Verification and Validation of Corrected Versions of RELAP5 for ATR Reactivity Analyses

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Verification and Validation of Corrected Versions of RELAP5 for ATR Reactivity Analyses

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Abstract

Two versions of the RELAP5 computer code, RELAP5/MOD2.5 and RELAP5/MOD3 Version 3.2.1.2, are used to support safety analyses of the Advanced Test Reactor (ATR). Both versions of RELAP5 contain a point reactor kinetics model that has been used to simulate power excursion transients at the ATR. Errors in the point kinetics model were reported to the RELAP5 code developers in 2007. These errors had the potential to affect reactivity analyses that are part of the ATR's safety basis. Consequently, corrected versions of RELAP5 were developed for analysis of the ATR. Four reactivity transients were simulated to verify and validate the corrected codes for use in safety evaluations of the ATR. The objectives of this paper are to describe the verification and validation of the point kinetics model for ATR applications and to inform code users of the effects of the errors on representative reactivity analyses.

Summary

Two versions of the RELAP5 computer code, RELAP5/MOD2.5 and RELAP5/MOD3 Version 3.2.1.2, are used to support safety analyses of the Advanced Test Reactor (ATR). Both versions of RELAP5 contain a point reactor kinetics model that has been used to simulate power excursion transients at the ATR. Errors in the point kinetics model were reported to the RELAP5 code developers in 2007. These errors had the potential to affect reactivity analyses that were part of the ATR's safety basis. Consequently, corrected versions of RELAP5 were developed for analysis of the ATR. Four reactivity transients were simulated to verify and validate the corrected codes for use in safety evaluations of the ATR. These test cases included a theoretical 0.10\$/s reactivity ramp, a theoretical 0.15\$ step reactivity insertion, an accident in the ATR Critical (ATRC) facility initiated by dropping a filler piece into the large inpile tube, and an ATRC accident initiated by a 0.45\$/s reactivity ramp.

The original version of RELAP5/MOD2.5 produced results that were in excellent agreement with the exact solution for the 0.15\$ reactivity step. Results from the original version were also in excellent agreement with the results from the PTKIN3 code, which was used in reactivity analyses of the ATRC before RELAP5, for the drop accident. Although the results from the original version were in reasonable agreement with the exact solution or PTKIN3 for the reactivity ramps with large time steps, they were in poor agreement at small time steps.

Code updates were generated in 2007 to correct the code's poor performance with small time steps during ramp insertions. The poor performance was attributed to two errors in the point kinetics model. The first error was reported to be due to erroneous indices involved in the calculation of terms associated with the delayed neutron groups. The second error was related to logic that determined when to apply a quasi-steady form of the point reactor kinetics equation. Calculations performed during this evaluation showed that the "correction" to the first error reported in 2007 actually caused slightly worse results for the reactivity step insertion. Specifically, the power remained constant during the first time step although it should have increased. A re-evaluation of the updates revealed that the first "error" reported in 2007 was not

actually an error. The contributions of the delayed neutron groups to the reactor power were correctly calculated in the original code, although subtleties in the coding could easily cause one to come to the opposite conclusion following a cursory examination. Consequently, a 2008 version of RELAP5/MOD2.5 was created for this analysis that included only the correction to the second error reported in 2007.

Both the 2007 and 2008 versions of RELAP5/MOD2.5 were evaluated using the four verification and validation cases described above. The 2007 and 2008 versions of RELAP5/MOD2.5 produced nearly identical results at small (≤ 0.001 s) time steps for all four cases. Small differences ($\leq 6\%$) were noted at large (0.01 s) time steps. At relatively large (0.002 - 0.01 s) time steps, the 2008 version generally agreed better with the exact solution or PTKIN3 than the 2007 version. The 2008 version also better represented the power at the end of the first time step following the step reactivity insertion. RELAP5 users from different organizations should use updates equivalent to those generated in 2008 instead of those generated in 2007. The updates required to generate both versions are included in the main body of this paper.

