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DIGITAL SOLUTION
OF THE REACTOR KINETIC EQUATIONS
BY THE THETA METHOD
FOR FAST (FFTF)
AND THERMAL REACTORS

February 1969

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AND THERMAL REACTORS

By

R. A. Burnett

Control and Instrumentation Department
Systems and Electronics Division

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ABSTRACT

Three variations of a digital integration formula known as the Theta method were used to solve the nuclear reactor point kinetics equations on a Digital Equipment Corporation PDP-7 computer. The equations were also solved by trapezoidal integration. A three-delay-group model was programmed with thermal reactor parameters. Printout solutions were obtained for a reactivity step input of -0.005 and were compared to an analytical solution. For other reactivity inputs, hybrid equipment was used to compare the digital results to an analog solution computed simultaneously on a Beckman EASE 2133 analog computer. The analytical and analog solutions were assumed to be the "true" solutions. Fast reactor constants were then inserted and the tests repeated. A simple modification of one of the weighting parameters displayed a definite accuracy advantage over integration by the trapezoidal rule in the calculation of fast transients, although it required nearly two and one-half times the solution time of the trapezoidal method. In the case of more slowly changing power levels, the trapezoidal rule was able to nearly match the accuracy of the Theta method. A simplified variation of the Theta method required only 20 to 35% more solution time than trapezoidal integration while handling fast transients nearly as well as the more complex Theta variation. With the fast reactor model, the Theta and trapezoidal methods produced nearly identical results; both had good accuracy.

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INTRODUCTION

Three variations of a digital integration formula known as the Theta method were used to solve the nuclear reactor point kinetics equations on a Digital Equipment Corporation PDP-7 computer. The equations were also solved by trapezoidal integration. The purpose of this study was to determine the relative accuracy and efficiency of each method in real-time simulation.

A three-delay-group model was programmed with thermal reactor parameters. Printout solutions were obtained for a reactivity step input of -0.005 and were compared to an analytical solution. For other reactivity inputs, hybrid equipment was used to compare the digital results to an analog solution computed simultaneously on a Beckman EASE 2133 analog computer. The analytical and analog solutions were assumed to be the "true" solutions. Fast reactor constants were then inserted and the tests repeated.

SUMMARY

A simple modification of one of the weighting parameters resulted in an improvement of the basic Theta method. With the thermal reactor model, the improved Theta method displayed a definite accuracy advantage over integration by the trapezoidal rule in the calculation of fast transients, although it required nearly two and one-half times the solution time of the

trapezoidal method. In the case of more slowly changing power levels, the trapezoidal rule was able to nearly match the accuracy of the Theta method. A simplified variation of the Theta method required only 20 to 35% more solution time than trapezoidal integration while handling fast transients nearly as well as the more complex Theta variation. With the fast reactor model, the Theta and trapezoidal methods produced nearly identical results; both had good accuracy.

DISCUSSION

The kinetics equations to be solved are:

$$\frac{dN(t)}{dt} = \frac{\rho - \beta}{\ell^*} N(t) + \sum_{i=1}^G \lambda_i C_i(t) \quad (1)$$

$$\frac{dC_i(t)}{dt} = \frac{\beta_i}{\ell^*} N(t) - \lambda_i C_i(t) \quad (i=1,2,\dots,G) \quad (2)$$

Three-delay-group representations were used in both the thermal reactor and fast reactor models. Except for a brief investigation involving Doppler feedback, the reactivity ρ was determined entirely by a specified input function: i.e., $\rho = \rho(t)$. Step and ramp inputs, both positive and negative, were selected.

The Theta method can be thought of as a modification of closed trapezoidal integration in which the averaging factor of 0.5, applied to the sum of the past and present values of the derivative, is replaced by one or more variable weighting parameters, θ_i , which may take on values between zero and one. The manner in which the values of θ_i are calculated determines the particular variation of the method.

The following variation, applied to the kinetics equations, has been found by others^(1,2,3) to be quite successful. It will hereafter be referred to as "Theta I":

$$\begin{aligned}
N^{j+1} = & N^j + \Delta t \theta_1^j \left(\frac{\rho^{j+1} - \beta}{\ell^*} \right) N^{j+1} \\
& + \Delta t \left(1 - \theta_1^j \right) \left(\frac{\rho^j - \beta}{\ell^*} \right) N^j \\
& + \sum_{i=1}^G \Delta t \lambda_i \left[\theta_2^j C_i^{j+1} + \left(1 - \theta_2^j \right) C_i^j \right]
\end{aligned} \tag{3}$$

$$\begin{aligned}
C_i^{j+1} = & C_i^j + \Delta t \left(\frac{\beta_i}{\ell^*} \right) \left[\theta_1^j N^{j+1} + \left(1 - \theta_1^j \right) N^j \right] \\
& - \Delta t \lambda_i \left[\theta_2^j C_i^{j+1} + \left(1 - \theta_2^j \right) C_i^j \right] \quad (i = 1, 2, \dots, G)
\end{aligned} \tag{4}$$

$$\theta_i = \begin{cases} \frac{1}{\omega_i \Delta t} - \frac{1}{\exp(\omega_i \Delta t) - 1} & |\omega_i \Delta t| > K \\ \frac{1}{2} - \frac{\omega_i \Delta t}{12} & |\omega_i \Delta t| \leq K \end{cases} \tag{5}$$

