PRE-TEST SIMULATIONS OF A 28-ELEMENT HIGH-TEMPERATURE THERMAL-CHEMICAL EXPERIMENT USING THE COMPUTER CODES CATHENA AND CHAN-II-WL *

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ABSTRACT

Pre-test simulations have been performed for the first out-of-pile 28-element high-temperature thermal-chemical experiment using the computer codes CATHENA (MOD-3.3h) and CHAN-II-WL (MOD-28a). The ongoing CHAN thermal-chemical experimental program at Whiteshell Laboratories provides experimental data on the integrated thermal-chemical transient behaviour of a CANDU^{**} fuel channel with low-pressure, single-phase steam as the only coolant inside the channel. The program also increases our understanding of the behaviour of fuel channels at high temperatures and their integrity during postulated accidents.

A parametric study was performed using the computer codes to examine effects of steam flow rates, unheated fuel element simulators, moderator temperatures, and other variables on the predicted outcome of the experiment. The results of this study were used to optimize the experimental input parameters and test procedures. This paper details the parametric study with emphasis on the predicted effects of the various steam flow rates on test section behaviour.

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1. INTRODUCTION

In a CANDU Pressurized Heavy-Water (PHW) reactor, the fuel and coolant are separated from the heavy-water neutron moderator by horizontal fuel channels. The fuel channel consists of a Zr-2.5 Nb pressure tube and a Zr-2 calandria tube, separated by a gas-filled annulus. To demonstrate the safety of current and future CANDU-PHW reactors during postulated severe accidents, it is important to have a thorough understanding of high-temperature fuel channel behaviour under postulated accident conditions.

This understanding is best achieved by studying the underlying phenomena using mathematical models and single-effect tests. These models are then coupled into an integrated code to predict fuel channel behaviour under accident conditions. Data for validation of the codes come from various integrated experiments involving the complex interaction of pressure, temperature, material properties, heat transfer and reaction kinetics on fuel channel components subjected to severe temperature transients. These experiments are called the CHAN Thermal-Chemical Experiments.

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^{**} CANadian Deuterium Uranium, registered trademark of AECL.

The methodology adopted in this experimental program has been to perform several series of tests, progressing from a single Fuel Element Simulator (FES), to seven elements, and ultimately, to 28-element geometries. The single- and seven-element series have been completed and reported [1,2]. The next stage in this program is, therefore, to perform a 28-element out-of-pile high-temperature thermal-chemical experiment. An important part of these 28-element experiments is to perform pre-test simulations to optimize the experimental input parameters.

The computer codes CATHENA (MOD-3.3h) [3] and CHAN-II-WL (MOD-7a) [4] have been used to model the thermal-chemical behaviour of several out-of-pile hightemperature fuel channel experiments as part of the post-test analysis. The codes have also been used in a blind simulation study where they adequately predicted the behaviour of a seven-element experiment when only the input parameters were known [5].

As a result of the codes' performance in the above tasks, CATHENA and CHAN-II-WL were used to do pre-test simulations for our first CHAN 28-element experiment. The objectives of this paper are to report a parametric study of factors that were predicted to affect test section behaviour and to outline the recommended experimental conditions and test procedures. The results of this study are also useful for future pre- and post-test analyses of the CHAN hightemperature thermal-chemical experiments.

2. DESCRIPTION OF THE CODES

2.1 <u>CATHENA</u>

The CATHENA code was developed primarily for the analysis of postulated lossof-coolant accidents in CANDU reactors [6]. CATHENA uses a full two-fluid representation of two-phase flow in piping networks. This results in a model where liquid and vapour phases may have different pressures, velocities, and temperatures. The code uses a staggered-mesh, one-step, semi-implicit, finitedifference solution method, which is not transit-time-limited.

The effects of thermal radiation, pressure-tube deformation, zirconium/steam reaction, steam starvation and the presence of noncondensables can all be included.

2.2 <u>CHAN-II-WL</u>

CHAN-II-WL [4] is a modified Whiteshell Laboratories' version of the original CHAN II computer code [7]. CHAN II is a fast-running stand-alone computer code that predicts the transient behaviour of a fuel channel when the internal coolant is superheated steam. With suitable changes in geometry and material properties, the CHAN II code has been used to calculate the transient thermalchemical responses of CANDU fuel channels during a postulated severe loss-ofcoolant accident when steam is the only coolant available.

