VERIFICATION AND VALIDATION OF A FUEL-ROD TEMPERATURE ANALYSIS CODE BIRCH

J. L. Ruan, Y. B. Zhu, J. G. Li

China Nuclear Power Technology Research Institute 47/F, Jiangsu Building, Shenzhen 518026, China ruanjialei@cgnpc.com.cn; zhuyuanbing@cgnpc.com.cn; lijinggang@cgnpc.com.cn

ABSTRACT

A fuel-rod temperature analysis code` for PWRs named BIRCH has been developed as part of the indigenous effort of China Guangdong Nuclear Power Corp. (CGNPC) to develop a full-spectrum software package for reactor design and safety analysis. The verification and validation of BIRCH are introduced in the paper.

BIRCH calculates the temperature distribution transient in a fuel rod cross section (pellet, pellet-cladding gap and cladding), as well as the transient heat flux at the cladding surface, using as input the nuclear power and the coolant parameters (pressure, flow rate, temperature). The code also calculates the energy stored in the pellet, the expansion of the pellet and the cladding and the pellet-cladding gap. The model representing the fuel permits BIRCH analyzing the integrity of the fuel and the cladding during rapid transients under accident thermal-hydraulic conditions, such as the rod ejection accident.

In BIRCH code, the fuel is represented by a series of concentric rings (sections). The heat transfer by conduction equations are solved simultaneously for each ring using the finite differences method in the form of a system of linear equations. Some auxiliary models, such as cladding surface heat transfer model, gap heat transfer model, zirconium water reaction model and fuel pellets melt model, are coupled in the code.

Verification and validation (V&V) of the software product is used to ensure that software adequately performs all intended functions and that it does not perform any unintended function that can degrade an intended function or the function of the complete code. The software verification and validation activities of the BIRCH code are presented herein.

The BIRCH V&V effort will be comprised of 2 different types of analyses: separate effect analyses and system effect analyses. The separate effect analyses are used to evaluate individual models against simple experiments or analytical solutions. The system effect analyses are designed to evaluate the ability of the code to calculate the overall response. For BIRCH, this part would be comparisons with analyses from a licensing code named FACTRAN.

KEYWORDS

BIRCH, fuel-rod temperature analysis code, verification, validation

1. INTRODUCTION

BIRCH is a fuel-rod temperature analysis code, which calculates the temperature distribution transient in a fuel rod cross section (pellet, pellet-cladding gap and cladding), as well as the transient heat flux at the

cladding surface, using as input the nuclear power and the coolant parameters (pressure, flow rate, temperature).

This code is particularly adapted for the following accident transient analyses:

- Rod withdrawal with sub critical core;
- Rod ejection during power operation;
- Rod ejection with sub critical core;
- Locked reactor coolant pump shaft.

A key requirement of the development process for computer programs that will be used to perform analyses providing licensing bases for nuclear reactor systems is that planned verification and validation activities must be performed. The software verification and validation activities planned for the BIRCH code are presented herein.

In this article, the first part provides a description of the programming structure. The second part provides the verification and validation plan of the BIRCH code. The third part consists of a description of the V&V activities and the result of each analysis.

2. GENERAL DESCRIPTION

BIRCH calculates the temperature distribution transient in a fuel rod cross section (pellet, pellet-cladding gap and cladding), as well as the transient heat flux at the cladding surface, using as input the nuclear power and the coolant parameters (pressure, flow rate, temperature). These parameters may be input as a function of time. The code also calculates the energy stored in the pellet, the expansion of the pellet and the cladding and the pellet-cladding gap.

The model representing the fuel permits BIRCH to be used for fast transients such as the rod ejection accident.

2.1 Representation of the fuel

The fuel is represented by a series of concentric rings (sections) as shown in Figure 1:

- The pellet is represented by a number of rings specified in the data input.
- Three additional rings are provided around the pellet to represent the pellet-cladding gap, the cladding and film existing between the cladding and the coolant under forced convection and after DNB occurs.