(i = 1, 2)

$$\omega_1^j = \begin{cases} \frac{\rho^j - \beta}{\ell^*} & \rho^j < \beta \\ 0 & \rho^j \geq \beta \end{cases} \tag{6}$$

$$\omega_2^j = \begin{cases} \frac{\ell^*}{\beta - \rho^j} \sum_{i=1}^G \lambda_i \left(\frac{\beta_i}{\ell^*} - \frac{\lambda_i C_i^j}{N^j} \right) & \rho^j < 0.1 \frac{(\beta - \rho^j)^2}{\ell^*} \\ \frac{\rho^j - \beta}{\ell^*} + \sum_{i=1}^G \lambda_i \frac{C_i^j}{N^j} & \rho^j \geq 0.1 \frac{(\beta - \rho^j)^2}{\ell^*} \end{cases} \quad (7)$$

The superscripts j and $j+1$ refer to the old and new variable values, respectively. A list of symbols appears on page 36. The integration step size is Δt . The PDP-7 was able to provide accurate computation of the θ function with $K = 0.8$. Notice that if $\theta_1 = \theta_2 = 0.5$, Equations (3) and (4) become identical to those which would result from an application of the trapezoidal rule to Equations (1) and (2).

Equation (4) can be solved for C_i^{j+1} and substituted into Equation (3) to obtain:

$$N^{j+1} = f_o(N^j, C_1^j, C_2^j, \dots, C_G^j, \rho^{j+1}, \rho^j) \quad (8)$$

$$C_i^{j+1} = f_i(N^{j+1}, N^j, C_i^j) \quad (i = 1, 2, \dots, G) \quad (9)$$

If this method is to be used in a real-time simulation, it is important that the frame time (time required by the computer to calculate a new set of variable values) be as small as possible while maintaining accurate solutions. It was therefore important to know the accuracy and frame time of Theta I and to investigate the possibility of altering this method to reduce the frame time without significantly impairing the accuracy.

It should be noted here that the Theta method, like the trapezoidal rule, is an implicit form of integration and therefore cannot predict a new solution ahead of the instant of time at which that solution is valid, unless the reactivity input is known ahead of time. If the reactivity input is an analog signal, the computer must monitor that input at time t^{j+1} before it can complete the calculation of N^{j+1} and C_i^{j+1} . The updating of the complete solution will thus experience a time delay equal to the frame time. If N^{j+1} is the only variable of interest to the remainder of the simulation system, then the delay will be somewhat less than the total frame time.

VARIATIONS

It is evident that a value for θ_1 at time t_{j+1} could be calculated, using Equation (5) with

$$\omega_1^{j+1} = \begin{cases} \frac{\rho^{j+1} - \beta}{\ell^*} & \rho^{j+1} < \beta \\ 0 & \rho^{j+1} \geq \beta \end{cases} \quad (10)$$

It would thus seem logical and beneficial to replace θ_1^j with θ_1^{j+1} in those terms in Equations (3) and (4) which multiply $(j+1)$ variables by θ_1 . This can be done with no increase in frame time. A corresponding change cannot be made with θ_2^{j+1} because of its dependency upon quantities which are not yet available (N^{j+1}, C_i^{j+1}). Equations (3) and (4) now become:

$$\begin{aligned}
N^{j+1} = & N^j + \Delta t \, \theta_1^{j+1} \left(\frac{\rho^{j+1}}{\ell^*} - \beta \right) N^{j+1} \\
& + \Delta t \, (1 - \theta_1^j) \left[\frac{\rho^j}{\ell^*} - \beta \right] N^j \\
& + \sum_{i=1}^G \Delta t \lambda_i \left[\theta_2^j C_i^{j+1} + (1 - \theta_2^j) C_i^j \right] \quad (11)
\end{aligned}$$

$$\begin{aligned}
C_i^{j+1} = & C_i^j + \Delta t \left(\frac{\beta_i}{\ell^*} \right) \left[\theta_1^{j+1} N^{j+1} + (1 - \theta_1^j) N^j \right] \\
& - \Delta t \lambda_i \left[\theta_2^j C_i^{j+1} + (1 - \theta_2^j) C_i^j \right] \quad (i = 1, 2, \dots, G) \quad (12)
\end{aligned}$$

Equations (5), (6), and (7), with the addition of Equation (10), still apply. This variation will be called Theta II. The final form of Equations (11) and (12), rearranged according to the manner of Equations (8) and (9), is listed in Appendix A.

