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Thermo Mechanical Calculations for Integrated High Fidelity Reactor Core Simulations

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The Numerical Nuclear Reactor is a collaborative US-ROK I-NERI project to develop a comprehensive high fidelity reactor core modeling capability for detailed analysis of current and advanced reactor design. One of the objectives of the US-ROK collaborative I-NERI project known as the "Numerical Reactor" is the application of thermo-mechanical techniques for structural calculations as part of integrated whole-core simulations. In the thermo-mechanics area, activities to date are focused on assessment of the thermo-mechanical response of fuel assemblies, development of an efficient computational methodology to simulate that response, and establishing an interface for coupling of this methodology with the CFD module. The mechanical response or bowing deflection of core assemblies due to thermal gradients, swelling and irradiation creep are being formulated as a function of location in the core and the assembly support structures for a typical PWR core. It is anticipated that these mechanical responses will be significant during startup, long term operation, and various transients, and examination of the effects of such geometric changes on reactor operations will be important.

KEYWORDS: Themo-mechanics, Rod Bowing, Thermal-hydraulics, coupled codes, computational fluid dynamics, CFD, numerical reactor, DNB

1. Introduction

As part of a US-ROK collaborative I-NERI project, a comprehensive high fidelity reactor core modeling capability is being developed for detailed analysis of current and advanced reactor designs. The work involves the coupling of advanced numerical models such as computational fluid dynamics (CFD) for thermal hydraulic calculations, whole core discrete integral transport for neutronics calculations, and thermo-mechanical techniques for structural calculations.

Previous papers have provided an overview of the project [1,2] and detailed discussions of the key phenomenological models and the interfaces for the coupling of these models. For conventional reactor applications, coupling of the thermo-mechanical and thermal hydraulics analyses can be used to assess the effects of rod bowing on flow and heat transfer, which may affect assessments of departure from nucleate boiling (DNB). In advanced reactors, where inherent safety characteristics may depend on structural and neutronic response to thermal transients, the ability to closely couple the three phenomena may lead to clearer demonstration of inherent safety or a reduction in overly conservative safety margins.

Thermal-mechanical activities are currently focused on the assessment of the impact of movements (deformations) of fuel pins or assemblies and what these changes in geometries have on the

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thermal-hydraulic and neutronics calculations. The project is using a three dimensional finite element code, NEPTUNE, developed at Argonne to simulate the response of reactor components to design basis and beyond the design basis loads.

The NEPTUNE code is a three-dimensional finite element program developed to simulate the response of reactor components in 3-D to design basis and beyond-design-basis loads [3]. The code can treat structures and structural components made from plate and/or shell structures, bar structures, and beam/column structures. An important feature of NEPTUNE is its ability to handle nonlinear problems which often occur during beyond-design-basis loads. The element formulations can properly treat large deformations (geometric nonlinearities), and the rate-type material models can handle large material strains (material nonlinearities). Explicit solution algorithms are used to economically solve short duration transient problems, and relaxation methods are employed for nonlinear static problems. Material models can handle metallic elastic and nonlinear elastoplasticity.

In order to assure the structural integrity of nuclear structures, it is necessary to simulate their response to anticipated loadings, both from a design basis and a beyond-design-basis viewpoint. To properly treat some of the important structures, it is necessary to perform three-dimensional numerical simulations; two-dimensional models cannot properly capture the mechanics. The above situation was recognized in the early seventies, and an effort was initiated to develop the three-dimensional finite element code NEPTUNE. The code can treat structures and structural components made from (1) plate and/or shell structures, (2) bar structures, (3) beam/column structures, and (4) reinforced concrete structures. One of the main features of NEPTUNE is the capability to handle large deformations, and the rate type material relationships can treat large material strains. The element library provides the user with elements to model bars, beams/columns, plates, shells and reinforced concrete walls/slabs. The solution algorithms can treat short duration transient problems in a very economical manner, and nonlinear static problems are solved using relaxation methods.

Interaction of the thermo mechanical code with the thermal-hydraulics CFD code involves the transfer of thermal field and fluid forces acting on the fuel pin cladding to NEPTUNE as loadings. NEPTUNE will feedback the resulting geometry changes (bowing) to the CFD analysis which may effect the flow paths. Thermal hydraulic analysis has been focused on the use of high fidelity computational fluids dynamics capabilities available in several commercial CFD software, with specific focus being applied to the STAR-CD[4] code at Argonne. Additionally, the interaction of the thermo mechanical code with the reactor physics neutronics code will be the transfer of geometry (bowing) from NEPTUNE. This interaction will not be discussed in the paper.