1.0 Introduction

Two versions of the RELAP5 computer code are used to support safety analyses of the ATR. These versions are RELAP5/MOD2.5 (Allison and Johnson, 1989) and RELAP5/MOD3 (RELAP5 Development Team, 1995) Version 3.2.1.2. The former code was used to simulate most of the events described in the ATR Safety Analysis Report (SAR) and all the reactivity events described in the ATR Critical (ATRC) facility SAR, while the latter code was used to simulate some of the experiment loop blowdown events described in the ATR SAR. RELAP5/MOD3 Version 3.2.1.2 is also generally used in the experiment safety analyses that support the irradiation of various tests.

Both versions of RELAP5 contain a point reactor kinetics model that has been used to simulate power excursion transients at the ATR. The point reactor kinetics model was validated against numerous exact solutions as described in the code manual. The model was also specifically verified and validated for ATR applications using three test cases involving reactivity insertions. These test cases included a theoretical 0.15\$ step reactivity insertion, an accident in the ATRC initiated by dropping a filler piece into the large inpile tube, and an ATRC accident initiated by a 0.45\$/s reactivity ramp. All of the validation calculations showed excellent performance of the RELAP5 point reactor kinetics model. However, errors in the point kinetics model were reported to the RELAP5 code developers in 2007. The errors were originally reported by researchers at Purdue University who were studying reactivity transients in an Argentine reactor.

Previous evaluations have shown that RELAP5/MOD2.5 and RELAP5/MOD3 Version 3.2.1.2 produced identical results for reactivity transients initiated by step and ramp insertions without reactivity feedback. Identical results were expected for these transients because the point reactor kinetics models are identical between versions. Consequently, this paper focuses on the verification and validation of ATR's version of RELAP5/MOD2.5.

The errors and corrections to the errors are described in Section 2. The verification and validation of the corrected version of RELAP5/MOD2.5 are described in Section 3. Conclusions and references are provided in Sections 4 and 5, respectively.

2.0 Error Corrections

Two errors in the point reactor kinetics model were reported to the RELAP5 code developers in 2007. The first error was in the calculation of terms associated with one of the six delayed neutron groups. The second error was related to logic that determined when to apply a quasi-steady form of the point kinetics equation rather than the fully transient form. The switch from the quasi-steady form to the transient form was done to prevent a possible loss in the number of significant digits when subtracting one from the reactivity. Recent experience has shown that the numerical value used to switch from the quasi-steady to transient forms of the point reactor kinetics equation was too large to obtain accurate solutions for some problems. Reducing the numerical value causes the code to generally use the fully transient solution, which results in better solutions for some problems. Note that the user has no control over the switch from the quasi-steady to transient forms of the point reactor to the stdy-st and *transnt* options that are entered on Card 100.

Preliminary testing during this evaluation showed that the "correction" to the first error reported in 2007 actually caused slightly worse results for the reactivity step insertion in that the power remained constant during the first time step. Physically, the power should increase immediately following a step insertion of reactivity. The original developer of the reactor point kinetics model was consulted (Wagner, 2008) about this anomaly. He re-evaluated the corrections generated in 2007 and concluded that the first reported "error" was not actually an error. The contributions of the delayed neutron groups were correctly calculated in the original code, although subtleties in the coding could easily cause one to come to the opposite conclusion following a cursory examination. This conclusion of the original developer was confirmed by calculations performed during this evaluation. The code version with the corrections to the second reported error but without the corrections to the first reported error produced results that were equivalent to, or slightly better than, the version with corrections to both reported errors. In particular, the code version without the first "correction" converged to the exact solution at larger time steps during the reactivity ramps.

The point reactor kinetics equations are solved within Subroutine *rkin*. The differences between Subroutines *rkin* in the original and the "corrected" version of RELAP5/MOD2.5 based on the updates generated in 2007 are shown in Table 1. This version of the code is hereafter referred to as the 2007 version. The table was created with the UNIX *diff* utility. The numerical value that controls the change between the fully transient and quasi-steady equations was reduced from 0.002 to 0.000001 at five places in the subroutine. All the other changes corrected the "error" in the evaluation of the terms associated with one of the delayed neutron groups.

