BRAZILIAN JOURNAL
OF
RADIATION SCIENCES
10-03A (2022) 01 14

Passive Autocatalytic Recombiner Perfomance Assessment Using COCOSYS

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ABSTRACT

The progression of severe accidents in nuclear reactors is characterized by a diversity of phenomena that are Beyond Design Basis (BDBA), such as Direct Containment Heating (DCH), Molten Corium Concrete Interaction (MCCI), hydrogen detonation, and others. Currently, there are several devices and systems that allow mitigating the progression of these events, avoiding the failure of the physical barriers between the nuclear power plant and the environment. In this context, the present work aims to reproduce the HR-14 experiment carried out at the Thermal-hydraulic, Hydrogen, Aerosols and Iodine (THAI) test facility through the Passive Autocatalytic Recombiners (PAR) performance assessment with the COCOSYS code. The analysis of the convergence of the results was performed using the Fast Fourier Transform Based Method (FFTBM) and showed that the results had sufficient accuracy with the experimental data.

Keywords: **Hydrogen, Passive Autocatalytic Recombiners, THAI test facility, Severe Accidents.**

ISSN: 2319-0612
DOI: https://doi.org/10.15392/2319-0612.2022.1906
Submitted: 2022-01-31
Accepted: 2022-11-27

1. INTRODUCTION

Severe Accident (SA) in Pressurized Water Reactor (PWR) are Beyond Design Basis Accidents (BDBA) that causes failures in structures, systems, and components, that could not allow the reactor core cooling system to work perfectly and therefore lead to its degradation [1].

One of the consequences of a reactor core cooling system failure is the oxidation of the fuel rods and core components, which culminates with hydrogen generation. The accumulation of this gas can cause a deflagration with a possible Deflagration to Detonation Transition (DDT), challenging the integrity of the protection barriers between the nuclear reactor and the environment [2].

Among the main hydrogen mitigation devices for PWR containment are the Passive Autocatalytic Recombiners (PAR) and the igniters, which are proving to be the most used option for current designs and reactors in operation [3].

Considering the point of view of nuclear reactors safety analysis, this paper aims to perform a computational assessment of PAR performance using COCOSYS V2.4 code [4] by means of the HR-14 experiment carried out in the Thermal-hydraulic, Hydrogen, Aerosols and Iodine (THAI) test facility [5].

2. MATERIALS AND METHODS

The Hydrogen Recombiner (HR) tests carried out at the THAI test facility had the objective to provide a wide spectrum of benchmark to verify the operational performance of the PAR units from the manufacturers: Siempelkamp-NIS, AECL, and AREVA, which contemplate practically all the existing PAR models [5].

The THAI containment is a test vessel manufactured in stainless steel with a volume of 60 m^3, 22 mm thickness, 9.2 m high, and 3.2 m in diameter. The installation can be operated up to 180 °C and 14 bar, with an internal geometry composed of steel structures and a thermally insulated external environment. Additionally, this test facility has advanced systems with instrumentation and sensors online and offline, specially for field measurements, and gas and aerosol diagnostics; see Figure **1** [6].