As a trial problem, the point kinetics equations were programmed using typical three-delay-group thermal reactor parameters. Provision was made such that Theta I, Theta II, or trapezoidal integration could be selected. The analytical solution to the problem of a step reactivity input of -0.005 was derived, using Laplace transforms, as a reference solution. The digital solutions were started from a steady-state condition with zero reactivity at $t_0 = 0$, and the reactivity was stepped to its full value at the first iteration ($t_1 = \Delta t$). If an analog reactivity signal were being monitored, the exact time at which the reactivity changed could have been anywhere from just after t_0 to just before t_1 . The average of the possibilities would be at $t = (t_0 + t_1)/2 = \Delta t/2$. It would seem likely, then, that the digital solutions should most nearly match the true solution to a reactivity step occurring at $t = \Delta t/2$. For this reason, comparison was made with the analytical solution stepped at $t = \Delta t/2$.

Table 1 shows the $N(t)$ solutions from zero to 3.5 sec with a time step of 0.1 sec. Let us examine their relative accuracies in two phases: the accuracy of the first few points of the transient, and the amount of error that has accumulated after 2 to 3 sec.

The Theta II variation was greatly superior in the calculation of the first two points of the transient, with Theta I running second and the trapezoidal rule coming in last. At 0.2 sec, the percent errors were 4.28, 0.93, and 0.12% for trapezoidal, Theta I, and Theta II, respectively. After five iterations, the Theta I solution converged to the same value as the Theta II solution and remained there to the termination of the test. The trapezoidal solution continued to be farthest from the analytical solution and was drifting from that solution at a slightly greater rate than the Theta solutions at the conclusion of the test.

Other reactivity inputs were applied, including step functions ranging from -0.020 to +0.003 and ramp functions ranging from -0.003t to +0.0015t, and the solutions were compared to points obtained from analog computer strip-chart solutions. The analog solutions to step inputs were started at $t = \Delta t/2$; solutions to ramp inputs were started at $t = 0$. The results were similar to those of Table 1 with moderate to large reactivity step changes. Theta II was able to follow reactivity ramps more closely than the other two methods. If the reactivity function was a slowly changing ramp or a small step, the differences in accuracy between the three methods nearly vanished. Increasing the integration step size generally had the expected effect of reducing the accuracy of all three digital solutions, but the relative accuracies among methods remained about the same.

TABLE 1. Thermal Reactor Response to a Reactivity
Step Change of -0.005 Occurring at
 $t = 0.05$: Theta Method Test Number 1.

<u>Time, sec</u>	<u>Trapezoidal Rule</u>	<u>Theta I</u>	<u>Theta II</u>	<u>Analytical Solution</u>
T	10 N	10 N	10 N	10 N
0.00	400.00	400.00	400.00	400.00
0.10	305.92	298.34	280.79	281.84
0.20	209.81	221.24	218.93	219.20
0.30	205.55	207.27	206.95	207.05
0.40	201.35	201.87	201.82	201.92
0.50	197.52	197.74	197.74	197.84
0.60	193.76	194.01	194.01	
0.70	190.05	190.37	190.37	
0.80	186.66	186.99	186.99	187.01
0.90	183.33	183.68	183.68	
1.00	180.17	180.47	180.47	
1.10	177.15	177.42	177.42	177.50
1.20	174.19	174.53	174.53	
1.30	171.47	171.74	171.74	171.79
1.40	168.70	169.07	169.07	
1.50	166.16	166.44	166.44	
1.60	163.63	164.04	164.04	
1.70	161.29	161.64	161.64	
1.80	159.01	159.39	159.39	159.43
1.90	156.73	157.14	157.14	
2.00	154.63	154.99	154.99	
2.10	152.59	152.97	152.97	
2.20	150.67	151.09	151.09	
2.30	148.88	149.22	149.22	149.34
2.40	146.97	147.40	147.40	
2.50	145.30	145.69	145.69	
2.60	143.64	143.97	143.97	
2.70	141.97	142.42	142.42	
2.80	140.49	140.93	140.93	141.05
2.90	139.00	139.43	139.43	
3.00	137.65	138.04	138.04	
3.10	136.23	136.60	136.60	136.79
3.20	134.81	135.25	135.25	
3.30	133.63	133.97	133.97	
3.40	132.40	132.74	132.74	
3.50	131.16	131.57	131.57	131.79

Another Theta variation resulted from a simplification of Theta II. It was observed that a significant reduction in frame time could be achieved if θ_2^j could be approximated by a

constant. A logical choice for this constant would be 0.5. Since θ_2^j is associated with the slowly changing precursor groups, Theta II normally calculates θ_2^j values which are very close to 0.5, so this approximation should be a good one. This variation, identical to Theta II except for the restriction of $\theta_2^j = 0.5$, will be called Theta III.

Table 2 lists the trapezoidal, Theta II, and Theta III solutions to the same problem solved in Table 1. Notice that the first few points of the transient are identical in the Theta II and Theta III solutions. Then Theta III begins to drift further from the "true" solution than does Theta II. At 3.5 sec the Theta III solution is only slightly more accurate than the trapezoidal solution (0.42% error for Theta III versus 0.48 and 0.17% for trapezoidal and Theta II, respectively). Other reactivity inputs and time step sizes produced similar results. Again, the differences between solutions were slight for small reactivity changes.