Table 1. Differences in Subroutine *rkin* based on updates generated during 2007.

```
299,300c299
         do 51 i = j, jd, 9
<
<
           tem = tem + rkfi(i)*rkdpvn(k)
___
         do 51 i = jp,jd,9
>
301a301
         tem = tem + rkfi(i)*rkdpvn(k)
>
304c304
         if (abs((rm1*rkdpvn(k) - tem)/tem) .lt. 0.002) rkdpvn(k) =
<
___
>
         if (abs((rm1*rkdpvn(k) - tem)/tem) .lt. 0.000001) rkdpvn(k) =
320,321c320
<
         do 61 i = j, jd, 9
<
          tem = tem + rkfi(i) * rkdpvn(k)
___
>
         do 61 i = jp, jd, 9
322a322
>
          tem = tem + rkfi(i)*rkdpvn(k)
325c325
<
         if (abs((rm1*rkdpvn(k) - tem)/tem) .lt. 0.002) rkdpvn(k) =
___
>
         if (abs((rml*rkdpvn(k) - tem)/tem) .lt. 0.000001) rkdpvn(k) =
345,346c345
         do 71 i = j,jd,9
<
          tem = tem + rkfi(i)*rkdpvn(k)
<
___
>
         do 71 i = jp, jd, 9
347a347
          tem = tem + rkfi(i)*rkdpvn(k)
>
350c350
         if (abs((rm1*rkdpvn(k) - tem)/tem) .lt. 0.002) rkdpvn(k) =
<
___
         if (abs((rm1*rkdpvn(k) - tem)/tem) .lt. 0.000001) rkdpvn(k) =
>
368,369c368
<
         do 81 i = j, jd, 9
<
           tem = tem + rkfi(i) *rkdpvn(k)
___
>
         do 81 i = jp,jd,9
370a370
         tem = tem + rkfi(i)*rkdpvn(k)
>
373c373
         if (abs((rm1*rkdpvn(k) - tem)/tem) .lt. 0.002) rkdpvn(k) =
<
___
         if (abs((rm1*rkdpvn(k) - tem)/tem) .lt. 0.000001) rkdpvn(k) =
>
395c395
         rept = abs((rm1*rkdpvn(k) - rksum(j))/rksum(j)) .lt. 0.002
<
___
         rept = abs((rml*rkdpvn(k) - rksum(j))/rksum(j)) .lt. 0.000001
>
```

The differences between the original and corrected versions of RELAP5/MOD2.5 generated during this evaluation are shown in Table 2. This code is hereafter referred to as the 2008 version. The changes listed in Table 2 are a subset of those listed in Table 1. The updates shown in Table 2 will be used for future analyses of the ATR. Similar updates will be made in

RELAP5-3D and are recommended for organizations using other versions of RELAP5. Note that the changes given in Table 2 do not represent true *error* corrections. Rather, they reflect a better *choice* of a numerical value that has almost no impact for most cases, but causes significantly improved results for the rare cases where the original model did not provide an accurate solution.

304c304	
<	if $(abs((rm1*rkdpvn(k) - tem)/tem)$.lt. 0.002) $rkdpvn(k) =$
> 325c325	<pre>if (abs((rml*rkdpvn(k) - tem)/tem) .lt. 0.000001) rkdpvn(k) =</pre>
<	<pre>if (abs((rm1*rkdpvn(k) - tem)/tem) .lt. 0.002) rkdpvn(k) =</pre>
> 350c350	<pre>if (abs((rml*rkdpvn(k) - tem)/tem) .lt. 0.000001) rkdpvn(k) =</pre>
<	<pre>if (abs((rml*rkdpvn(k) - tem)/tem) .lt. 0.002) rkdpvn(k) =</pre>
> 373c373	<pre>if (abs((rml*rkdpvn(k) - tem)/tem) .lt. 0.000001) rkdpvn(k) =</pre>
<	<pre>if (abs((rml*rkdpvn(k) - tem)/tem) .lt. 0.002) rkdpvn(k) =</pre>
> 395c395	if $(abs((rm1*rkdpvn(k) - tem)/tem)$.lt. 0.000001) rkdpvn(k) =
<	<pre>rept = abs((rm1*rkdpvn(k) - rksum(j))/rksum(j)) .lt. 0.002</pre>
>	<pre>rept = abs((rm1*rkdpvn(k) - rksum(j))/rksum(j)) .lt. 0.000001</pre>

Table 2. Differences between the original and 2008 versions of RELAP5/MOD2.5.