The CHAN II code assumes the complex fuel bundle pin geometry can be represented by an equivalent cylindrical ring geometry. It divides the simulated fuel channel into several axial segments. Each segment is radially subdivided into fuel rings, flow ring subchannels, the pressure tube, and the calandria tube. The code considers each fuel segment to be axisymmetric and axially isothermal.

3. DESCRIPTION OF THE EXPERIMENT

3.1 <u>Experimental Apparatus</u>

The 28-element test section consisted of three rings of fuel element simulators concentrically located inside a Zr-2.5 Nb pressure tube (Figure 1). Each fuel element simulator consisted of Zr-4 cladding (15.2-mm OD and 14.4-mm ID) within which annular alumina pellets (14.3-mm OD, 6.1-mm ID and 16 mm in length) electrically insulated the cladding from a graphite rod heater. The 6-mm-diameter graphite rod heater was coated with tungsten carbide to minimize the reaction between the alumina and the graphite at high temperatures. The length of the graphite rod heaters was 1800 mm.

The fuel element simulator bundle was surrounded by a 2105-mm-long section of autoclaved Zr-2.5 Nb pressure tube mounted inside a 1780-mm-long Zr-2 calandria tube (Figure 2). The test-section annulus (gap between the pressure and calandria tubes) contained an Inconel X-750 garter spring located at the test section centreline. The calandria tube was surrounded by heated, nonflowing water in an open tank. The top surface of the calandria tube was covered by at least 250 mm of water throughout the experiment.

Five spacer plates, machined out of 0.90-mm-thick Zr-4, were symmetrically placed in the heated zone of the test section (Figure 2). Their purpose was to simulate the effects of CANDU bundle end plates on steam flow patterns through the fuel element simulator bundle, and to help minimize sag of the bundle at high temperatures.

A schematic of the entire test apparatus is shown in Figure 3. Steam produced in the boiler passes through the steam superheater and into the test section. The steam picks up energy from the hot fuel element simulators as it passes through the test section and some of the steam reacts exothermically with the zirconium, releasing hydrogen.

The hot steam-hydrogen mixture exiting the test section is directed through a condenser to condense the steam. The resulting mixture of condensate and hydrogen enters a water trap where the condensate is collected. The remaining hydrogen gas flows through a mass flowmeter and is vented to the atmosphere.

3.2 Instrumentation

The fuel element simulators are connected in parallel to a DC power supply. The power to the test section will be determined using measured voltage drops across the test section and measured current flow through the fuel element simulators. Power distribution throughout the fuel element simulator bundle is designed to be similar to that found in a Pickering-type fuel bundle. Normalized pin powers will be roughly 1.111, 0.894 and 0.775 for the outer, middle, and inner fuel-element-simulator rings, respectively. Thermocouples were used to monitor temperatures of the inside surface of the fuel element simulators, outer surface of the pressure and calandria tubes, steam flow, and moderator water. The fuel element simulator bundle was radially subdivided into six rings for instrumentation purposes (Figure 1). The thermocouples inside the fuel element simulators were Al_2O_3 insulated C-Type (tungsten rhenium) with 0.25-mm-diameter sensing wires. These thermocouples were threaded through small holes in the Al_2O_3 insulators of the fuel element simulator, less than 1 mm away from the inner surface of the cladding.

The thermocouples monitoring temperatures of the pressure tube, calandria tube, steam flow, and moderator water were standard R-Type or K-Type, depending on the expected temperature range. The individual sensing wires for the pressureand calandria-tube thermocouples were slightly separated and spot-welded directly onto the tube surface.

3.3 Proposed Experimental Procedures

The proposed experimental procedures for the 28-element thermal-chemical experiment are as follows:

- Heat the water surrounding the calandria tube to 85°C (for degassing), and then reduce it to 75°C for the test.
- Purge the inside of the end hubs, including the fuel element simulators, with helium, and heat the test section in argon.
- 3) Purge the annulus between the pressure tube and the calandria tube with CO_2 (Stage 1). The purge flow will be high initially but reduced to 6 L/min prior to the start of the test.
- 4) Steam will be introduced into the superheater and the argon flow stopped at the end of Stage 1. The steam flow will likely be 10 g/s and the electric power to the test section will be 10 kW (Stage 2). The entire proposed test section power profile for this experiment is given in Figure 4.
- 5) Once the test section temperatures have stabilized in Stage 2, test section power will be ramped to 40 kW to start Stage 3. Stage 3 is designed to be a pseudo steady-state portion at a reasonably high power.
- 6) The test section power will then be ramped from 40 to 135 kW to start Stage 4. Power will be left at this value until maximum recorded fuel-element-simulator temperatures exceed 1700°C. Electric power to the test section will then be turned off to study the energy released from the exothermic zirconium/steam reaction at elevated temperatures (Stage 5).
- 7) The test will be terminated when test section temperatures are observed to decrease. The test will be terminated by shutting off the steam flow to the test section and introducing an argon purge, thus shutting down the zirconium/steam reaction.

4. MODELLING ASSUMPTIONS

The CATHENA (MOD-3.3h) and CHAN-II-WL (MOD-28a) computer codes were used to perform the pre-test simulations. The main modelling assumptions were as follows:

- 1) Geometrical deformation and buoyancy-induced free convection were neglected.
- 2) The test section was axially discretized into 12 equal lengths. A 90-degree symmetry pin model was used in the CATHENA simulation while a ring model was used in the CHAN-II-WL simulation (Figure 5). CATHENA modelled seven fuel element simulators, each divided into an inner and outer surface. A quarter of the pressure tube was sectored to three equal-length portions. Thus CATHENA employed 17 isothermal surfaces at each axial segment. For CHAN-II-WL, the 28 fuel element simulators were grouped into three concentric rings, each divided into an inner and outer surface. CHAN-II-WL used seven isothermal surfaces at each axial segment.
- 3) Subchannel steam flows were assumed to be completely mixed at the end of each axial segment for CHAN-II-WL, but only at spacer plates for CATHENA.
- 4) The Urbanic-Heidrick equations [8] were used to calculate the zirconium/steam reaction rates. At temperatures over 1850°C, a constant reaction rate was used to approximate the molten zirconium/steam reaction. The flow area blockage due to molten material and bundle relocation were ignored.
- 5) Emissivities of the pressure-tube inner and outer surfaces were assumed constant and equal to 0.8. The emissivity of the calandria tube inner surface was assumed to be constant at 0.3.

5. PARAMETRIC STUDIES

5.1 <u>Overview</u>

Electric power to the test section was constrained to 5.4 kW per fuel element simulator to ensure integrity of the fuel element simulators up to 1700°C. Hence, the maximum total power to the test section was proposed to be 135 kW (5.36 kW for each outer-ring fuel element simulator) for this experiment (Figure 4). Other parameters affecting the performance of the experiment and the simulations were:

- steam flow rate,
- unheated fuel element simulators,
- moderator water temperature,
- use of different zirconium oxidation correlations,
- flow mixing assumptions,
- surface emissivities used in the computer codes, and
- pressure-tube deformation and/or bundle slump.

Effects of using different zirconium oxidation correlations were not assessed at the present time since CATHENA (MOD-3.3h) offers only one correlation (Urbanic-Heidrick [8]). Effects of flow mixing assumptions were examined for the purpose of confirming the significance of Assumption 3. Effects of surface emissivities and pressure-tube deformation were also examined to some degree during this study.

The main thrust of the present work is to study the effects of the first three parameters. The steam flow rate was found to be a key factor since it has a dual effect on the experimental results. High steam flow rates provide adequate steam for the zirconium/steam reaction and significant steam cooling to the test section. Low steam flow rates, however, have negligible cooling effects but may result in a steam starvation situation. Steam starvation limits the heat generation from the zirconium/steam reaction and may, in turn, lower test section temperatures.

5.2 <u>Effect of Steam Flow Rates</u>

A total of five CATHENA simulations were performed to study the effect of steam flow rates on test section temperatures and hydrogen production. Steam flow rates of 5, 8, 9, 10, and 15 g/s were examined while other conditions were kept unchanged.

A common simulation restart file was produced for these five runs. This file covered the low-power stages 1, 2 and 3 (up to 900 s), providing a common starting point for subsequent simulations. Test conditions for this file were a steam flow rate of 5 g/s, an electric power profile of 2, 10, and then 40 kW as per Figure 4, all fuel element simulators powered, a steam inlet temperature of 700°C, and a moderator water temperature of 75°C.