Strip-chart displays of the Theta II, Theta III, trapezoidal, and analog computer responses to various reactivity inputs are shown in Figures 1 through 9. An error signal, the difference between the digital solution and the analog solution, was plotted for each digital method. The large time steps were used primarily to amplify the error differences in the various methods. Smaller time steps would result in smoother solutions. In a hybrid simulation where analog signals are dependent upon the continuous result of the digitally calculated power level, a smooth solution would be desirable. An all-digital simulation, working with discrete points for all variables, would be more concerned with the accuracy of the points than the continuity of the solution and could thus accept larger time steps. In a complete reactor plant simulation, the lower limit on the time step

TABLE 2. *Thermal Reactor Response to a Reactivity
Step Change of -0.005 Occurring at
 $t = 0.05$: Theta Method Test Number 2.*

<u>Time, sec</u>	<u>Trapezoidal Rule</u>	<u>Theta II</u>	<u>Theta III</u>	<u>Analytical Solution</u>
T	10 N	10 N	10 N	10 N
0.00	400.00	400.00	400.00	400.00
0.10	305.92	280.79	280.79	281.84
0.20	209.81	218.93	218.93	219.20
0.30	205.55	206.95	206.95	207.05
0.40	201.35	201.82	201.87	201.92
0.50	197.52	197.74	197.69	197.84
0.60	193.76	194.01	193.95	
0.70	190.05	190.37	190.37	
0.80	186.66	186.99	186.94	187.01
0.90	183.33	183.68	183.57	
1.00	180.17	180.47	180.41	
1.10	177.15	177.42	177.36	177.50
1.20	174.19	174.53	174.48	
1.30	171.47	171.74	171.58	171.79
1.40	168.70	169.07	168.96	
1.50	166.16	166.44	166.35	
1.60	163.63	164.04	163.83	
1.70	161.29	161.64	161.47	
1.80	159.01	159.39	159.12	159.43
1.90	156.73	157.14	156.92	
2.00	154.63	154.99	154.78	
2.10	152.59	152.97	152.81	
2.20	150.67	151.09	150.82	
2.30	148.88	149.22	148.90	149.34
2.40	146.97	147.40	147.13	
2.50	145.30	145.69	145.36	
2.60	143.64	143.97	143.76	
2.70	141.97	142.42	142.15	
2.80	140.49	140.93	140.60	141.05
2.90	139.00	139.43	139.16	
3.00	137.65	138.04	137.72	
3.10	136.23	136.60	136.33	136.79
3.20	134.81	135.25	134.94	
3.30	133.63	133.97	133.64	
3.40	132.40	132.74	132.42	
3.50	131.16	131.57	131.24	131.79

FIGURE 1. *Solution Timing for Step Inputs*

FIGURE 2a. Normalized Thermal Reactor Response to a Reactivity Step Change of -0.005 Occurring at $t = 0.05$. $\Delta t = 0.1$ sec.

FIGURE 2b. Error Signals Expressed as a Fraction of Initial Neutron Level.

$$E_i(t) = |N_i(t) - N_1(t)| \quad (i = 2, 3, 4)$$

FIGURE 3a. Normalized Thermal Reactor Response to a Reactivity Step Change of -0.005 Occurring at $t = 0.20$.
 $\Delta t = 0.4$ sec

FIGURE 3b. Error Signals

FIGURE 4a. Normalized Thermal Reactor Response to a Reactivity Step Change of -0.005 Occurring at $t = 0.40$.
 $\Delta t = 0.8$ sec

FIGURE 4b. Error Signals

FIGURE 5a. Normalized Thermal Reactor Response to a Reactivity Step Change of -0.020 Occurring at $t = 0.05$.
 $\Delta t = 0.1$ sec

FIGURE 5b. Error Signals

FIGURE 6a. Normalized Thermal Reactor Response to a Reactivity Step Change of -0.020 Occurring at $t = 0.20$.
 $\Delta t = 0.4$ sec

FIGURE 6b. Error Signals

FIGURE 7a. Normalized Thermal Reactor Response to a Reactivity Step Change of +0.003 Occurring at $t = 0.05$.
 $\Delta t = 0.1$ sec

FIGURE 7b. Error Signals

FIGURE 8a. Normalized Thermal Reactor Response to a Reactivity Ramp Input of $+0.001t$ Occurring at $t = 0$.
 $\Delta t = 0.1$ sec

FIGURE 8b. Error Signals for
Figure 8a

FIGURE 9a. Normalized Thermal Reactor Response to a Reactivity Ramp Input of $-0.003t$ Occurring at $t = 0$.
 $\Delta t = 0.1$ sec

FIGURE 9b. Error Signals for
Figure 9a

size would be determined by the frame time of the digital portion of the entire simulation. However, roundoff error could further restrict the minimum Δt , especially with fixed-point arithmetic.

The PDP-7 solution time required by each method is given in Table 3, along with the calculation times of various phases of the solution. Programming was done in symbolic assembly language. The PDP-7 is an 18-bit octal fixed-point computer with a cycle time of 1.75 μ sec. More information about this computing system can be found in Reference 4.