Figure 1. Representation of the Fuel

2.2 Code structure and flow chart

The core model in the computer code is the fuel rod heat transfer model. It calculates the temperature distribution of the fuel rod and cladding surface heat flux at steady-state or transient condition, based on the volume heat release rate and coolant heat transfer coefficient. Note that:

- 1) This model only consider the radial thermal conductivity of the fuel rod, the circumferential direction and the axial direction are not considered;
- 2) Thermal properties of each material are temperature-dependent variable;
- 3) Heat of zirconium water reaction is taken into account.

The parameters required by core model is provided by some auxiliary models, such as

- Heat transfer model between cladding and coolant;
- Heat transfer model across the pellet-cladding gap;
- Water-zircaloy reaction model;
- Fuel melting;
- Radial power distribution model;
- Physical properties model of fuel pellet and cladding material.

The operation of BIRCH and the linking of its subprograms are summarized in the following flow sheet:



3. VERIFICATION AND VALIDATION PLAN

A key requirement of the development process for computer programs that will be used to perform analyses providing licensing bases for nuclear reactor systems is that planned verification and validation activities must be performed. Ongoing testing and evaluation is performed during the development process to ensure that the basic design requirements are achieved, but verification and validation of the software product is used to ensure that software adequately performs all intended functions and that it does not perform any unintended function that can degrade an intended function or the function of the complete code. The software verification and validation activities planned for the BIRCH code are presented herein.

The BIRCH verification and validation effort will be comprised of 2 different types of analyses:

1. Separate Effect Problems

These problems are devised to confirm the correct and accurate behavior of one or several specific models. These problems are based on the analysis of experimental data and manual calculation, and comparison of these results with those determined by a BIRCH model.

2. System Effect Problems

These problems provide evidence that the collection of individual models function collectively in predicting the behavior of more complex models. BIRCH's predictions of integral system parameters, such as reacted Zircaloy, heat flux at the outside surface of the cladding, and temperatures for each time step, are used to assess overall accuracy of the code.

The test cases for each problem category are summarized in the Table I.

Assessment Objective(s)	Involved Case/Correlation	Assessment Method	
Separate Effect Problems			
Heat-conduction differential equations	One-dimensional steady-state heat	Analytic calculation	
	One dimensional unsteady state heat		
	conduction equation	Numerical calculation	
Heat transfer model between cladding and coolant	D-B correlation ^[1]	Manual calculation	
	S-T correlation ^[2]	Manual calculation	
	Михеев correlation ^[2]	Experimental data	
	Chen correlation ^[3]	Experimental data	
	Jens-Lottes correlation ^[4]	Manual calculation	
	Incropera correlation ^[5]	Experimental data	
	Thom correlation ^[6]	Experimental data	
Heat transfer model across	Thermal conductivity correlation of Ar, H2,	Experimental data	
the pellet-cladding gap	He, Kr, N2, O2, Xe	Experimental data	
Water-zircaloy reaction	Baker-Just correlation ^[7]	Manual calculation	
model	Cathcart-Pawel correlation ^[8]	Manual calculation	
Physical properties model of fuel pellet and cladding material	Thermal conductivity of the pellet	Experimental data	
	Specific heat capacity of the pellet	Experimental data	
	Thermal conductivity of the cladding	Experimental data	
	Specific heat capacity of the cladding	Experimental data	
System Effect Problems			
Locked Rotor	Assess transient specific key parameters	Comparisons with FACTRAN code	

Table I. Verification and Validation Assessment Matrix

4. VERIFICATION AND VALIDATION RESULT

This section describes the V&V results of BIRCH code. The results take the form of absolute deviation and relative deviation, which are defined as follows:

Absolute deviation

$$\varepsilon = |VALUE_{\text{STANDARD}} - VALUE_{BIRCH}|$$

Relative deviation

$$\delta = \frac{VALUE_{\text{STANDARD}} - VALUE_{\text{BIRCH}}}{VALUE_{\text{STANDARD}}}$$

4.1 Heat-conduction differential equations

The fuel rod thermal model of BIRCH code is a one-dimensional, containing internal heat source heat conduction model. In a one-dimensional radial cylindrical coordinate system, the thermal differential equation is:

$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} (k \cdot r \frac{\partial T}{\partial r}) + S$$

Where c_p is the specific heat capacity, k is the thermal conductivity, and S is the internal heat source. Analytical solutions and numerical solutions are respectively used to verify the correctness of the thermal model in steady-state and unsteady-state cases.