2. Example Simulation for Thermal Induced Bowing

The thermal expansion from a hypothetical fuel rod is presented for a proof of concept to capture “bowing” behavior with the NEPTUNE code. An elastic beam is assumed to be subjected by a fluid motion (force). A beam with pinned stayed ends at the top and bottom, (i.e. rotation unrestrained, axial and lateral displacement restrained) is shown in Fig. 1, so nodes 1 and 13 are partially restrained. A lateral load, P, is applied at the mid-height of the beam at node 7 of the mesh. This will simulate a force, which would develop due to fluid motion. Several analyses were performed using different values of lateral forces, a lateral force transient is shown in Fig. 2. Essentially the transient is a ramped force that is held constant after a time of 0.8 seconds. Three different lateral forces are assumed and vary from 0.4N, 4 N and 40N force. The analysis is done with the central difference integration in NEPTUNE using a time step of 2.10^{-5} s.

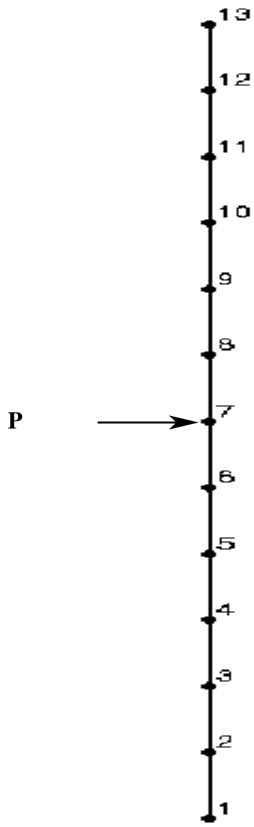

Fig. 1. Finite Element Mesh of Beam

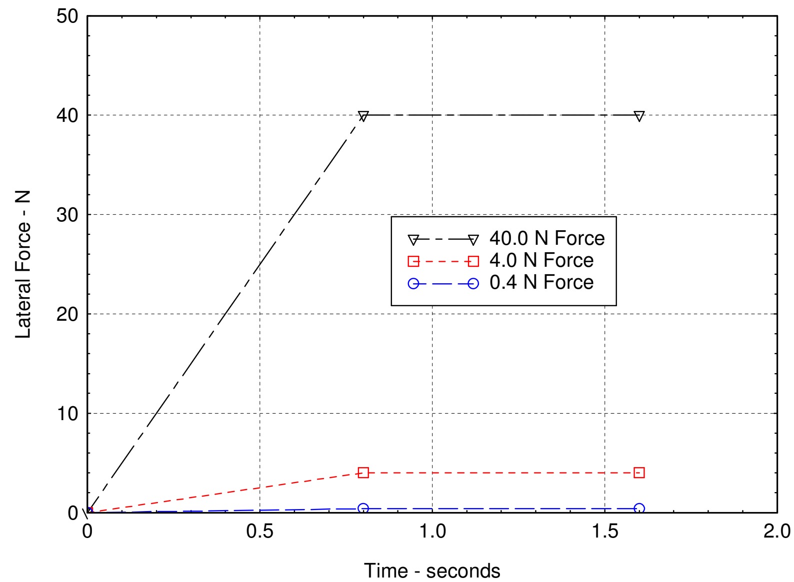

Fig. 2. Assumed Lateral Force Transient from Fluid Flow

A thermal load increment of 55C and 110C is applied to entire beam as a ramped load as depicted in Fig. 3. The temperature is constant up to time of 1.0 seconds, an increase in temperature is applied over a time of 0.1 seconds and held constant afterwards.

The resulting lateral deflections of the beams at mid height are given in Fig. 4a and 4b for a thermal transient of 55C and 110C respectively. The amount of lateral load is varied, however the final deflection after a short time is the essentially the same value and is independent of the initial lateral load. The response is consistent for bowing behavior, a compressive force is generated from the thermal loading and the lateral load triggers the bowing effect. Thus, the bowing displacement is independent from the lateral load but is dependent on the thermal load for the amount of bowing. The lateral load determines the direction of the bowed shape which is shown in Fig. 5 and is the same configuration (direction) independent of the amount of the thermal gradient.

