\varphi} - \mathrm{AA}^M$ gives the information about time shift contribution. This expression is further normalized to:

$$I = \frac{\mathrm{AA}^{M\varphi} - \mathrm{AA}^M}{\mathrm{AA}^M} = \frac{\mathrm{AA}^{\varphi}}{\mathrm{AA}^M}, \qquad (5)$$

where the *I* tells how the compared time signals are shifted and therefore it is called time shift indicator. Larger the value of the time shift indicator *I*, larger is the contribution of the time shift to $\mathrm{AA}^{M\varphi}$ of the error signal. A large value of *I* (I>2) indicates, that the compared signals are maybe only shifted in time.

2.3 Spectral interpolation

As for AA^M calculation the sum is made from the difference of magnitudes there was a need to increase the number of samples in the frequency domain (to make the frequency spectrum more continuous) to correctly calculate the magnitude differences. This was done through zero padding briefly described below. For more details the reader is referred to [6]. The Discrete Time Fourier Transform (DTFT) can be viewed as the limiting form of the Discrete Fourier Transform (DFT) when its length N is allowed to approach infinity. The DTFT, which produces a continuous spectrum, is not suitable for a practical application because we can store only a finite number of samples, and we are able to compute the spectrum only at specific discrete values of frequency. However, spectral interpolation can be done by zero padding.

Because appending zeros does not change the input sampling rate, the frequency span of the FFT output will remain the same. The new output remains an evenly distributed set of samples spread over 0 to f_c. The sample spacing of the new output must decrease to fit more samples over the same frequency range. The decreased spacing is in the sampled output of the FFT and corresponds to a resolution increase in those samples.

2.4 Other proposals

As previously mentioned the advantage of the transformed error signal is that both the magnitude and the phase of compared signals are used for the accuracy assessment. Therefore it is suggested that all operations related for a more reasonable accuracy assessment are made already in the time domain, as it is very difficult to make any adjustments during the comparison of spectra in the frequency domain. For example, if a time shift is needed it should be done in the time domain. When the nature of the phenomenon is logarithmic (logarithmic plots) it makes sense to log the time signals before making the error function. In the case of numerous oscillations, like at flows, generally the D'Auria AA is very high as the oscillations of the experimental and calculated signals are usually not in phase. If these oscillations are measuring or are not important from the physical point of view, they should be filtered in the time domain by the moving average of the signal.

3 INPUT MODEL AND TEST DESCRIPTION

3.1 MELCOR input model description

In the following only a brief description of the input model is provided. For details the reader is referred to [7]. The hydrodynamic nodalization of the bundle and circuit was developed strictly following the recommendations on noding for the reference case simulation provided in the ISP-46 Specification Report [1].

The core nodalization of the bundle was modelled with the COR package. The bundle was modelled with two radial rings. In the first radial ring there are the control rod, the control rod guide tube and the inner 8 irradiated fuel rods. In the second radial ring there are the outer 10 irradiated fuel rods, the 2 fresh fuel rods and the stiffeners. The support plate and the two spacer grids were distributed in both radial rings according to the rings surface area. The shroud was considered as a heat structure and was not modelled with the COR package.

Because of the small size of the bundle in the Phebus facility, each ring of the core nodalization contains only one layer of fuel rods. Thus, an “average” rod in a ring has a much better view of the adjacent ring than would be the case in a full-scale reactor core. In addition the fuel rods in the inner ring can see not only the fuel rods in the outer ring but also directly the shroud.

Therefore the default radiative exchange factor 0.25 was increased to 0.75 to get the best agreement with the experimental measurements.

The Radionuclide package of MELCOR has three different radionuclide release models available. It was decided to perform the final simulation with the CORSOR-M model since the results were the best.

3.2 Phebus FTP1 test description

The ISP-46 was conducted as an open exercise, with all the relevant experimental results being available to the participants. It was divided into four phases:

- Fuel degradation, hydrogen production, fission product and structural material release (‘bundle’, phase 1).
- Fission product and aerosol transport in RCS (‘circuit’, phase 2).
- Thermal hydraulics and aerosol physics in containment (‘containment’, phase 3).
- Iodine chemistry in containment (‘chemistry’, phase 4).