3.0 Verification and Validation

Four cases were simulated to verify and validate the changes to the point reactor kinetics model in the ATR version of RELAP5/MOD2.5. The first case involved comparisons of an exact solution of a 0.10\$/s reactivity ramp with calculations from the original and corrected versions of RELAP5/MOD2.5. This test case was obtained from Information Systems Laboratories (Mortensen, 2008) and is described in Section 3.1.

The verification and validation calculations of the original point reactor kinetics model performed specifically for ATR were repeated with the corrected code. These cases included an exact solution for a theoretical 0.15\$ step insertion and comparisons between the RELAP5/MOD2.5 and PTKIN3 codes for accidents in the ATRC initiated by dropping a filler piece into the large inpile tube and a 0.45\$/s ramp. The PTKIN3 code was used to simulate reactivity accidents in earlier versions of the ATRC SAR. The results from these repeated calculations are shown in Sections 3.2 through 3.4.

The breadth of the verification and validation is illustrated in Figure 1, which shows the total reactivity from each of the four transients. The transients were all initiated by insertion of positive reactivity. Reactor scram was not simulated in the first two transients, but was simulated in the latter two. Reactivity feedback was not simulated in any of the transients.

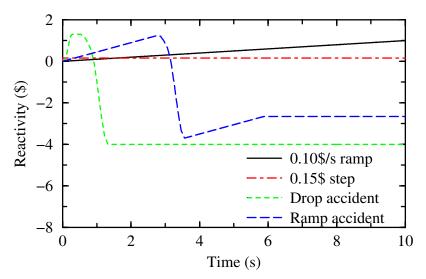


Figure 1. Total reactivity for the verification and validation transients.

3.1 0.10\$/s Reactivity Ramp

A calculation was performed to demonstrate the effect of the errors in the original RELAP5 point reactor kinetics model. Van den Eynde (2006) reported a high-fidelity numerical solution to a transient caused by a reactivity ramp of 0.1\$/s in a letter to the editors of Nuclear Science and Engineering. The high-fidelity numerical solution is hereafter referred to as the exact solution. The calculated results with a time step of 0.0001 s are compared with the exact solution in Figure 2. Table 3 shows the effect of time steps on the calculated power at 10 s with the original, 2007, and 2008 versions of the code.

The results with the original, 2007, and 2008 versions of RELAP5/MOD2.5 agreed closely, and were in excellent agreement with the exact solution, until 6 s. After 8 s, the calculated powers with the original version diverged significantly from the exact solution whereas the values from the 2007 and 2008 versions remained in excellent agreement. Table 3 shows that the results with the original code were not converged near 10 s. Although the results were in good agreement with the exact solution for a time step of 0.01 s, the agreement worsened as the time step decreased. With the 2007 and 2008 versions, the calculated results agreed better with the exact solution as the time step was reduced. The 2007 version of the code gave similar results to the 2008 version except at the largest time step.

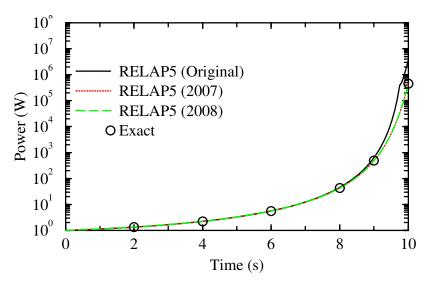


Figure 2. A comparison of RELAP5 results and the exact solution for a 0.10\$/s reactivity ramp.

	Calculated power / exact power at 10 s		
Time step (s)	Original 2007 2008		
0.01000	1.0015	0.9399	0.9998
0.00100	1.0468	0.9938	1.0000
0.00010	8.2112	0.9994	1.0000

Table 3. Results of convergence study for a 0.10\$/s reactivity ramp.