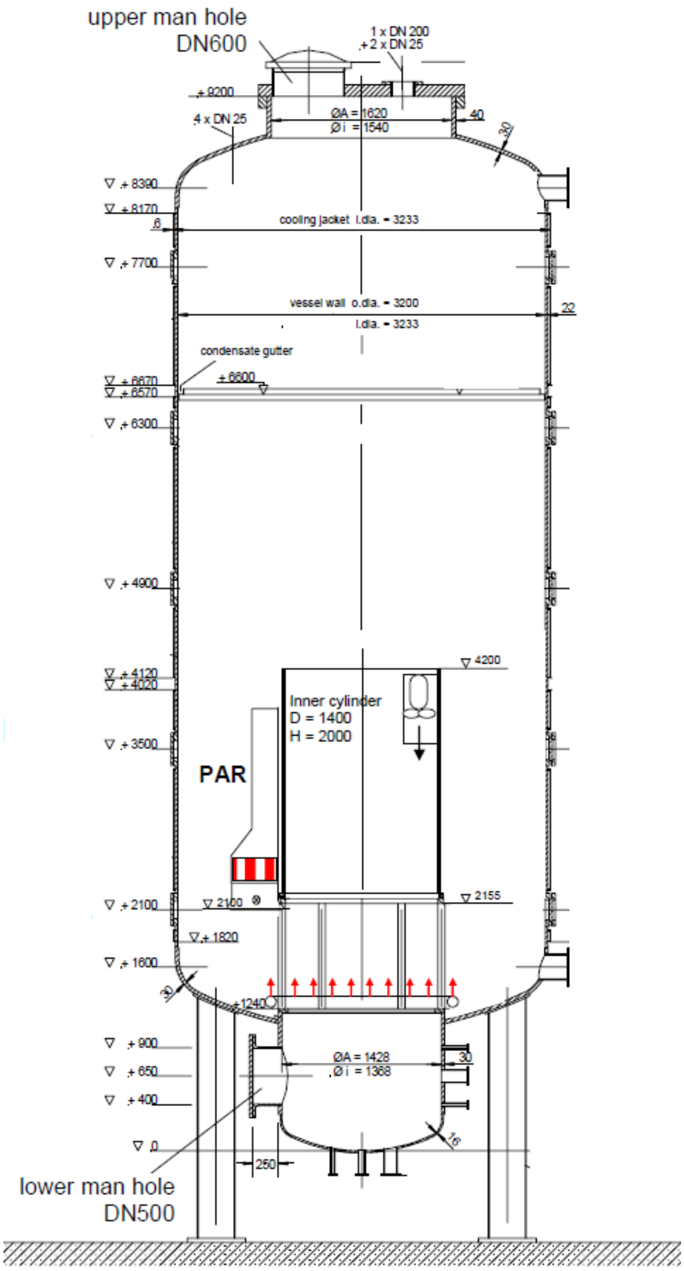

Figure 1: THAI test facility overview for the HR-14 experiment [7]

The PAR model used in the HR-14 experiment was the Siempelkamp-NIS ⅛, also commercially known as NIS-PAR 11 (Figure), which contains 11 cartridges coated with austenitic steel and filled with the catalyst material (Aluminum oxide as carrier and Palladium as catalytic coating) [5].

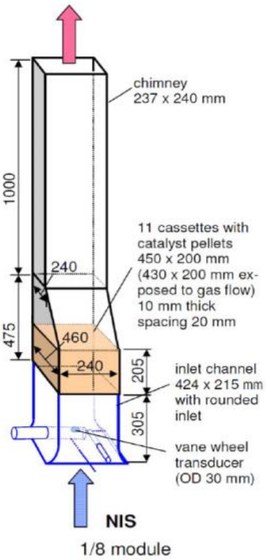

Figure 2: Siempelkamp-NIS 1/8 overview [8]

PAR are devices that convert hydrogen and oxygen into water through the exothermic reaction, equation (1), releasing approximately 238 kJ/mol [9]:

$$2H_2 + O_2 \rightarrow 2H_2O + \text{energy} \tag{1}$$

The PAR is referred to as a passive device because it operates without any energy source (a good approach for a station blackout event) and autocatalytic because it uses catalytic substances in order to reduce the activation energy of the reaction.

The mass flow rates of hydrogen and nitrogen applied in the HR-14 experiment to evaluate PAR performance are presented in Figure **3**. The nitrogen injection occurs in order to verify PAR performance in a mixed atmosphere and under oxygen starvation conditions.