4.1.1 Steady-state heat conduction

Steady-state heat conduction problem is simplified to a problem with uniform internal heat and constant thermal properties.

By integrating, the radial temperature distribution function of the fuel rod can be written in the following form.

For pellets

$$T = T_1 + \frac{S}{4k_1} \cdot \left(r_1^2 - r^2\right)$$

For gap

$$T = T_1 + \frac{T_2 - T_1}{\ln(r_2 / r_1)} \ln(r / r_1)$$

For cladding

$$T = T_2 + \frac{T_s - T_2}{\ln(r_s / r_2)} \ln(r / r_2)$$

Where r_1 , r_2 and r_s are radius of pellet surface, cladding inner surface and cladding outer surface,

respectively; T_1 , T_2 and T_s are temperature of pellet surface, cladding inner surface and cladding outer surface, respectively; k_1 is the pellets thermal conductivity. If T_s is given, T_2 and T_1 can be calculated accordingly:

$$T_2 = T_s + \frac{S \cdot r_1^2}{2k_s} \ln\left(r_s / r_2\right)$$

Where k_2 and k_s are thermal conductivities of gap and cladding respectively.

In this test, the fuel rod is divided into 14 nodes in the radial direction, wherein the fuel pellet contains 11 nodes, and the gap, the cladding and the coolant film respectively contain 1 node.

The results of analytic calculation and BIRCH for Steady-state heat conduction are shown in **Figure 3**. The maximum relative deviation between BIRCH and analytic calculation is only 0.91 ‰. Therefore, it can be concluded that BIRCH fuel rod heat transfer model is correct for the one-dimensional steady-state heat conduction.



Figure 3 The Results of Steady-State Heat Conduction Test

4.1.2 Unsteady-state heat conduction

This case assumes a uniform distribution of the initial temperature, a non-varying heat source and constant physical properties. It is researched under the third boundary condition:

$$\frac{\partial T}{\partial r}\Big|_{r=0} = 0$$
$$-k \frac{\partial T}{\partial r}\Big|_{r=R} = h \left(T_{r=R} - T_{\infty}\right)$$

Where h is the convective heat transfer coefficient between cladding and the coolant.

In this case, the node division of fuel rod is the same as section 4.1.1. The temperature relative deviations between numerical calculation and BIRCH for unsteady-state heat conduction are shown in Figure 3.



Figure 4 Temperature Relative Deviations of Unsteady-State Heat Conduction Test

The relative deviation between BIRCH and numerical calculation increases with the radial position and time, and the maximum absolute value is 3.6%, which is due to the gradual magnification of input parameters truncation-error along with the iterative process. The deviations are in a reasonable range, and BIRCH fuel rod heat transfer model is correct for the one-dimensional unsteady-state heat conduction.

4.2 Separate Effect Problems

These problems are devised to confirm the correct and accurate behavior of one or several specific models, and experimental data or manual calculation would be verification criteria.

4.2.1 Heat transfer model between cladding and coolant

In BIRCH, there are several correlations in the cladding-coolant heat transfer model, including Dittus-Boelter correlation^[1], Sider-Tate correlation^[2], Muxees correlation^[2], Chen correlation^[3], Jens-Lottes correlation^[4], Incropera correlation^[5], Thom correlation^[6], etc.

Dittus-Boelter correlation and Sider-Tate correlation are widely used in textbooks, engineering projects and nuclear analysis softwares, so BIRCH results of these two correlations are only compared with manual calculations to ensure that the corresponding code is correct. The results show that the average relative deviation of Dittus-Boelter correlation is -4.72×10^{-7} , while the maximum relative deviation is -5.93×10^{-6} ; and the average relative deviation of Sider-Tate correlation is -8.02×10^{-5} , while the maximum relative deviation is -1.05×10^{-4} .

Михеев correlation and Chen correlation are verified by the experimental data of MIT Forced Convection Heat Transfer Tests^[4]. The results are shown in Figure 5.