Table 3 shows that a three-delay-group model requires a maximum PDP-7 frame time of 2.40 msec with Theta I or II and 1.34 msec with Theta III. Corresponding times for a six-delay-group model would be 3.93 and 1.94 msec. A frame time of 3.20 msec has been achieved by Porsching⁽¹⁾ on a Philco 2000-212 computer for a six-delay-group model using Theta I. A Univac 1108 computer produced frame times of 0.780 and 0.414 msec for Theta II and Theta III, respectively, with a reactivity input of 0.0037 and a three-delay-group model.⁽³⁾

The Theta III variation proved to be as accurate as Theta II in the calculation of rapidly changing neutron levels, while Theta II was shown to be superior in the case of slow, long-term level changes. Some advantage could thus be gained by selecting Theta II or Theta III according to the anticipated rate of change of the neutron level. Such a program, called Theta Selective, was written with typical results listed in Table 4. In this program, Theta II was used to calculate N^{j+1} unless either of the following two conditions prevailed, in which case Theta III was selected:

$$(a) \quad |\rho^{j+1} - \rho^j| \geq 0.001 \quad ;$$

$$\text{or (b)} \quad \left| \frac{N^j - N^{j-1}}{N^{j-1}} \right| \geq 0.1 \quad .$$

TABLE 3. *PDP-7 Solution Times for Theta Methods and Trapezoidal Rule: Three-Delay-Group Thermal Reactor Kinetics*

	Method	Solution Time, msec
a) Frame time, total solution:	Theta I and II	$\left\{ \begin{array}{l} 2.40 (\rho < 0.00133)^{(a)} \\ 2.21 (0.00133 \leq \rho \leq 0.0022) \\ 2.03 (\rho > 0.0022) \end{array} \right.$
	Theta III	$\left\{ \begin{array}{l} 1.34 (\rho < 0.00133)^{(a)} \\ 1.15 (\rho \geq 0.00133) \end{array} \right.$
	Trapezoidal	0.98
b) Time required to update $N(t)$:	Theta I and II	$\left\{ \begin{array}{l} 1.71 (\rho < 0.00133)^{(a)} \\ 1.52 (0.00133 \leq \rho \leq 0.0022) \\ 1.34 (\rho > 0.0022) \end{array} \right.$
	Theta III	$\left\{ \begin{array}{l} 0.77 (\rho < 0.00133)^{(a)} \\ 0.58 (\rho \geq 0.00133) \end{array} \right.$
	Trapezoidal	0.41
c) Additional time required to add one delay group:	Theta I and II	$\left\{ \begin{array}{l} 0.51 (\rho \leq 0.0022) \\ 0.43 (\rho > 0.0022) \end{array} \right.$
	Theta III	0.20
	Trapezoidal	0.20

a. *Reactivity break-point based on a time step (Δt) of 0.1 sec. A larger time step would cause an increase in this break point; e.g., if $\Delta t > 0.1$, then Theta II frame time = 2.40 msec if $\rho < \rho_k$, where $\rho_k > 0.00133$.*

The comparison numbers are not necessarily optimal but were chosen to give approximately the desired effect. Since the frame time of Theta II is approximately twice that of Theta III, the time step used by Theta II (Δt_2) was also twice that used by Theta III (Δt_3). In this manner the total percentage of simulation time consumed by the kinetics equations was held nearly constant. By using the faster Theta III variation and the smaller time step for calculation

TABLE 4. *Thermal Reactor Response to a Reactivity Step Change of -0.005 Occurring at $t = 0.025$; Theta Selective.*
 $\Delta t_3 = 0.05$; $\Delta t_2 = 0.10$ sec

100 $\Delta t = 5.00$

1000 $\rho(0) = 0.00$

1000 $\rho(0+) = -5.00$

1000 Times Slope of ρ Ramp = 0.00

100 T	0.1 C1	0.1 C2	C3	Theta	Analytical
				10 N	10 N
0.00	100.81	383.83	379.64	400.00	400.00
5.00	100.81	383.70	378.77	326.41	326.71
10.01	100.79	383.46	375.08	253.92	254.21
15.01	100.77	383.09	369.97	225.79	226.18
20.02	100.74	382.73	364.44	214.21	214.52
30.03	100.68	382.12	353.22	205.66	205.53
40.04	100.62	381.38	342.38	201.06	200.83
50.05	100.56	380.65	332.01	197.11	196.87
60.06	100.50	379.92	322.08	193.31	193.12
70.07	100.44	379.19	312.59	189.72	189.57
80.08	100.38	378.45	303.50	186.26	186.17
90.09	100.32	377.72	294.83	182.98	182.93
100.10	100.26	376.99	286.52	179.79	179.77
110.11	100.20	376.26	278.59	176.78	176.76
120.12	100.13	375.53	270.99	173.95	
130.13	100.07	374.79	263.73	171.17	171.10
140.14	100.01	374.06	256.79	168.56	
150.15	99.94	373.33	250.15	165.93	165.91
160.16	99.88	372.60	243.79	163.53	
170.16	99.81	371.74	237.71	161.17	161.14
180.17	99.73	370.89	231.89	158.87	
190.13	99.66	370.03	226.32	156.73	156.73
200.19	99.59	369.18	220.98	154.59	
210.20	99.51	368.32	215.88	152.56	152.63
220.21	99.44	367.47	211.00	150.63	
230.22	99.36	366.61	206.31	148.77	148.88
240.23	99.29	365.76	201.83	147.00	
250.24	99.22	364.91	197.54	145.24	145.41
260.25	99.15	364.05	193.43	143.52	
270.26	99.07	363.20	189.49	142.03	142.20
280.27	99.00	362.34	185.72	140.48	
290.28	98.93	361.49	182.10	139.03	
300.29	98.85	360.63	178.65	137.59	137.78