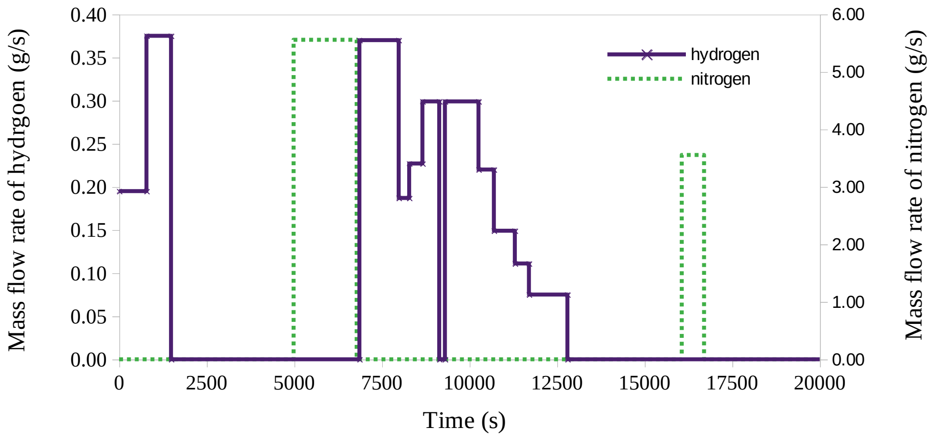

Figure 3: Hydrogen and nitrogen injection curves for experiment HR-14

2.1. THAI Containment Model in COCOSYS v2.4

The THAI Containment (Figure **4**) was modeled in the COCOSYS V2.4 code with 44 Control Volumes (CV) distributed radially and axially as shown in Figure **4**. The COCOSYS V2.4 deals separately with the transposition of fluids and gas/vapor, so the junctions are also presented between the control volumes for these types of flows. The heat structures (blue line) that represent the containment and the internal structures were modeled according to the information obtained from the experiment.