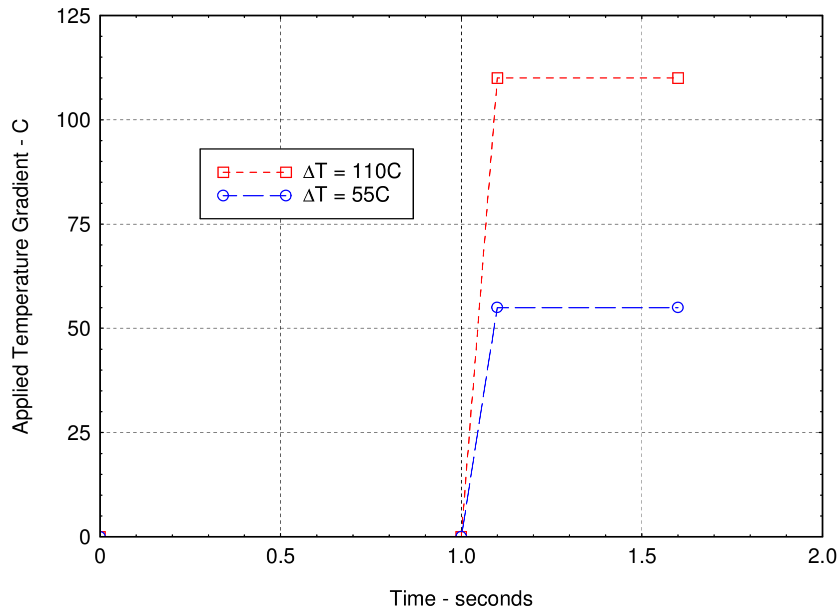

Fig. 3. Assumed Thermal Transient Acting in Beam

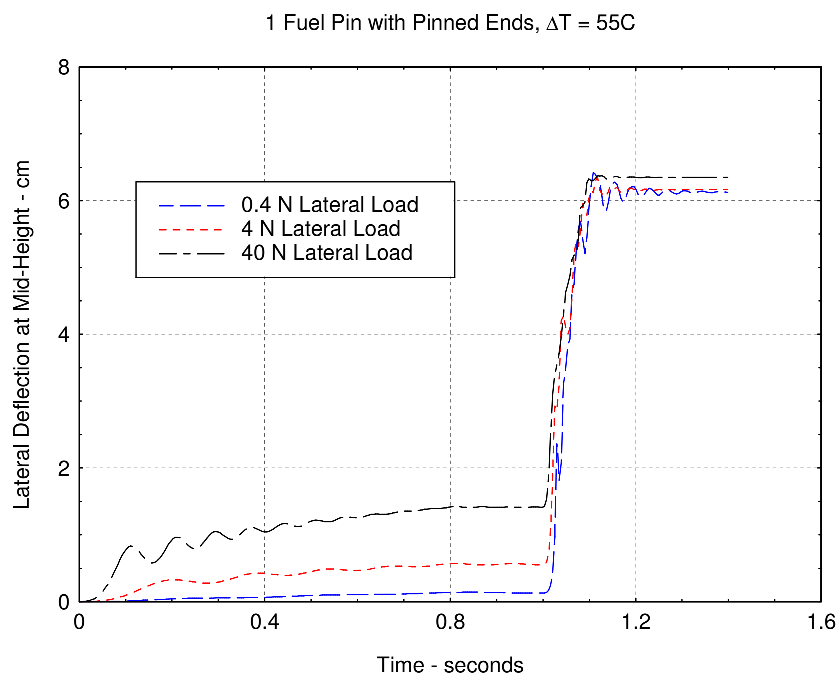

Fig. 4a. Lateral Deflection of Beam due to Lateral Force and Thermal Transient for 55C