With MELCOR phases 1 and 2 were simulated (first 18660 s). The degradation of the fuel was realised by a progressive increase of the nuclear power, up to the formation of a molten pool in the lower part of the bundle. The first cladding rupture occurred at 5700 s, cladding oxidation and hydrogen release at 8580 s, degradation of the control rod at 9690 s and the first fuel movement at around 11000 s. The total amount of hydrogen released was about 96 g, corresponding to 64% of the total zircaloy inventory in the bundle. At 11170 s the release of fission products (FPs) from the fuel started. A significant amount of FPs and structure material was released. The released materials were transported by the steam flow in the experimental circuit, comprising a hot leg at 970 K, the primary side of a steam generator at 420 K, and a cold leg at 420 K. Deposition of vapour and aerosols in various parts of the circuit was measured, as well as the flow rates in circuit. The deposition took place mainly in the two zones with abrupt temperature changes, just above the fuel bundle and in the rising line of the steam generator. For the other phases the reader is referred to [8].

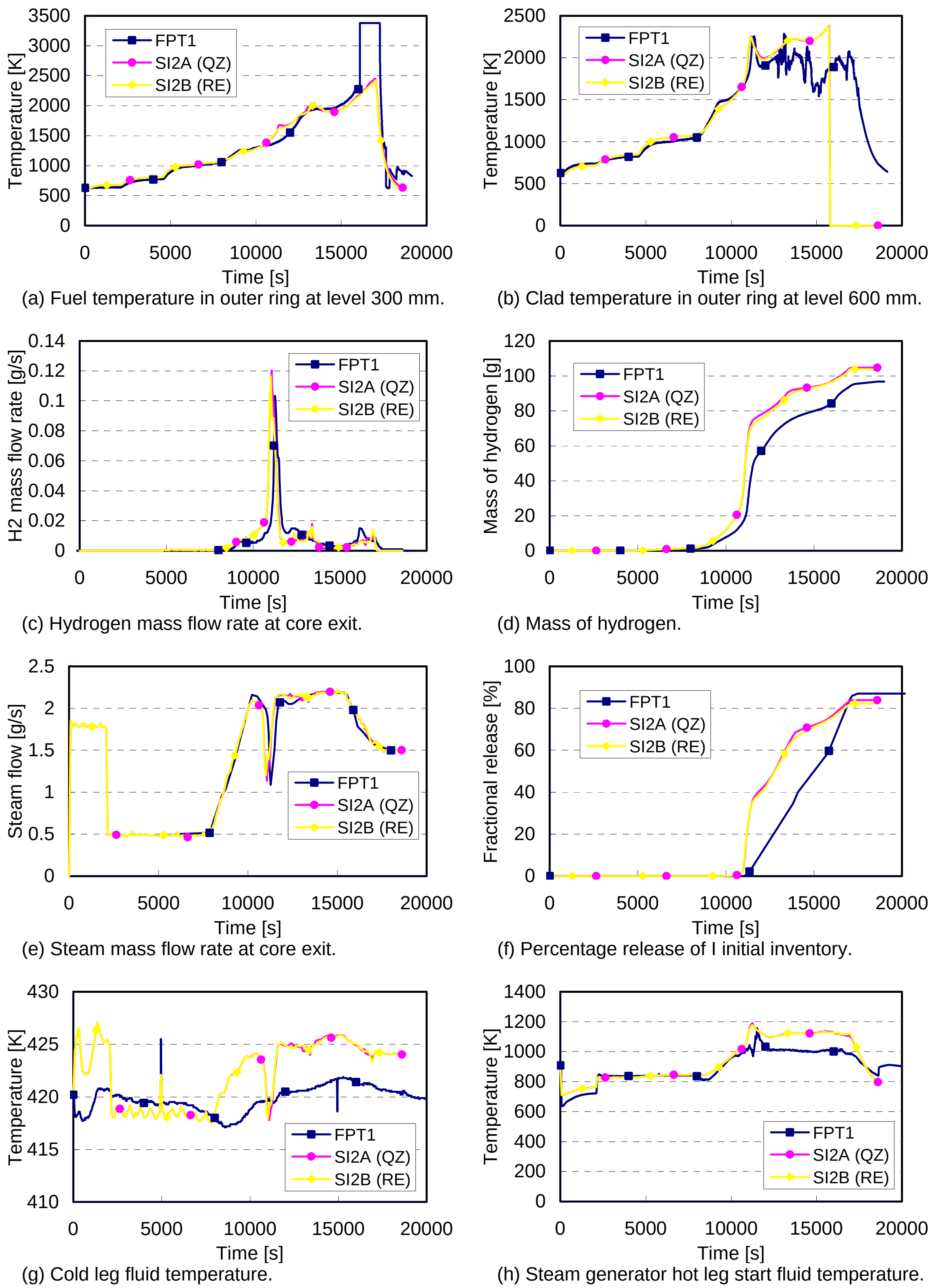
4 QUANTITATIVE ASSESSMENT OF THE CALCULATED RESULTS

The qualitative analysis with the conclusions is described in [7]. In order to perform a quantitative assessment a brief qualitative analysis based on visual observation was done first. The plots are shown in Fig. 1. The time dependent AA for parameters shown in Fig. 1 are shown in Fig. 2. Finally, Table 1 shows the quantitative results for all selected variables.