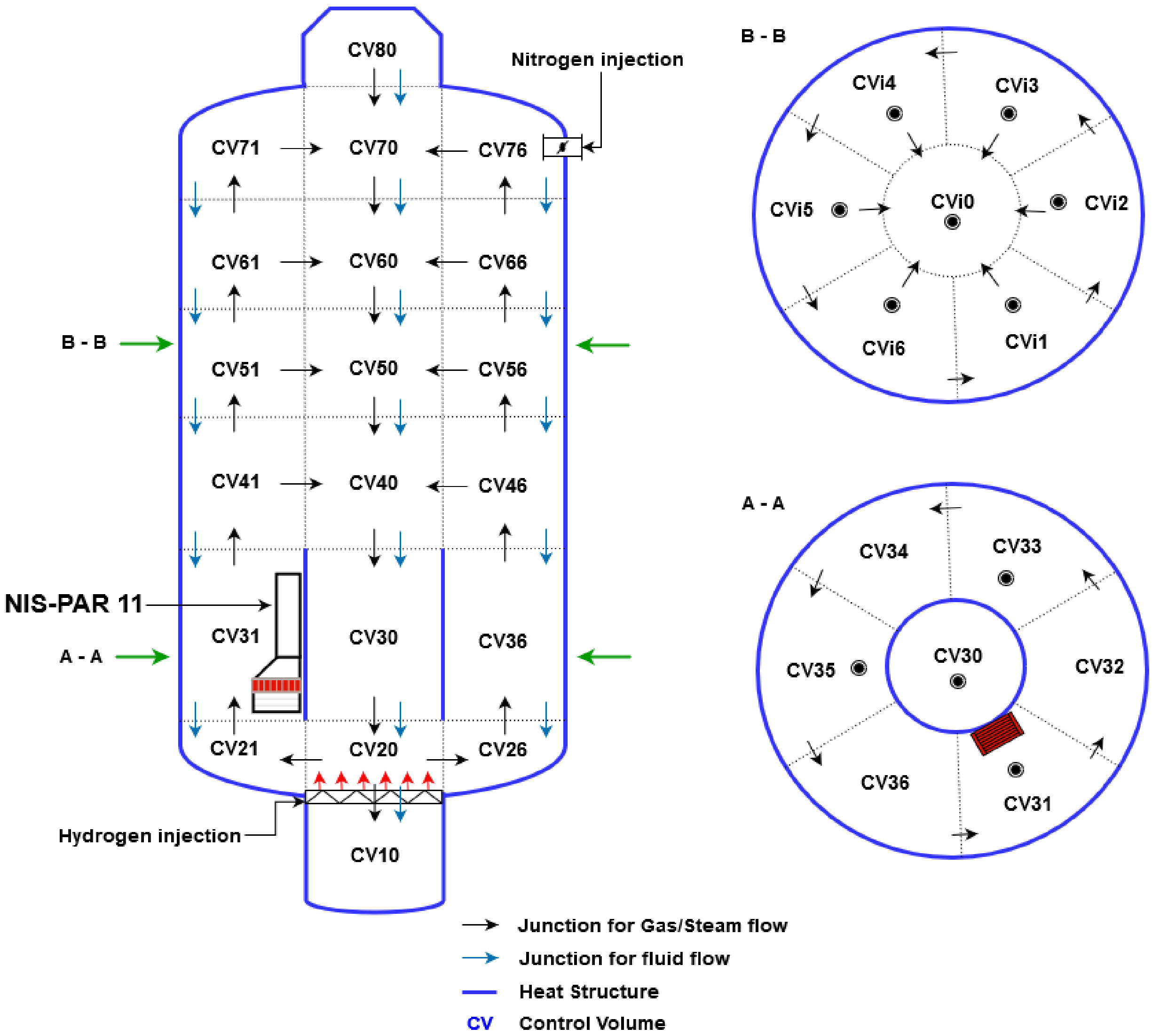

Figure 4: Nodalisation of THAI containment in COCOSYS v2.4

2.2. Fast Fourier Transform Based Method

The Fast Fourier Transform Based Method (FFTBM) [10] [11] [12] was applied to the results obtained for accuracy quantification. The FFTBM shows the measurement–prediction discrepancies in the frequency domain and quantifies the discrepancy magnitude. The FFTBM initially considers the error function between the Fast Fourier Transformation (FFT) of the calculated values (COCOSYS V2.4) and the experimental values, according to the equation (2):

$$(F(f_n)\Delta \vee)\left(\tilde{F}(f_n)_{\text{calc}} - \tilde{F}(f_n)_{\text{exp}}\right) \tag{2}$$

By definition, the two representations of the Fourier transform equations (3) and (4):

$$\tilde{F}(f) = \int_{-\infty}^{+\infty} \tilde{F}(t) e^{2\pi \mathrm{ift}} \mathrm{dt} \tag{3}$$

$$F(t) = \int_{-\infty}^{+\infty} \tilde{F}(f) e^{-2\pi \mathrm{ift}} \mathrm{df} \tag{4}$$

Discretizing the function in the time domain, for a set of N intervals, with spacing τ, it is obtained according to the equation (5):

$$F_k = \mathrm{F}(t_k), \quad t_k \equiv \mathrm{k}\tau \quad \mathrm{k}=0,1,2,\ldots,\mathrm{N}-1 \tag{5}$$

The approximation of the integral in equation (2) by discrete sum gives:

$$\tilde{F}(f_n) = \int_{-\infty}^{+\infty} \tilde{F}(t) e^{2\pi \mathrm{i} f_n t} \mathrm{dt} \approx \sum_{\mathrm{k}=0}^{N-1} F_k\, e^{2\pi \mathrm{i} f_n t_k} \tau = \tau \sum_{\mathrm{k}=0}^{N-1} F_k\, e^{2\pi \mathrm{ikn}/N} \tag{6}$$

With discrete values, the average amplitude (AA) is calculated by the sum of FFT error function, normalized by FFT of the experimental data, according to the equation (7):

$$AA = \frac{\sum_{n=0}^{2^m} |\Delta \tilde{F}(f_n)|}{\sum_{n=0}^{2^m} |\tilde{F}_{exp}(f_n)|} \tag{7}$$

To obtain the overall accuracy quantification for the computational model, the calculation of the total amplitude is performed by equation (8), which associates a weight factor by equation (9) that characterizes the simulated variable [10] [11].

$$\mathrm{AA}_{\mathrm{tot}} = \sum_{\mathrm{i}=1}^{\mathrm{Nvar}} (\mathrm{AA})_i \left(w_f\right)_i \tag{8}$$

$$\left(w_f\right)_i = \frac{\left(w_{\mathrm{exp}}\right)_i (w_{\mathrm{saf}})_i (w_{\mathrm{norm}})_i}{\sum_{\mathrm{i}=1}^{\mathrm{Nvar}} \left(w_{\mathrm{exp}}\right)_i (w_{\mathrm{saf}})_i (w_{\mathrm{norm}})_i} \tag{9}$$

The Table **1** show the weight factors components.