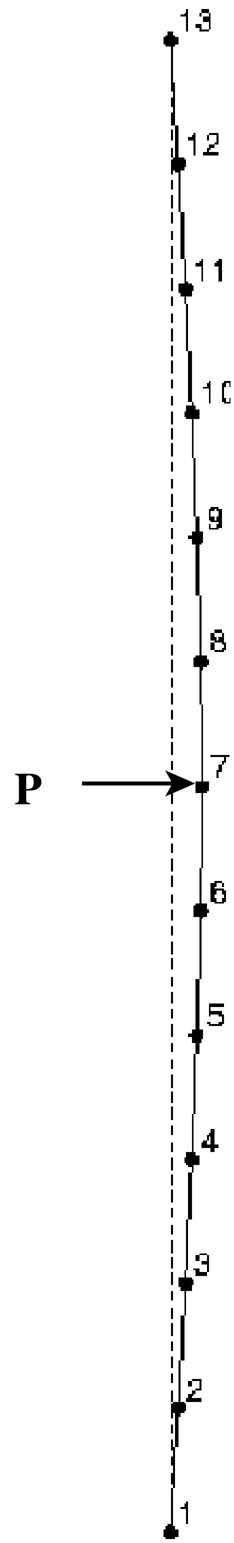

Fig. 5. Bowing of Beam due to Lateral Force and Thermal Transient

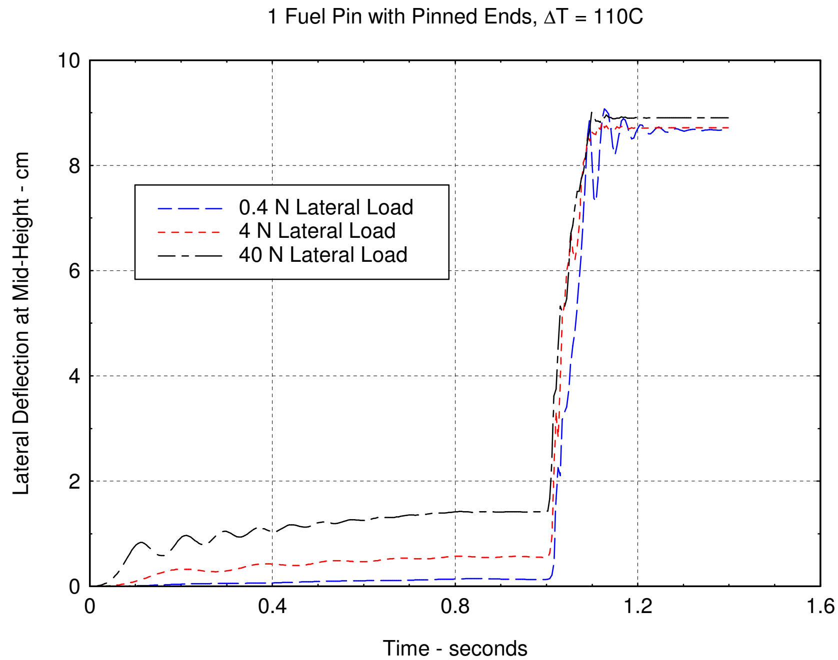

Fig. 4b. Lateral Deflection of Beam due to Lateral Force and Thermal Transient for 110C

3. Analysis of Thermal-Hydraulic Implications of Pin Deformation Using STAR-CD

To assess the basic STAR-CD capabilities for coupling of the CFD models with the thermo-structural analysis module in problems involving a deforming mesh, initially a simple 2-D flow between parallel plates was studied (Fig.6). Starting from a steady state solution, the calculations continued for a transient deformation of the mesh between the plates to determine its effect on flow and heat transfer. In all simulations reported here, the standard k-ε model is used to simulate the turbulent flow and heat transfer using logarithmic wall-functions to resolve the near-wall boundary layers. Comparison of the results with the initial steady state solution indicate some sensitivity to rapid transient deformation of the CFD mesh; however, the quality of the overall flow field is preserved assuring the consistency of the solution. The careful examination of the flow field confirms that the code properly conserves mass, momentum and energy after the computational cells start deforming. However, the results show that calculated heat flux along the heated walls is somewhat sensitive to the mesh

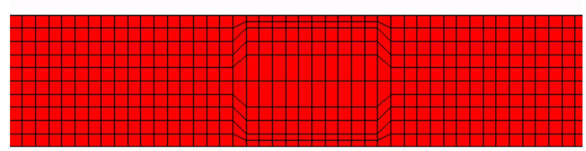

Fig. 6. Deformed mesh structure for 2-D flow between parallel plates.