When comparing the AA of increasing time interval for thermalhydraulic variables shown in Fig. 2 with the trends of variables shown in Fig. 1, we see that AA changes with progressing into the transient and that each discrepancy influences AA. An abrupt decrease in accuracy is observed especially at the edges (sudden drop or increase of the variable). This is intrinsic to FFTBM as many harmonic components are generated [see Figs. 1(e) and 2(e)]. An abrupt decrease in accuracy occurs also when the experimental signal is very small compared to the calculated signal (for example, earlier prediction of some phenomenon). The earlier prediction of the release is shown in Figs. 1(c), 1(d) and 1(f), respectively and the corresponding AA of increasing time interval in Figs. 2(c), 2(d) and 2(f), respectively. From Fig. 2 it can be concluded that the temperatures in the fuel and clad agree very well during most of the transient. The accuracy of the fuel temperature [see Figs. 1(a) and 2(a)] decreases after 16000 s when the very sharp increase was not predicted and the accuracy of the clad temperature decreases after 12000 s [see Figs. 1(b) and 2(b)] when the clad temperature was under predicted for a few hundred K. The hydrogen mass flow rate accuracy was judged as poor due to the time shift of signals while the mass of hydrogen was judged as good at the end of the transient [see Figs. 1(f) and 2(f)] as the calculated released fraction was close to the experimental one. The steam flow rate was also predicted good as shown in Figs. 1(e) and 2(e). The accuracy of the Iodine (I) release at the end of the transient [see Figs. 1(f) and 2(f)] is similar to release of hydrogen. The circuit cold leg temperature was predicted very well as shown in Figs. 1(g) and 2(g) while the accuracy of the steam generator hot leg start temperature [see Figs. 1(h) and 2(h)] is comparable with the accuracy of the fuel and clad temperatures.

Finally, in Table 1 the accuracy for all selected parameters is shown. We can see that there are not only time functions and that the intervals for variables are different. The reason for different time intervals is that outside the interval the measured data are not correct or available or the calculation is not valid due to the MELCOR definition that the temperature of non-existing component is zero. Different intervals makes difficult to calculate the total accuracy. Another difficulty was a need to define new weighting factors for parameters occurring during severe accidents. As the selection of weighting factors for the total accuracy is subjective and requires several experiments to be fixed, the total accuracy was not calculated. Instead, the need to define a new figure of merit independent (or little dependent) on the weights was identified and this will be investigated in the future. The results show reasonable agreement for all selected parameters. For parameters, which are functions of time, AA is below 0.7 giving an average AA (can be considered as total accuracy) around 0.34. For radionuclide depositions logarithmic scale was used. Using moving average for experimental signal further increases the accuracy.