3.2 0.15\$ Step Reactivity Insertion

Lamarsh (1972) provides an exact solution for a 0.15\$ step insertion of reactivity in an infinite U^{235} reactor for six groups of delayed neutrons. Short-term results from the exact solution and the original and corrected RELAP5/MOD2.5 codes are compared in Figure 3. The power from the 2007 version did not change during the first time step, but otherwise, all versions gave answers in excellent agreement with the exact solution through 50 seconds as shown in Figure 4. The original code predicted a small (0.2%) step increase in the normalized power at 0.098 s when the code switched from the transient to steady-state logic as shown in Figure 5. The small increase in power did not occur in the exact solution or with either of the corrected codes.

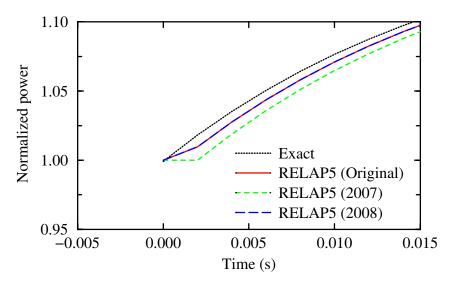


Figure 3. Normalized power following a step insertion of 0.15\$ reactivity (short term).

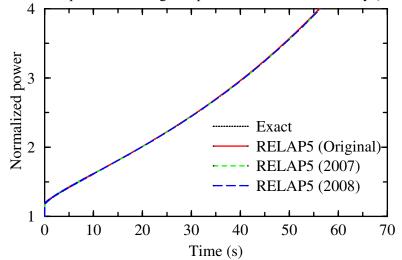


Figure 4. Normalized power following a step insertion of 0.15\$ reactivity (long term).

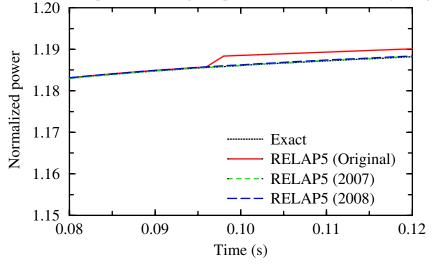


Figure 5. Normalized power near 0.10 s following a step insertion of 0.15\$ reactivity.

The results shown in Figures 3 through 5 were generated with time steps of 0.002 s before 1 s and 0.01 s afterwards. A time step convergence study was performed by multiplying these time steps by factors of 5, 0.5, and 0.05. The results were not significantly affected by the time step size, indicating that all codes were adequately converged. For example, Table 4 shows that the maximum variation from the exact solution was 0.1% at 1 s. The maximum variation at 70 s was 0.3%.

	Calculated power / exact power at 1 s		
Time step (s)	Original	2007	2008
0.01	1.0010	0.9997	0.9999
0.002	1.0012	1.0001	1.0001
0.001	1.0012	1.0001	1.0001
0.0001	1.0012	1.0001	1.0002

Table 4. Results at 1 s of the convergence study for a 0.15\$ step insertion.

3.3 ATRC Drop Accident

The third verification and validation case simulated an accident in the ATRC initiated by dropping a filler piece into the large inpile tube. The falling filler piece replaced water with metal, causing an average reactivity insertion rate of 4.6\$/s. The reactivity insertion caused the power to increase until a scram signal was generated and the safety rods were released.

Reactor powers calculated with the three versions of RELAP5/MOD2.5 and PTKIN3 are compared in Figure 6 for the drop accident. All results were generated with a time step of 0.002 s. The results from all four computer codes were similar, but the maximum power calculated with the 2007 version was about 2% higher than the peak powers from the other codes. As shown in Table 5, the 2007 and 2008 versions were in excellent agreement with PTKIN3 when the time step was reduced to 0.001 s or less. Although the magnitude of the deviation was small, the largest difference between the original version and the other codes occurred at the smallest time step, indicating a lack of convergence in the original version.

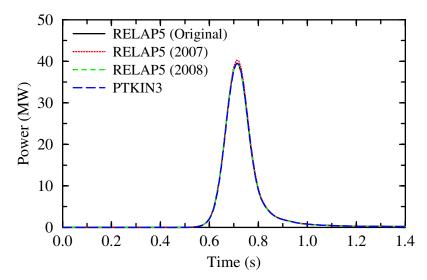


Figure 6. A comparison of calculated powers during the drop accident.