Figure 5 The Comparison of Михеев Correlation, Chen Correlation and MIT Data

The same as Dittus-Boelter correlation and Sider-Tate correlation, Jens-Lottes correlation is widely used and only need to be compared with manual calculations to ensure that the corresponding code is correct. The result shows that the average relative deviation of Jens-Lottes correlation is 1.44×10^{-7} , while the maximum relative deviation is 1.78×10^{-6} .

Incropera correlation and Thom correlation are verified by the experimental data of UCLA Local Boiling Heat Transfer Tests^[4]. The results of Incropera correlation and Thom correlation are compared with experimental data, as shown in Figure 6.



Figure 6 The Comparison of Incropera Correlation, Thom Correlation and UCLA Data

4.2.2 Heat transfer model across the pellet-cladding gap

In general, this model only considers heat conduction, and natural convection is not considered. Optional gap gases include Ar, H2, He, Kr, N2, O2, Xe, etc. The thermal conductivity correlations of these gases are verified by several experimental data, and the results are listed inTable II.

Gas	Average Relative Deviation	Maximum Relative Deviation
Ar	-0.298%	7.88%
H_2	1.13%	29.8%
He	0.438%	-17.6%
Kr	0.136%	9.95%
N_2	3.14%	9.12%
O_2	1.04%	-2.20%
Xe	-1.15%	6.20%

Table II. Relative deviations of gas thermal conductivity

4.2.3 Water-zircaloy reaction model

BIRCH provides Baker-Just correlation ^[7] and Cathcart-Pawel correlation ^[8] to simulate cladding oxidation progress. These two correlations are widely used and only need to be compared with manual calculations to ensure that the corresponding code is correct. The result shows that the average relative deviation of Baker-Just correlation is 8.3×10^{-8} , while the maximum relative deviation is 1.43×10^{-6} ; and the average relative deviation of Cathcart-Pawel correlation is -1.82×10^{-8} , while the maximum relative deviation is 1.47×10^{-6} .

4.2.4 Physical properties model of fuel pellet and c ladding material

Physical properties model contains pellet thermal conductivity model, pellet specific heat capacity model, cladding thermal conductivity model, and cladding specific heat capacity model.

The pellet thermal conductivity model is tested by the experimental data of Bates et al. ^[9], Godfrey et al. ^[10], Weilbacher et al. ^[11], Gibby et al. ^[12], and Hobson et al. ^[13]. The results are shown in Figure 7.



Figure 7 The Comparison of UO₂Thermal Conductivity and Experimental Data

The pellet specific heat capacity model is tested using the experimental data of Hein et al.^[14], Leibowitz et al.^[15], and Gronvold et al.^[16]. The results are shown in Figure 8.



Figure 8 The Comparison of UO2 Specific Heat Capacity and Experimental Data

In BIRCH, the cladding material includes Zr-2, Zr-4 and M5. The thermal conductivity and specific heat capacity of these three materials are all tested using the experimental data. Take Zr-2 as an example, its thermal conductivity is compared with Anderson et al. ^[17], Lucks et al. ^[18], and Powers et al. ^[19] experimental data, as shown in Figure 9; and its specific heat capacity is compared with Eldridge et al. ^[20] experimental data, as shown in Figure 10.



Figure 9 The Comparison of Zr-2 Thermal Conductivity and Experimental Data



Figure 10 The Comparison of Zr-2 Specific Heat Capacity and Experimental Data

4.3 System Effect Problems

FACTRAN is a licensed fuel-rod temperature analysis code developed by Westinghouse. It has similar physical models and features with BIRCH, so it is suitable as a benchmark program to validate the system effect. That is, same parameters are inputted into each code, and the output parameters are compared.

In this article, an AP1000 locked rotor case was chosen to be calculated. In this case, the pellet was radially divided into 10 sections; the maximum calculating time was 10seconds, and the time step was 0.1second. The result shows that the average relative deviation of pellet temperature is 0.289%, while the

maximum relative deviation is 2.29%, as shown in Figure 11. The average relative deviation of convective heat transfer coefficient is 0.140%, while the maximum relative deviation is 0.237%.