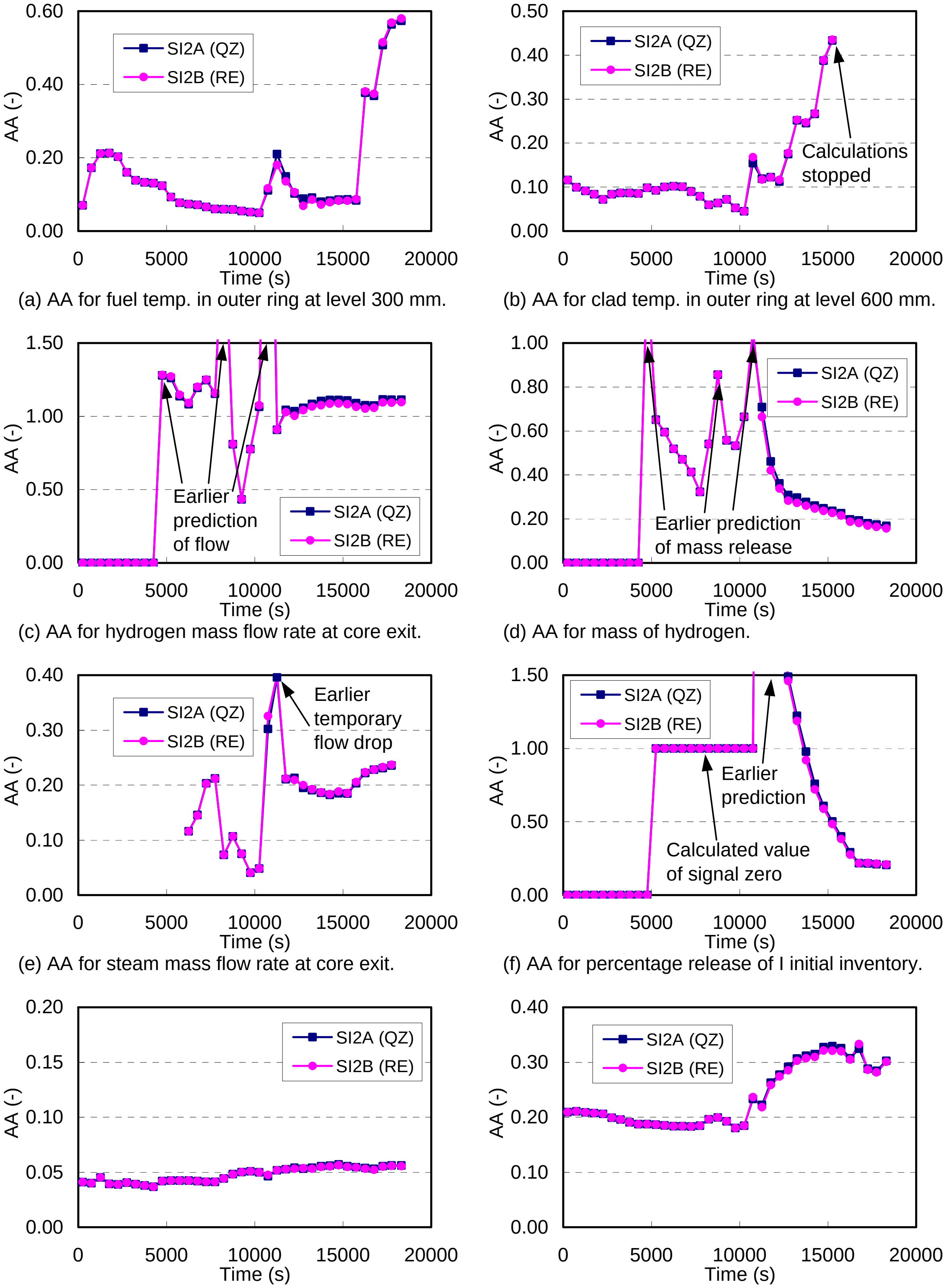
When comparing the above conclusions based on FFTBM with the qualitative analysis performed at participation in ISP46, they agree rather well. In [7] it was stated that the agreement of thermal-hydraulic variables is quite good, that the agreement of total releases for most radionuclide classes is satisfactory, and that the radionuclide depositions are somewhat over predicted (regarding to the total releases). It was also stated that the differences between the simulation results of both versions of MELCOR are negligible for thermal-hydraulic variables, small for radionuclide releases and the timing of key events, and significant for



(a) Fuel temperature in outer ring at level 300 mm.
(b) Clad temperature in outer ring at level 600 mm.
(c) Hydrogen mass flow rate at core exit.
(d) Mass of hydrogen.
(e) Steam mass flow rate at core exit.
(f) Percentage release of I initial inventory.
(g) Cold leg fluid temperature.
(h) Steam generator hot leg start fluid temperature.

Figure 1: Visual observation of measured and calculated parameters.

radionuclide depositions and bundle degradation. This statement also holds in the case when the moving average of signals and the logarithmic scale were used. Taking the moving average is justified as the calculation was performed for a few locations while in the



(a) AA for fuel temp. in outer ring at level 300 mm.

(b) AA for clad temp. in outer ring at level 600 mm.

(c) AA for hydrogen mass flow rate at core exit.

(d) AA for mass of hydrogen.

(e) AA for steam mass flow rate at core exit.

(f) AA for percentage release of I initial inventory.

(g) AA for cold leg fluid temperature.

(h) AA for SG hot leg start fluid temperature.

Figure 2: AA of increasing time interval for calculated parameters.

experiment the releases were measured every mm. Without using moving average the measured data oscillate as shown in Fig. 3. Figure also shows that in the case of deposition of radionuclides the oscillations are not very important from the physical point of view.

Table 1: Results of quantitative analysis.