Table 1: Weight factors components [12]

Variable analyzed	w_{exp}	w_{saf}	w_{norm}	$w_{exp*wsaf*wnorm}$
Pressure drops	0.5	0.7	0.7	0.245
Mass inventories	0.8	0.9	0.9	0.648
Flowrates	0.5	0.5	0.8	0.200
Primary pressure	1.0	1.0	1	1.000
Secondary pressure	1.0	0.6	1.1	0.660
Fluid temperatures	0.8	0.8	2.4	1.536
Clad temperatures	0.9	1.0	1.2	1.080
Collapsed levels	0.8	0.9	0.6	0.432
Core power	0.8	0.8	0.5	0.320

The FFTBM should consider some important restrictions, such as those listed below, for its correct calculation [10]:

I. The FFTBM must be applied for interpolated values in a range of $2^9 – 2^{12}$ points;

II. The sampling must be satisfied (sampling frequency at least 2 times the highest frequency);

III. The FFTBM considers the maximum value equal to 0.4 of total amplitude for an acceptable adherence of the obtained results [10]. Above this value, the nodalization model must be refined to better interpret the phenomenology of the considered experiment.

The FFTBM approach was developed with SCILAB software [13]. Initially, the model was applied to a practical example already performed. In this case, one of the results of the IAEA-SPE-4 experiment [14] (cold leg rupture simulation) in the PMK-2 integral test facility [15] as an initial evaluation of the FFTBM calculation and it showed a good agreement with the experimental data.

3. RESULTS AND DISCUSSION

Initially, the first test carried out with the computational model was the verification of the initial condition parameters of HR-14 experiment in order to reach steady state conditions as shown in Table **1**. In addition, the model was tested for an interval of 500 seconds of computer simulation, and the stability of steady-state values was verified, Table **2**.

Table 2: Initial condition of HR-14 [7] and COCOSYS V2.4 calculation

HR-14 test	P (bar)	T (°c)	C_{steam}(vol.%
Specified	1.500	74.0	25.0
Measured	1.442	73.5	24.2
COCOSYS v2.4	1.442	73.5	25.1

The HR-14 experiment at THAI was monitored by a large number of sensors that acquired data at different positions of its containment [5], however, as the main object of this work is to assess the performance of the NIS-PAR 11, the results that are presented (Figures **5**, **6**, **7** and **8**) are related only to the Control Volume of PAR position (CV 31).

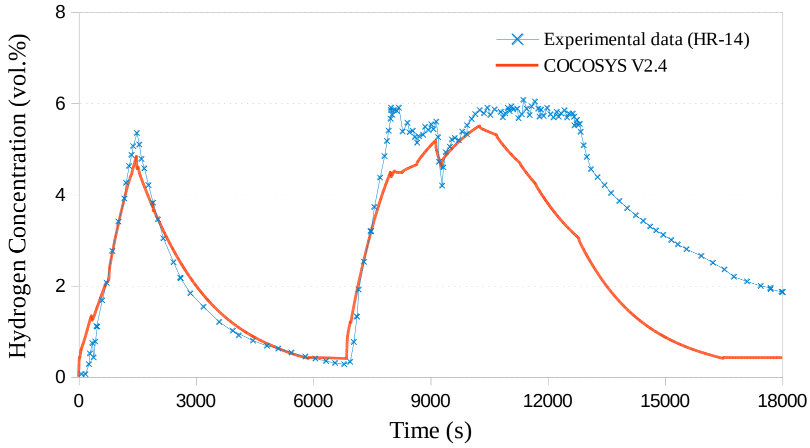

Figure 5: Hydrogen concentration inside containment (CV 31)