Electric power to the test section for each simulation was turned off when the maximum fuel-element-simulator cladding temperature reached 1700°C. Results of these simulations are summarized in Table 1.

Maximum values for the heat generation from the zirconium/steam reaction are plotted versus the steam flow rate in Figure 6. These values, as well as maximum values for the hydrogen production rate, fuel-element-simulator cladding temperature, and steam exit temperature (Table 1) increased with increasing steam flow rates and reached maximums at a steam flow rate of 8 g/s. These predicted results then decreased with further increases in steam flow rates. This was due to insufficient steam supply (steam starvation) for steam flow rates less than 8 g/s and increasing steam cooling for steam flow rates greater than 8 g/s.

Effects of steam flow rates on cladding temperatures of the inner-ring fuel element simulators, 1425 mm into the heated zone, are illustrated in Figure 7. Predicted test section temperatures continued to increase after the electric power was turned off in all the cases studied. This uncontrolled temperature escalation indicated the zirconium/steam reaction was self-sustaining at certain locations in the test section. Maximum predicted test section temperatures occurred at a steam flow rate of 8 g/s. At 8 g/s, there was enough steam to fuel the zirconium/steam reaction but not enough to contribute any significant excessive cooling. Steam starvation was predicted to occur at steam flow rates \leq 8 g/s and anything above 8 g/s helped cool the test section.

5.3 Effect of Unheated Fuel Element Simulators

Concerns about having unheated fuel element simulators to facilitate the experimental instrumentation had not been previously addressed in this experimental program. The following comparisons were made to determine potential differences between the predicted results when 28 pins are powered (Case 1) and the results when the four inner-ring fuel element simulators are not powered (Case 2).

Two CATHENA simulations were performed using a steam flow rate of 10 g/s, a moderator water temperature of 75°C, and identical electric power per heated pin. Total maximum test section electric powers, however, were different for the two cases, reflecting the fact that the four central pins were not powered in Case 2. The powers were 135 kW for Case 1 and 120 kW for Case 2. Figure 8 shows CATHENA predicted differences between the two cases for inner-ring fuel-element-simulator cladding temperatures, 1425 mm into the heated zone, and the heat generated by the zirconium/steam reaction.

To allow test section temperatures to reach 1700°C, the 120-kW full power was left 91 s longer for Case 2 than Case 1. Test section temperatures for Case 2 were significantly lower than for Case 1 prior to turning the electric power off. Temperature differences for these two cases, however, became insignificant once maximum test section temperatures exceeded 1700°C and the electric power was returned to zero. There were no significant differences in heat generation rates from the zirconium/steam reaction between the two cases other than a slight time delay for the case having four unheated pins.

5.4 Effect_of_Moderator_Temperature

The effects of moderator water temperatures of 75 and 25°C were studied. The predicted test section temperatures and hydrogen production showed negligible differences between these two cases. The predicted heat fluxes from the calandria tube to the moderator were below the critical values. Therefore, the predicted effect was expected since moderator water temperature does not significantly affect nucleate pool-boiling heat transfer on the external surface of the calandria tube.

5.5 <u>Effects of Other Parameters</u>

The effects of the number of times the subchannel flows were assumed to be well mixed were assessed by CATHENA and CHAN-II-WL. In the CATHENA simulations, more complete flow mixing locations along the test section tended to yield slightly higher predicted test section temperatures, but overall the differences were not significant. CHAN-II-WL was more sensitive to the flowmixing assumptions. From the CHAN-II-WL predictions, temperature differences between 12 complete flow mixes and no flow mix were as high as 150°C.

The effects of pressure-tube deformation and surface emissivities for various test section components on the predicted results were examined to some degree in this work. Further studies are needed for conclusive assessments on these effects.

6. COMPARISON OF CATHENA AND CHAN-II-VL PREDICTIONS

The purpose of comparing CATHENA and CHAN-II-WL predictions in this report was not to judge which code was more suitable for this pre-test simulation work, but rather to gain confidence in the predicted results and to make a proper proposal for the conditions of the upcoming experiment.

A simulation was performed using CATHENA and CHAN-II-WL. The test conditions assumed were 10 g/s steam flow rate, 75°C moderator water temperature, 135-kW maximum electric power to the test section, and complete subchannel mixing at 12 axial locations.