			Interval 0 - 18600 s			
			SI2A		**SI2B**	
ID	**Label**	**Description of variable**	**AA**	***I***	**AA**	***I***
1	TCCLE	Cold leg fluid temperature	0.06	0.53	0.06	0.53
2	TCSGHS	Steam generator hot leg start fluid temperature	0.30	0.48	0.30	0.47
3	TCVLL	Lower vertical line fluid temperature	0.30	0.40	0.30	0.39
4	TSH1	Inside shroud temperature at level 800 mm	0.24	1.24	0.22	1.20
6	TU3R	Fuel temperature in outer ring at level 300 mm	0.57	0.16	0.58	0.17
8	Ag	Percentage release of Ag initial inventory	0.11	0.47	0.10	0.47
9	Cs	Percentage release of Cs initial inventory	0.20	0.48	0.20	0.46
10	I	Percentage release of I initial inventory	0.21	0.52	0.21	0.49
11	H2TOT	Mass of hydrogen	0.17	0.27	0.16	0.30
12	H2MFTOP	Hydrogen mass flow rate at core exit	1.11	2.05	1.10	3.06
12[a]	H2MFTOP	Hydrogen mass flow rate at core exit	0.65	0.76	0.49	0.83
13	TFLTOP	Fluid temperature at core exit	0.28	0.66	0.27	0.65
			Interval 0 - 15500 s			
5	TC3R	Clad temperature in outer ring at level 600 mm	0.43	0.67	0.44	0.67
			Interval 0 - 10000 s			
7	TABS	Absorber temperature at level 700 mm	0.09	0.60	0.09	0.60
			Interval 6000 - 18000 s			
14	STMFTOP	Steam mass flow rate at core exit	0.24	0.97	0.24	0.91
			Interval -2.42 – 0.26 m			
15[b]	Ag_d	Deposition of Ag	0.79	0.32	0.76	0.31
16[b]	Cs_d	Deposition of Cs	0.83	0.26	0.82	0.31
17[b]	I_d	Deposition of I	0.81	0.40	0.80	0.50
15[c]	Ag_d	Deposition of Ag	0.34	0.26	0.29	0.32
16[c]	Cs_d	Deposition of Cs	0.40	0.38	0.35	0.54
17[c]	I_d	Deposition of I	0.47	0.56	0.40	0.80

[a] calculated signal delayed 300 s, [b] logarithmic scale for all signals, [c] logarithmic scale for all signals plus moving average of the experimental signal

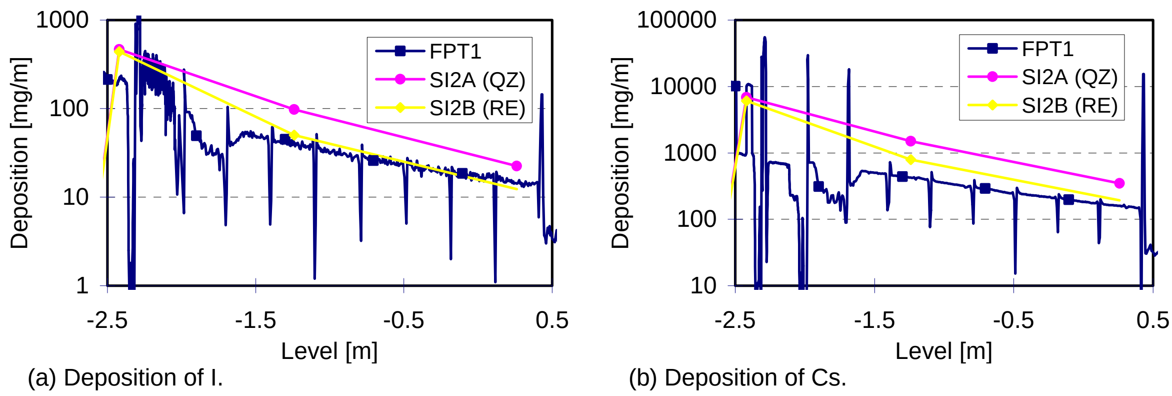


Figure 3: Deposition of radionuclides.

5 CONCLUSIONS

In the work the accuracy of the calculations of the severe accident International Standard Problem ISP-46 (Phebus FPT1), performed with two versions of the MELCOR

1.8.5, was quantitatively assessed. The improved FFTBM with the capability to calculate time dependent code accuracy was successfully adapted for the use within severe accidents field. New measure for the indication of the time shift between the experimental and the calculated signal was proposed. It was also suggested to make all operations in the time domain, as it is very difficult to make the adjustments in the frequency domain (e.g. logarithmic scale, moving average).

The quantitative results confirmed the qualitative conclusions done in the framework of ISP-46 participation. Finally, the quantitative FFTBM results showed that for the Phebus FPT1 severe accident experiment the accuracy of thermal-hydraulic variables calculated with the MELCOR severe accident code is rather high, despite the complex non-linear oxidation processes, which significantly influence the thermal-hydraulic behaviour.

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