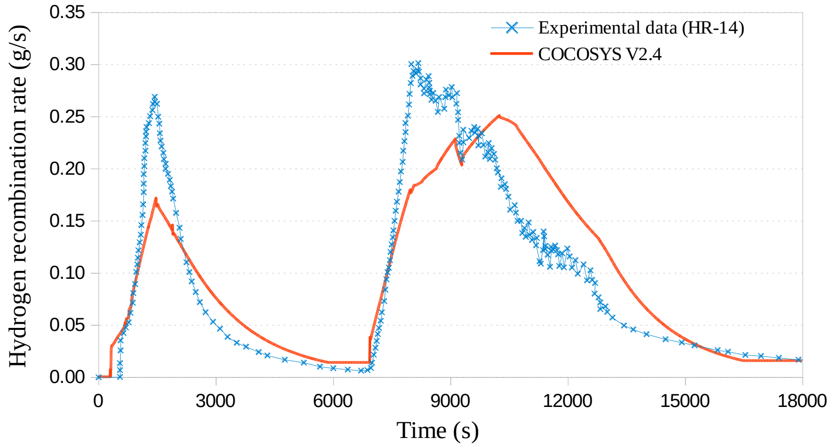

Figure 6: NIS-PAR 11 recombination rate

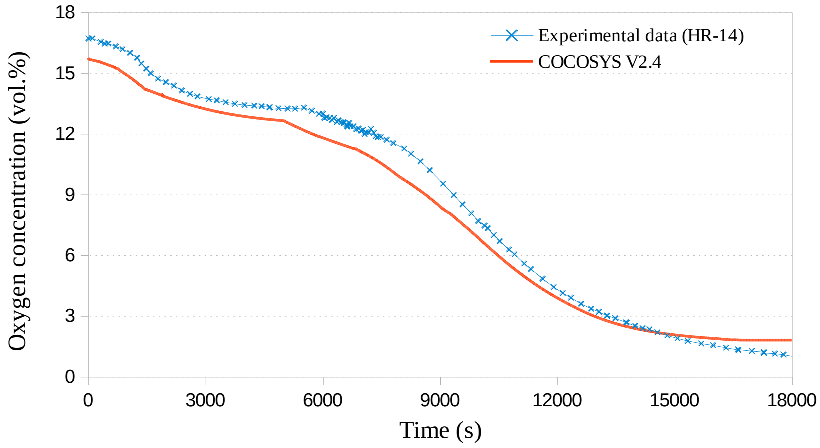

Figure 7: Oxygen concentration inside containment (CV 31)

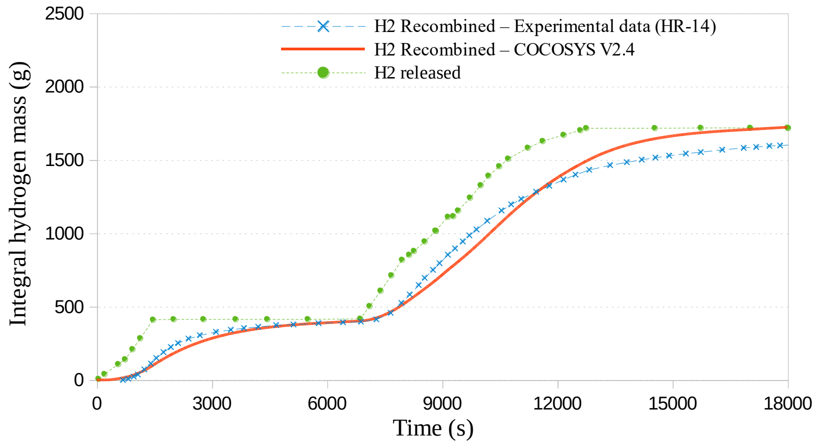

Figure 8: Integral hydrogen masses injected and recombined

As observed in Figures **5** and **6**, the NIS-PAR performance in the COCOSYS model was very consistent with the experimental data for lower values of hydrogen concentration, but when the hydrogen concentration becomes higher, it was observed in the experiment, the escape of bright particles from the PAR housing, which justifies the assumption of an additional mass recombination that occurs outside the range of the catalytic plates [16].

At the beginning of the second feeding phase, the model is in agreement with the measurements, but when the hydrogen concentration becomes higher, the simulation deviates from the experimental values due to the absence of the model's capacity to interpret this additional gain effect due to recombined mass.

The results presented in Figure **7** show a good agreement for oxygen concentration, including periods of decreased PAR efficiency and nitrogen injection.

The Integral hydrogen mass recombined in COCOSYS v2.4 was found to be in over-estimation within the relative error of 7% as show in Figure **8**.

The results of applying the FFTBM for PAR performance with COCOSYS v2.4 for HR-14 experiment are shown in Table **3**. The accuracy quantification was calculated considering the sensitivity analysis of cut frequency.

Table 3: FFTBM results

f_{cut} - Cut frequency (Hz)	0.011	0.022	0.033	0.044	0.056
AA_{tot} - Total accuracy	0.324	0.336	0.343	0.348	0.351

acceptability factor is $AA_{tot} < 0.4$

4. CONCLUSION

The results for accuracy quantification obtained applying the FFTBM show that the simulation model with COCOSYS v2.4 for HR-14 experiment reproduced with a good agreement the experimental data, as can be verified in Table 3 with all acceptability factors lower than 0.4, even considering the deviations observed during the assessment of the simulation results.

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