Test section temperatures predicted by CHAN-II-WL were consistently higher than CATHENA predictions during the medium- and high-power stages 3 and 4 (Figure 9). As a result of these differences, electric power to the test section was left on 49 s longer in the CATHENA simulation in order for maximum cladding temperatures to reach 1700°C. Peak cladding and pressure-tube temperatures, however, were higher for the CATHENA prediction. One possible reason for the difference is in the way the two codes model the thermal characteristics of the fuel element simulator bundle, i.e., ring versus pin model.

Predicted heat generation from the zirconium/steam reaction using the two codes is also shown in Figure 9. There appears to be a time lag between the two code predictions, with CATHENA lagging behind CHAN-II-WL. This "time lag" relates back to the slower test section heating rates predicted by CATHENA during Stages 3 and 4. Differences in the peak hydrogen production rates and the cumulative amount of hydrogen were small despite the differences in timing of the events.

In summary, predictions by CATHENA and CHAN-II-WL follow similar trends but differ slightly with the timing of event and maximum test section temperatures achieved. Differences in the ring and pin approaches to characterize the fuel element simulator bundle and in the convective models used in the two codes may be the main source of the differences observed.

7. RECOMMENDATION

Based on the above pre-test simulation results, we recommended the following test conditions for the first out-of-pile 28-element thermal-chemical test:

- steam inlet temperature of 700°C and flow rate of 10 g/s;
- moderator water temperature of 75°C;
- electric power profile of 2, 10, 40, and 135 kW for Stages 1 through 4 respectively (Figure 4); and
- to turn off the electric power to the test section when maximum recorded fuel-element-simulator temperatures exceed 1700°C to study the energy released from the exothermic zirconium/steam reaction.

The recommendation for using a steam flow rate of 10 g/s was largely based on having enough steam available for the zirconium/steam reaction without having too much excessive steam cooling. We did not recommend 8 g/s because of concerns of having some of the steam flow bypass the bundle after the test

section began to slump at high temperatures. Steam starvation would occur with a flow rate of 8 g/s if any of the steam bypassed the bundle or was not well mixed at each spacer plate.

Another concern was with the oxidation rates used by CATHENA (MOD-3.3h) at high temperatures. Recent work by Prater and Courtright [9] have reported significantly higher oxidation rates at high temperatures than those used in CATHENA. A steam flow rate of 8 g/s would result in significant steam starvation if the Prater and Courtright correlation was used. In fact, even a steam flow rate of 10 g/s would result in steam starvation using this correlation, but not to the same extent as with 8 g/s.

8. A FULL SIMULATION USING THE PROPOSED CONDITIONS

A full pre-test simulation (i.e., from time = 0 s) employing the proposed test conditions was performed using CATHENA. The purpose of this simulation was to give an overall picture of the test section behaviour prior to conducting the experiment and to further confirm the proposed test procedures outlined in Section 3.3.

Selected predicted transient temperatures of the test section at one axial location are shown in Figure 10. Stages 3, 4 and 5 with electric power of 40, 135, and 0 kW, respectively, are shown. All predicted temperatures continued to increase after the electric power was returned to zero, indicating the zirconium/steam reaction was self-sustaining under these test conditions. Predicted radial temperature gradients were higher in Stage 5 than in other stages because of the higher reaction rates in the well-insulated inner- and middle-ring fuel element simulators. Temperatures increased sharply and then decreased during Stage 5, indicating the complete oxidation of the cladding at some axial and radial locations.

The predicted energy balance for this simulation is given in Figure 11. Maximum energy generated by the zirconium/steam reaction was 103 kW and occurred just after turning the electric power off. Near that time, 60 kW of heat was removed radially through the pressure and calandria tubes to the moderator water, and 15 kW was removed axially by the steam flowing in the pressure tube. The shaded area in the plots represents the period when the cumulative reaction heat from the entire test section was larger than the total heat removal. This indicates the zirconium/steam reaction will be self-sustaining, especially in the high temperature zone near the end of the test section.