Figure 11 Pellet temperature relative deviation between FACTRAN and BIRCH

5. CONCLUSION

The BIRCH verification and validation effort is comprised of separate effect problems and system effect problems. Analytical solutions and numerical solutions of the heat-conduction differential equations show that this model can simulate the internal temperature distribution of the fuel rods accurately. Separate effect verification shows that constitutive relations are in good agreement with manual calculations or experimental data, and hence the individual models are accurate. System effect verification shows that the results of BIRCH are in good agreement with a licensed code FACTRAN, and the deviations are within a reasonable range.

REFERENCE

- [1] F. W. Dittus, L. M. K. Boelter. Heat transfer in automobile radiators of the tubular type. Int. Comm. Heat Mass Transfer, 1985, 12: 3-22.
- [2] Yang Shiming, Tao Wenquan. Heat Transfer [M], Third Edition. Beijing: China Higher Education Press (CHEP), 1998:164.
- [3] Chen J. C, Correlation for Boiling Heat Transfer to Saturated Fluids in Convective Flow. I&EC Process Design & Development. 1966, 5, 322-328.
- [4] Jens W. H., Lottes P. A., Analysis of heat transfer, burnout, pressure drop and density data for high-pressure water, ANL-4627, 1951.
- [5] Incropera F. P., DeWitt D. P. Introduction to heat transfer. 3rd ed. New York: John Wiley & Sons, 1996. 403-406.
- [6] Yu Zhenwan. The basic equation of two-phase flow and pressure drop calculation. Nuclear Power Engineering. 1982, 3: 82-88.

- [7] L. Baker, L. C. Just. Studies of metal-water reactions at high temperatures III. Experimental and theoretical studies of the zirconium-water reaction. AEC research and development report, ANL-6548, 1962.
- [8] Pawel K. E., Cathcart J. V., Mckee R. A. Electrochem Sci Techol, 1979; 126: 1105.
- [9] J. Lambert Bates, High Temperature Thermal Conductivity of "Round Robin" Uranium Dioxide, BNWL-1431, July 1970.
- [10] T. G. Godfrey et al., Thermal Conductivity of Uranium Dioxide and Armco Iron by an Improved Radial Heat Flow Technique, ORNL-3556, June 1964.
- [11] J. C. Weilbacher, "Diffusivite Thermique de l'Oxyde d'Uranium et de l'Oxyde de Thorium a Haute Temperature," High Temperatures--High Pressure, 4, 1972, pp. 431-438.
- [12] R. L. Gibby, "The Effect of Plutonium Content on the Thermal Conductivity of (U, Pu)O2 Solid Solutions," Journal of Nuclear Materials, 38, 1971, pp. 163-177.
- [13] I. C. Hobson, R. Taylor, and J. B. Ainscough, "Effect of Porosity and Stoichiometry on the Thermal Conductivity of Uranium Dioxide," Journal of Physics Section D: Applied Physics, 7, 1974 pp. 1003-1015.
- [14] A. Hein and P. N. Flagella, Enthalpy Measurements of UO2 and Tungsten to 3,260 K, GENMPO-578, February 1968.
- [15] L. Leibowitz et al., "Enthalpy of Liquid Uranium Dioxide to 3,500 K," Journal of Nuclear Materials, 39, 1971, pp. 115-116.
- [16] F. Gronvold et al., "Thermodynamics of the UO2+x Phase I. Heat Capacities of UO2.017 and UO2.254 from 300 to 1,000 K and Electronic Contributions," Journal of Chemical Thermodynamics, 2, 1970, pp. 665-679.
- [17] W. K. Anderson, C. J. Beck, A. R. Kephart, and J. S. Theilacker "Zirconium Alloys," Reactor Structural Materials: Engineering Properties as Affected by Nuclear Reactor Service, ASTMSTP-314, 1962, pp. 62-93.
- [18] C. F. Lucks and H. W. Deem, Progress Relating to Civilian Applications During June, 1958, R. W. Dayton and C. R. Tipton, Jr., (eds.), BMI-1273, 1958, pp. 7-9.
- [19] A. E. Powers, Application of the Ewing Equation for Calculating Thermal Conductivity from Electrical Conductivity, KAPL-2146, April 7, 1961.
- [20] H. W. Deem and E. A. Eldridge, Specific Heats and Heats of Transformation of Zircaloy-2 and Low Nickel Zircaloy-2, USAEC BM1-1803, May 31, 1967.