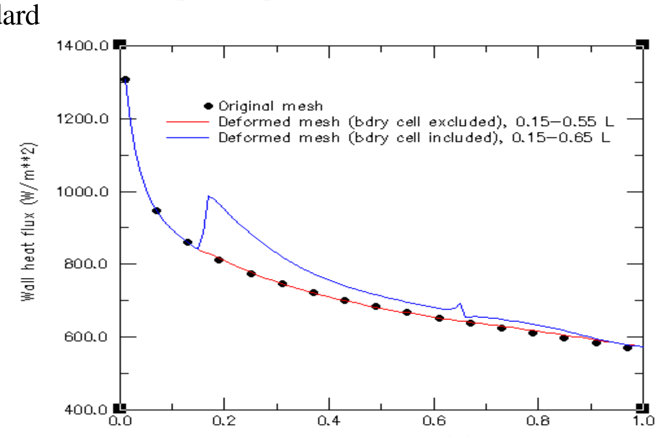

Fig. 7. Comparison of heat fluxes for the abruptly deformed mesh over 50% of the channel length to the case with the cell adjacent to the wall (boundary layer) kept the same size as the original mesh.

structure, particularly the structure of the boundary layer.

Fig. 7 compares the heat flux from the top or bottom wall at constant temperature for the abruptly deformed mesh over 50% of the channel length with the heat flux for mesh deformed over the same length, but with the cell layer adjacent to the wall kept at the same size as the original mesh. The heat flux for the case with a constant cell size adjacent to the wall is almost identical to the heat flux for the original un-deformed mesh case suggesting that the spurious heat transfer effects due to mesh deformation can be minimized by deforming only the cells away from the heated wall, maintaining the y+ value near the wall.

As an extension, the deformation of the lower wall boundary is also considered to investigate the performance for moving boundary cases. In this model, shown in Fig. 8, the upper wall is considered adiabatic and the deforming bottom wall is considered at a constant temperature. In one case, the near-wall cell layer is allowed to deform consistent with overall mesh deformation, and in another case, the thickness of the near-wall cell layer is preserved. A comparison of the calculated heat fluxes from the deforming bottom surface and the corresponding y+ values in the near-wall cell layer are provided in Fig. 9. As expected, the deforming boundary alters the flow field and, as a result, the heat flux distributions significantly: Due to velocity increase in the contracted region, the heat flux is about 2.5 times greater with deformed mesh in the mid-channel. The maximum heat flux differs only by about 4% between the two deformed cases, despite significant difference in y+ values as shown in Fig. 9. When the boundary layer is allowed to deform consistent with overall grid deformation, the y+ value near the mid-channel goes out of allowed range of 30<y+<300; however, this does not influence the calculated heat flux significantly.

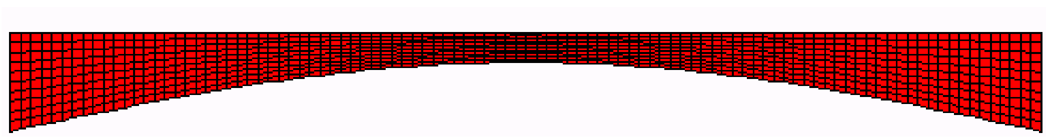

Fig. 8. 2D flow model with deformed boundary.

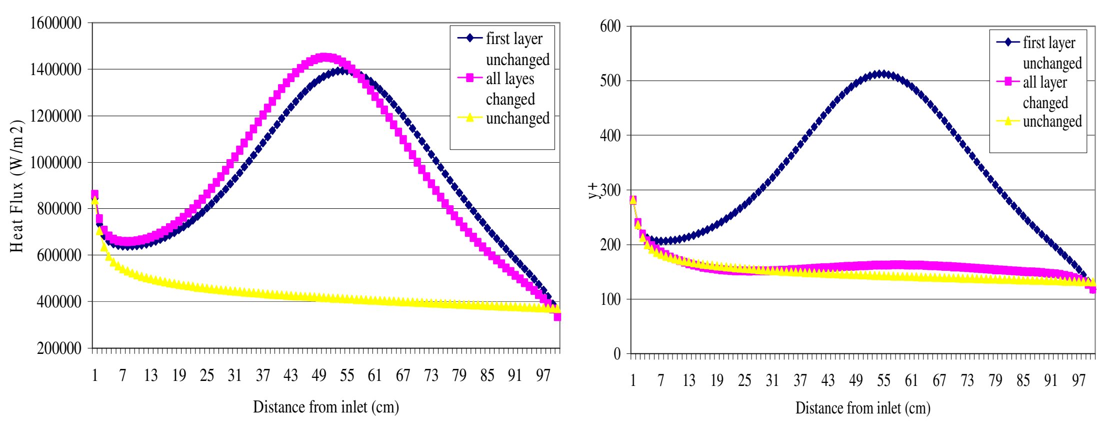

Fig. 9. Heat flux and y+ comparisons on the constant-temperature lower wall in Fig.8.