9. SUMMARY

Pre-test simulations of the first out-of-pile 28-element thermal-chemical experiment have been successfully performed using CATHENA (MOD-3.3h) and CHAN-II-WL (MOD-28a). A parametric study has been done to optimize the experimental input parameters for this test. From this work, the following key points are summarized:

1) The proposed steam flow rate of 10 g/s was based on providing steam-rich conditions for the exothermic zirconium/steam reaction and relatively

low heat removal by steam. Local steam starvation, however, may still occur at this steam flow rate owing to possible bundle or pressure-tube deformation, zirconium melt relocation, or flow area blockage.

- 2) The simulations indicated no adverse consequences associated with disconnecting electric power to the four inner-ring fuel element simulators except for a slight time delay caused by the lower bundle power. Maximum predicted cladding temperatures and hydrogen production rates were similar for the case where all 28 fuel element simulators were powered and the case where no electric power was provided to the four central fuel element simulators.
- 3) Moderator water temperatures had insignificant effects on test section temperatures under the conditions of this experiment.
- 4) Predicted test section temperatures continued to increase after electric power was returned to zero. This indicated a self-sustaining exothermic zirconium/steam reaction.
- 5) Peak cladding temperatures for most of the simulations were above 2000°C because of local temperature escalation caused by the exothermic zirconium/steam reaction. Simulation uncertainties above 2000°C are significant and difficult to estimate owing to limited verification data.

The results of this pre-test investigation were used to design a 28-element high-temperature thermal-chemical experiment. The experiment has since been successfully completed and post-test analysis of the results is ongoing. The experiment used the steam flow rate of 10 g/s and steam inlet temperature of 700°C, and moderator water temperature of 45°C, with one central fuel element simulator that was not electrically powered. Local temperature escalations caused by the self-sustaining of the zirconium/steam reaction were observed when electric power to the test section was shut off. These preliminary results correspond with our pre-test simulation results.

10. REFERENCES

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Table 1 Effect of Steam Flow Rates on CATHENA Predictions					
Description	Run 1	Run 2	Run 3	Run 4	Run 5
Steam flow rate (g/s)	5	8	9	10	15
Maximum cladding tem- perature of inner-ring fuel element simulators (°C)	2218	2337	2193	2273	1987
Maximum H ₂ production rate (mole/s)	0.30	0.35	0.31	0.29	0.25
Maximum heat generation by the Zr/H_2O reaction (kW)	82.4	95.2	6 8.1	80.6	66.7
Maximum steam exit temperature (°C)	1391	1633	1584	1512	1351
Local steam starvation ?	YES	YES	NO	NO	NO



FIGURE 1: Cross Section of the Test Section and Thermocouple Radial Locations



FIGURE 2: Schematic of the Test Section (not to Scale)



FIGURE 3: Schematic of the Test Apparatus



FIGURE 4: Proposed Electric Power Profile for the CHAN 28-Element Experiment



FIGURE 5: CATHENA 90-Degree Symmetry Model and CHAN-II-WL Entire Ring Model Used for the Simulation of the CHAN 28-Element Experiment



FIGURE 6: CATHENA Predicted Effects of Steam Flow Rates on Maximum Heat Generation from the Zirconium/Steam Reaction



FIGURE 7: CATHENA Predicted Effects of Steam Flow Rates on Cladding Temperatures of the Inner-Ring Fuel Element Simulators, 1425 mm into the Heated Zone



FIGURE 8: CATHENA Predicted Effects of Having Unheated Pins on Cladding Temperatures of Inner-Ring Fuel Element Simulators, 1425 mm into the Heated Zone (a), and Heat Generation from the Zirconium/Steam Reaction (b)

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FIGURE 9: Comparison of CATHENA and CHAN-II-WL Predictions: Inner-Ring Fuel-Element-Simulator Cladding Temperatures (a) and Pressure-Tube Temperatures (b), 1425 mm into the Heated Zone, and Heat Generated by the Zirconium/Steam Reaction (c)



FIGURE 10: CATHENA Prediction of Test Section Temperatures, 1575 mm into the Heated Zone, Using the Proposed Test Conditions: Steam Flow Rate = 10 g/s, All 28 Pins Heated, and Moderator Water Temperature = 75°C



FIGURE 11: CATHENA Prediction for Heat Input (a), Heat Removal (b), and Total Heat Input/Removal (c) Using the Proposed Test Conditions: Steam Flow Rate = 10 g/s, All 28 Pins Heated, and Moderator Water Temperature = 75⁶C