		Maximum p	ower (MW)	
Time step (s)	Original	2007	2008	PTKIN3
0.01	39.15	41.04	39.15	41.64
0.002	39.54	40.43	39.54	39.52
0.001	39.56	39.55	39.55	39.55
0.0001	39.98	39.55	39.55	39.55

Table 5.	Results of	convergence	study for	the drop	accident.

3.4 ATRC Ramp Accident

The last verification and validation case simulated an accident in the ATRC initiated by a 0.45\$/s reactivity ramp. The reactivity insertion caused a reactor scram on high neutron level. Reactor powers calculated with all four codes are compared in Figure 7 for the ATRC ramp accident. These results were obtained with a time step size of 0.002 s. The results from all four computer codes were nearly identical, as the peak powers differed by 0.2%.

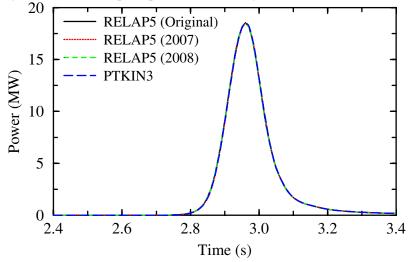


Figure 7. A comparison of calculated powers during the ramp accident.

Table 6 shows the effect of time step size on calculated peak power. The 2008 version of RELAP5/MOD2.5 and PTKIN3 gave nearly identical answers at all time steps. The maximum variation in the calculated peak power was 0.3%. The calculated peak values with the corrected version of RELAP5/MOD2.5 and PTKIN3 changed by less than 0.04% as the time steps were reduced from 0.002 to 0.0001 s, indicating that a reasonably converged solution had been obtained. The 2007 version gave similar results to the 2008 version, except at the largest time step where the peak powers differed by about 5%. The maximum values from the original version of RELAP5/MOD2.5 were within 1% of the values from PTKIN3 at the three larger time steps. However, the maximum power with the original version of RELAP5/MOD2.5 increased by more than a factor of two when the time step was decreased from 0.001 to 0.0001 s. Although the original version of RELAP5/MOD2.5 produced an accurate solution at relatively large time steps, the original numerical scheme diverged at very small time steps.

	Maximum power (MW)			
Time step (s)	Original	2007	2008	PTKIN3
0.01	18.45	17.54	18.45	18.51
0.002	18.53	18.50	18.49	18.50
0.001	18.67	18.50	18.50	18.50
0.0001	37.64	18.50	18.50	18.49

Table 6. Results of convergence study for the ramp accid
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4.0 Conclusions

The original version of RELAP5/MOD2.5 produced results that were in excellent agreement with the exact solution or PTKIN3 for the step insertion and ATRC drop accidents. Although the calculated results were in good agreement with the exact solution or PTKIN3 for the reactivity ramps with large time steps, they were in poor agreement at small time steps, indicating a lack of convergence in the original model.

The 2007 and 2008 versions of RELAP5/MOD2.5 converged to the correct solutions at small time steps for all four cases evaluated. The performance of the 2008 version was better at large time steps. RELAP5 users from different organizations should use updates equivalent to those generated in 2008 rather than those generated in 2007.

The 2008 version of RELAP5/MOD2.5 should be used to perform future reactivity analyses for the ATR and ATRC facilities.

5.0 References

Allison, C. M., and E. C. Johnson (eds.), SCDAP/RELAP5/MOD2 Code Manual, Volumes, 1, 2, and 3, NUREG/CR-5273, EGG-2555, September 1989.

Lamarsh, J. R., Introduction to Nuclear Reactor Theory, Addison-Wesley Publishing Company, Reading MA, 1972, p. 427.

Mortensen, G. A., Information Systems Laboratories, Personal communication, April 2008

RELAP5 Development Team, RELAP5/MOD3 Code Manual, Volumes 1, 2, and 4, NUREG/CR-5535, INEL-95-0174, August 1995.

Van den Eynde, G., Comments on "A Resolution of the Stiffness Problem of Reactor Kinetics," Nuclear Science and Engineering, 153, 2006, pp. 200-202.

Wagner, R. J., Innovative Systems Software, Personal communication, September 2008.

6.0 Acknowledgment

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