of sudden neutron level changes, more and closer points on the transient curve could be obtained. When the power level was changing slowly, the larger time step was used to take advantage of the now-superior accuracy of the Theta II variation. The Theta Selective comparison instructions added less than 100 μ sec per iteration to the total solution time.

REACTIVITY FEEDBACK CONSIDERATIONS

A Doppler feedback term, ρ_{fb} , was added to the total reactivity input to the thermal reactor model. The 2133 analog computer generated this term continuously as a function of the neutron level. Identical feedback functions were provided for each of the digital solutions and the analog solution. Typical results are shown in Figure 10.

This hybrid computation did not require any modifications in the digital programs, since they were already monitoring an analog voltage for the reactivity input. However, some problems would occur if the feedback reactivity were to be calculated digitally. Namely, ρ_{fb}^{j+1} and N^{j+1} become functions of each other, and their interdependence cannot be simply resolved. Since the feedback reactivity cannot change abruptly, ρ_{fb}^{j+1} could be predicted fairly accurately by a linear extrapolation of its last two points in advance of the calculation of N^{j+1} and then corrected after N^{j+1} has been calculated. Alternatively, explicit (backward-difference) integration formulae could be used to predict new fuel and coolant temperatures and hence new feedback reactivity values. Similar techniques could be used for other types of reactivity feedback.

FAST REACTOR KINETICS

The Theta III and trapezoidal methods were applied to the kinetics equations of a fast reactor with a mean effective neutron lifetime (ℓ^*) of 3.5×10^{-7} sec. Frame times

FIGURE 10a. Normalized Thermal Reactor Response to a Reactivity Step Change of -0.005 Occurring at $t = 0.05$, with Doppler Feedback. $\Delta t = 0.1$ sec

FIGURE 10b. Error Signals for
Figure 10a

and computation times were similar to those listed for the thermal kinetics problems. Table 5 is a listing of the two digital solutions to a reactivity step of -0.005 using a time step of 0.1 sec, together with a set of approximate points taken from an analog computer solution of the same problem. The time step was changed to 0.4 sec, yielding the solutions listed in Table 6. In each case the digital solutions were both quite accurate and nearly identical. A constant value of $\theta_1^j = \theta_1^{j+1} = 0.75$ was inserted into the equations, and again the results did not change significantly. The Theta III and trapezoidal solutions remained well matched for all of the reactivity functions selected, although a small difference gradually developed with increasing positive reactivity values such that Theta III was slightly more accurate. The reason for these rather surprising results can be better understood by making an approximate analysis of the Theta equations. This is done in Appendix B.

TABLE 5. *Fast Reactor Response to a Reactivity Step Change of -0.005 Occurring at $t = 0.05$: Theta Method Test Number 3. $\Delta t = 0.1$ sec*

<u>Time, sec</u>	<u>Trapezoidal Rule</u>	<u>Theta III</u>	<u>Analog Computer Solution</u>
T	100 N	100 N	100 N
0.00	200.00	200.00	200.00
0.10	77.26	77.14	76.80
0.20	75.26	75.38	75.10
0.30	73.81	73.69	73.50
0.40	71.95	72.08	72.00
0.50	70.69	70.54	70.60
0.60	68.95	69.08	69.20
0.70	67.85	67.69	67.80
0.80	66.21	66.36	66.50
0.90	65.25	65.09	65.20
1.00	63.72	63.88	63.90
1.10	62.87	62.72	62.70
1.20	61.45	61.61	61.60
1.30	60.73	60.56	60.50
1.40	59.37	59.55	59.40
1.50	58.74	58.58	58.40
1.60	57.51	57.65	57.50
1.70	56.93	56.78	56.60
1.80	55.78	55.93	55.80
1.90	55.27	55.13	55.00
2.00	54.20	54.35	54.20
2.10	53.77	53.60	53.50
2.20	52.75	52.89	52.80
2.30	52.38	52.21	52.10
2.40	51.42	51.56	51.50
2.50	51.10	50.94	50.90

TABLE 6. *Fast Reactor Response to a Reactivity Step Change of -0.005 Occurring at $t = 0.20$: Theta Method Test Number 3. $\Delta t = 0.4$ sec*