As the next step, the deformation of square profile fuel pin with uniform heat generation in the middle of a coolant channel is studied (Fig. 10). The periodic boundary conditions are specified on the right and left surfaces of the coolant channel to simulate unidirectional deformation of several pins in an assembly. The direction of flow in the coolant channel is along the fuel pin with inlet at the bottom and outlet at the top. The remaining boundaries of the computational domain are assumed to have symmetry boundary conditions.

Consistent with the earlier observations on 2-D flow between parallel plates, the calculated heat flux along the solid-fluid boundary is found to be somewhat sensitive to the thickness of the near-wall cell layer. The comparison of the calculated heat fluxes for the front (left side of the pin in Fig.10), back (right side of the pin in Fig.10), and side surfaces are provided in Figs. 11-13. Each chart shows heat fluxes for an undeformed pin, a bowed pin with a deformed boundary layer, and a bowed pin with the size of the cell adjacent to the wall unchanged (identified as "intact"). These results clearly highlight the importance of proper treatment of pin deformation particularly in terms of its effect on calculated heat fluxes with implications on DNB limits. Based on the experience gained with the models studied thus far, the deformation of a cylindrical fuel pin in a standard coolant channel and under prototypical operating conditions is currently being studied.

4. Summary and Conclusion

The paper presents the current results for the coupling of thermo mechanical analysis and thermal-hydraulics code. The thermo mechanical code can simulate rod bowing. The rod bowing is triggered by the net fluid forces and thermal gradients acting on the fuel pin. The load direction from the net fluid forces determines the position (direction) of the bowed fuel pins but does not directly determine the magnitude of bow (displacement). The temperature change (thermal gradient) directly determines the magnitude of fuel pin bowing (displacement) but not the position (direction) of the bow.

STAR-CD capabilities for simulations involving deforming mesh and boundaries have been studied for a variety of problems ranging from 2-D flow between parallel plates to prescribed bowing of a single pin in a coolant channel. The results show that mass, momentum and energy are all properly conserved when the computational domain is deformed and the mesh structure is distorted dynamically. However, the calculated heat fluxes along the heated surfaces are sensitive to the mesh structure of the boundary layer. These observed heat-flux differences can be minimized by maintaining the thickness of the cells adjacent to the wall during to mesh deformation to keep the nondimensional thickness (y+) of the near-wall cell layer within the allowable range for the turbulence model being used.

Thermo-structural capability when coupled with the CFD & neutronics codes will enable the study of "Departure from Nucleate Boiling" (DNB) penalty for subchannel analysis. DNB is important for the safety margin assessment in PWRs power density design. This aspect of the coupling capability is currently being investigated.

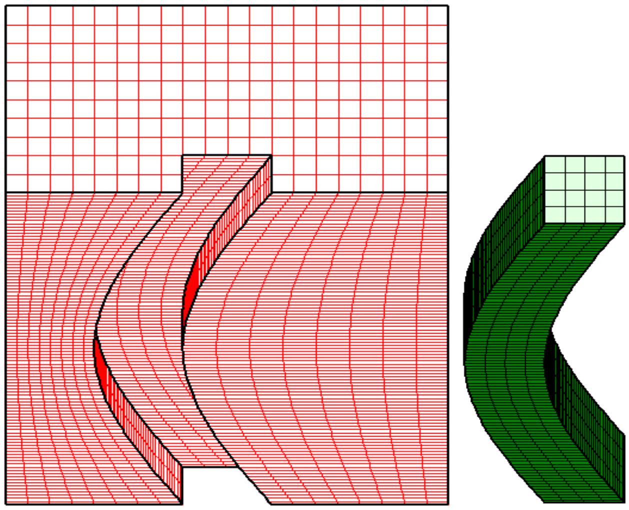

Fig. 10. Bowed configuration of square profile heated fuel pin (right) in the middle of a square profile coolant channel (only half shown on left).