<u>Time, sec</u>	<u>Trapezoidal Rule</u>	<u>Theta III</u>	<u>Analog Computer Solution</u>
T	100 N	100 N	100 N
0.00	200.00	200.00	200.00
0.40	74.74	74.67	74.30
0.80	68.43	68.50	68.10
1.20	63.44	63.37	63.20
1.60	59.05	59.11	59.00
2.00	55.62	55.54	55.40
2.40	52.50	52.57	52.40
2.80	50.12	50.05	50.00
3.20	47.89	47.93	47.90
3.60	46.19	46.12	46.10
4.00	44.53	44.58	44.40
4.40	43.31	43.24	43.00
4.80	42.03	42.08	41.90
5.20	41.14	41.05	40.90
5.60	40.11	40.15	40.00
6.00	39.43	39.36	39.20

CONCLUSIONS

The introduction of θ_1^{j+1} into the Theta equations resulted in a basic improvement in the method. With thermal reactor parameters, the Theta II variation displayed superior accuracy over trapezoidal integration but required more than twice the solution time. Theta III was more accurate than the trapezoidal rule while requiring only a slightly longer solution time; Theta III was less accurate than Theta II. In general, the superiority of the Theta methods was most noticeable when large negative reactivity steps were applied and when the integration time step was large.

Theta Selective combined the advantages of Theta II and Theta III with only a small increase in the effective frame time. This technique is recommended for complex simulations of thermal reactor systems in which the kinetics

equations are a small fraction of the total digital simulation. Strict use of Theta II would be desirable if the digital part of the total simulation is small enough to permit it. In either case, the frame time is small enough and the accuracy is good enough to provide an excellent real-time or faster kinetics simulation.

Because of the nature of the Theta equations, the fast reactor parameters created a situation in which trapezoidal integration performed as well as Theta integration for most reactivity inputs. Thus, in fast reactor simulations requiring an absolute minimum overall frame time, trapezoidal integration would be recommended. In most cases, however, Theta III would be preferable here because of its slightly greater accuracy in response to positive reactivity inputs.

LIST OF SYMBOLS

<u>Symbol</u>	<u>Definition</u>
$N(t)$	Neutron concentration (neutron/cm ³). Proportional to power level.
$C_i(t)$	Concentration of i th delayed neutron precursor (nuclei/cm ³)
G	Total number of delayed neutron groups
β	Total delayed neutron fraction (dimensionless)
β_i	Delayed neutron fraction from i th group (dimensionless)
λ_i	Decay constant of i th precursor (sec ⁻¹)
ℓ^*	Mean effective neutron lifetime (sec)
ρ	Total reactivity (dimensionless)
ρ_{fb}	Doppler feedback reactivity (dimensionless)
Δt	Integration step size (sec)
θ_1, θ_2	Weighting parameters, Theta method (dimensionless)

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APPENDICES

APPENDIX A

THETA II: FINAL EQUATIONS

$$N^{j+1} = \frac{1}{D_0} \left\{ \left[1 + \Delta t (1 - \theta_1^j) \right] (R^j - A_0) \right. \\ \left. + \sum_{i=1}^G \frac{\Delta t^2 A_{i\lambda_i} \theta_2^j (1 - \theta_1^j)}{D_i} \right] N^j + \sum_{i=1}^G \frac{\Delta t \lambda_i C_i^j}{D_i} \left. \right\} \quad (13)$$

$$C_i^{j+1} = \frac{1}{D_i} \left\{ \Delta t A_i \left[\theta_1^{j+1} N^{j+1} + (1 - \theta_1^j) N^j \right] \right. \\ \left. + C_i^j \left[1 - \Delta t \lambda_i (1 - \theta_2^j) \right] \right\} \quad (i = 1, 2, \dots, G) \quad (14)$$

where

$$A_0 = \frac{\beta}{\ell^*}$$

$$A_i = \frac{\beta_i}{\ell^*}$$

$$R^j = \frac{\rho^j}{\ell^*} \quad R^{j+1} = \frac{\rho^{j+1}}{\ell^*}$$

$$D_0 = \left[1 - \Delta t \theta_1^{j+1} (R^{j+1} - A_0) - \sum_{i=1}^G \frac{\Delta t^2 A_{i\lambda_i} \theta_2^j \theta_1^{j+1}}{D_i} \right]$$

$$D_i = \left[1 + \Delta t \lambda_i \theta_2^j \right]$$

$\theta_1^j, \theta_1^{j+1}, \theta_2^j$ defined by equations (5), (6), (7), (10)

OTHER VARIATIONS

Theta I: Substitute θ_1^j in place of every θ_1^{j+1} .

Theta III: $\theta_2^j = 0.5$

Trapezoidal Rule: $\theta_1^j = \theta_1^{j+1} = \theta_2^j = 0.5$

APPENDIX B

FAST KINETICS SOLUTION ANALYSIS

The lack of significant difference between the Theta and trapezoidal solutions in the fast reactor study can be better understood with the aid of the following approximate analysis of the Theta Equations (13) and (14).

First, we observe that the primary difference between the fast neutron constants and the thermal constants is the size of λ^* . With the short life-time of the fast kinetics, the magnitude of $(R - A_0)$ is quite large (>9000 when $\rho \leq 0$) unless $\rho \approx \beta$.

Now suppose that $\theta_1^j = \theta_1^{j+1} = \theta_1 = 0.5$ or some constant near 0.5 such that neither θ_1 nor $(1 - \theta_1)$ is excessively small. Trapezoidal integration meets this requirement. Next, if Δt is large enough such that

$$\left| \Delta t (1 - \theta_1) (R^j - A_0) \right| \gg 1$$

and

$$\left| \Delta t \theta_1 (R^{j+1} - A_0) \right| \gg 1,$$

and yet Δt is small enough such that

$$\left| \Delta t (1 - \theta_1) (R^j - A_0) \right| \gg \left| \sum_{i=1}^G \frac{\Delta t^2 A_i \lambda_i \theta_2^j (1 - \theta_1)}{D_i} \right|$$

and

$$\left| \Delta t \theta_1 (R^{j+1} - A_0) \right| \gg \left| \sum_{i=1}^G \frac{\Delta t^2 A_i \lambda_i \theta_2^j \theta_1}{D_i} \right|$$

then Equation (13) can be approximated by

$$N^{j+1} \approx - \left[\frac{1 - \theta_1}{\theta_1} \right] \left[\frac{R^j - A_0}{R^{j+1} - A_0} \right] N^j - \left[\frac{1}{\theta_1 (R^{j+1} - A_0)} \right] \left[\sum_{i=1}^G \frac{\lambda_i C_i^j}{D_i} \right]$$

In the initial steady state, with $R^j = R^{j+1} = 0$,

$$N^{j+1} = N_0 \approx - \left[\frac{1 - \theta_1}{\theta_1} \right] N_0 + \left[\frac{1}{\theta_1 A_0} \right] \left[\sum_{i=1}^G \frac{\lambda_i C_{i0}}{D_i} \right]$$

Solving for the initial precursor density term:

$$\sum_{i=1}^G \frac{\lambda_i C_{i0}}{D_i} = A_0 N_0$$

Thus the first iteration after a reactivity step change should produce

$$N_1 \approx \left[\frac{1 - \theta_1}{\theta_1} \right] \left[\frac{A_0}{R_1 - A_0} \right] N_0 - \left[\frac{A_0}{\theta_1 (R_1 - A_0)} \right] N_0$$

or

$$N_1 \approx \left[\frac{A_0}{A_0 - R_1} \right] N_0 = \left[\frac{\beta}{\beta - \rho_1} \right] N_0$$

This is the magnitude of the "prompt jump" given in nuclear engineering textbooks as the initial response to a step reactivity input.

Having achieved this degree of accuracy on the first iteration, the trapezoidal rule is then able to compute the remaining slowly changing portion of the transient quite easily.

It shall now be shown that the Theta methods will also give approximately this same first point of the step response.

If $\omega_1 \Delta t = (R - A_0) \Delta t$ is large in magnitude ($\gg 1$) and negative in sign, then θ_1 can be very accurately given by

$$\theta_1 \approx \frac{(R - A_0) \Delta t + 1}{(R - A_0) \Delta t}$$

Substituting into Equation (13), one obtains:

$$N^{j+1} = \left\{ \frac{1 + \Delta t (R^j - A_0) \left[1 - \frac{(R^j - A_0) \Delta t + 1}{(R^j - A_0) \Delta t} \right]}{1 - \Delta t (R^{j+1} - A_0) \left[\frac{(R^{j+1} - A_0) \Delta t + 1}{(R^{j+1} - A_0) \Delta t} \right]} \right\} N^j$$

$$+ \left\{ \frac{1}{1 - \Delta t (R^{j+1} - A_0) \left[\frac{(R^{j+1} - A_0) \Delta t + 1}{(R^{j+1} - A_0) \Delta t} \right]} \right\} \left\{ \sum_{i=1}^G \frac{\Delta t \lambda_i C_i^j}{D_i} \right\}$$

where the summation terms containing Δt^2 have again been neglected. Simplifying, one obtains

$$N^{j+1} = - \left[\frac{1 + \Delta t (R^j - A_0) - \Delta t (R^j - A_0) - 1}{\Delta t (R^{j+1} - A_0)} \right] N^j$$

$$- \left[\frac{1}{(R^{j+1} - A_0)} \right] \left[\sum_{i=1}^G \frac{\lambda_i C_i^j}{D_i} \right]$$

$$N^{j+1} = - \left[\frac{1}{R^{j+1} - A_0} \right] \left[\sum_{i=1}^G \frac{\lambda_i C_i^j}{D_i} \right]$$

Initial values are

$$N^{j+1} = N_0 = \frac{1}{A_0} \sum_{i=1}^G \frac{\lambda_i C_{i0}}{D_i}$$

$$\sum_{i=1}^G \frac{\lambda_i C_{i0}}{D_i} = A_0 N_0$$

and the first iteration yields

$$N_1 \approx - \left[\frac{A_0}{R_1 - A_0} \right] N_0 = \left[\frac{\beta}{\beta - \rho_1} \right] N_0$$

which is the same "prompt jump" as that generated by the trapezoidal rule.

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