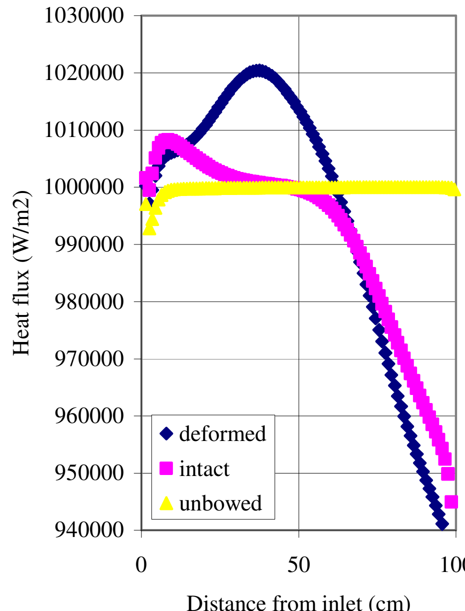

Fig. 11. Heat flux comparisons for the front surface (left surface of the pin in Fig.5).

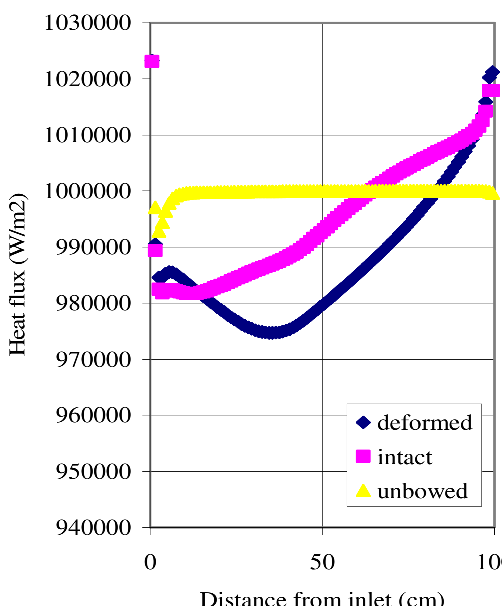

Fig. 12. Heat flux comparisons for the back surface (right surface of the pin in Fig.5).

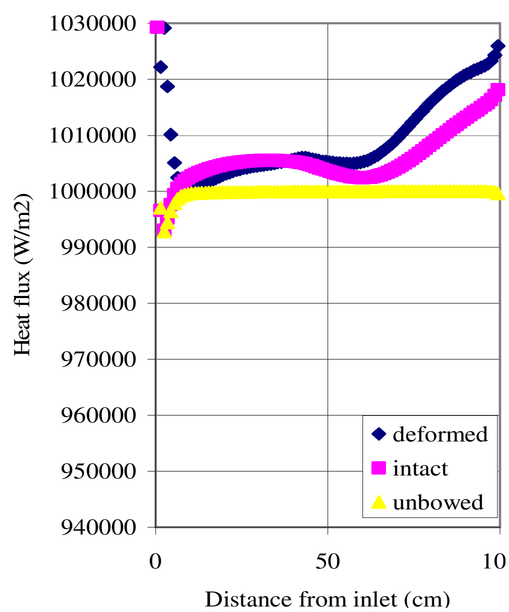

Fig. 13. Heat flux comparisons for two side surfaces.

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References

1) D. P. Weber, T. Sofu, P. A. Pfeiffer, W. S. Yang, T. A. Taiwo (ANL), H. G. Joo, J. Y. Cho, K. S. Kim, T. H. Chun (KAERI), T. J. Downar, J. W. Thomas, Z. Zhong (Purdue University), C. H. Kim (Seoul National University), The Numerical Nuclear Reactor for High Fidelity Integrated Simulation of Neutronic, Thermal-Hydraulic and Thermo Mechanical Phenomena, PHYSOR 2004, Chicago, IL, April 25-29, 2004.

2) D. P. Weber, T. A. Taiwo, W. S. Yang, P. A. Pfeiffer, P. H. Froehle, C. P. Tzanos, J. E. Cahalan, T. Sofu, Integrated 3-D Simulation Of Neutronic, Thermal-Hydraulic And Thermo-Mechanical Phenomena, The 10th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-10) Seoul, Korea, October 5-9, 2003.

3) R. F. Kulak and C. Fiala, "NEPTUNE: A System of Finite Element Programs for Three-Dimensional Nonlinear Analysis," *Nuclear Engineering and Design*, **106** (1988) 47-68.

4) STAR-CD, Version 3.150A, CD-Adapco Group, Melville, NY.