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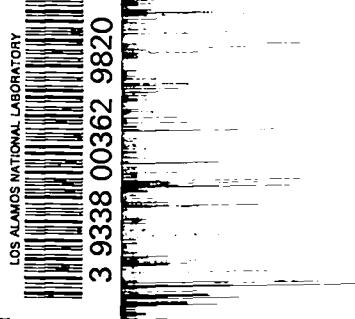
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**A FORMULATION FOR NUMERICAL SOLUTION  
OF THE INVERSE PROBLEM  
OF THE GENERALIZED REACTOR KINETICS EQUATIONS**



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**A FORMULATION FOR NUMERICAL SOLUTION  
OF THE INVERSE PROBLEM  
OF THE GENERALIZED REACTOR KINETICS EQUATIONS**

by

J. W. Evans



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## ABSTRACT

The general solution of the space independent reactor kinetics equations formulated by Keepin takes the form of an integral equation in which the neutron density is an implicit function of the time dependent reactivity. The equation also involves a set of tabulated constants. In this report the problem of specifying the reactivity required to yield a given neutron density function is solved by exhibiting an explicit solution for the reactivity in terms of the density function and a set of constants related to those tabulated by Keepin. The only mathematical restriction on the density function is that it be positive and differentiable. The solution is suitable for numerical computation, and methods for calculating the constants are developed. As a simple application the reactivity required to yield a constant density is shown to be a sum of negative exponentials.

## ACKNOWLEDGMENT

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Keepin<sup>1</sup> formulated a general solution of the space independent reactor kinetics equations for the neutron density. Keepin's formulation was particularly applicable for numerical solutions for arbitrary time dependence of the reactivity and required only that certain constants be tabulated for each fissile species.

If the direct problem of kinetics is finding the neutron density, given the time behavior of the reactivity, then the inverse problem is the determination of the time behavior of the reactivity necessary to produce a given neutron density.

The present report presents a formulation of the inverse problem similar to Keepin's formulation of the direct problem. The solution given is in many cases more readily determined numerically than the solution to the direct problem.

The neutron density,  $n(t)$ , satisfies the equation (in a source free medium)

$$n(t) = n(0) + \sum_{j=0}^{j_{\max}} A_j \int_0^t e^{S_j(t-u)} n(u) D(u) du, \quad t \geq 0, \quad (1)$$

where the  $A_j$  and  $S_j$  are constants determined and given by Keepin, and  $D(t) = k(t) - 1$  is the time dependent reactivity. In the inverse problem

$n(t)$  is supposed known and, for convenience, differentiable. The properties of the constants<sup>1</sup> which will be needed are

$$A_j > 0, \quad j \geq 0 \quad \text{and}$$

$$s_0 = 0, \quad s_0 > s_1 > s_2 > \dots > s_{j_{\max}}.$$

It is permissible to differentiate (1) giving

$$\frac{dn}{dt} = \sum_{(j)} A_j s_j e^{s_j t} \int_0^t e^{-s_j u} n(u) D(u) du + \sum_{(j)} A_j n(t) D(t),$$

or

$$n(t) D(t) = \frac{1}{\sum A_j} \left[ n'(t) - \sum_{(j)} A_j s_j \int_0^t e^{s_j(t-u)} n(u) D(u) du \right]. \quad (2)$$

Let  $y(t) = n(t) D(t)$ ,  $t \geq 0$ . For convenience, let  $a = \frac{1}{\sum A_j}$ .

Then

$$y(t) = a \left[ n'(t) - \sum_{(j)} A_j s_j \int_0^t e^{s_j(t-u)} y(u) du \right].$$

$$\text{Let } Y(s) = \int_0^\infty e^{-st} y(t) dt.$$

Then

$$Y(s) = a \int_0^\infty e^{-st} n'(t) dt - a \sum_{(j)} A_j s_j \int_0^\infty e^{-st} \left[ \int_0^t e^{s_j(t-u)} y(u) du \right] dt.$$

By the Convolution Theorem:

$$\begin{aligned}
 Y(s) &= a \int_0^\infty e^{-st} n'(t) dt = a Y(s) \sum_{(j)} A_j S_j \int_0^\infty e^{-st} \cdot e^{\frac{S_j t}{s-S_j}} dt \\
 &= a \int_0^\infty e^{-st} n'(t) dt = a Y(s) \sum_{(j)} \frac{A_j S_j}{s-S_j},
 \end{aligned}$$

or

$$Y(s) = \frac{a}{1+a \sum_{(j)} \frac{A_j S_j}{s-S_j}} \int_0^\infty e^{-st} n'(t) dt.$$

But

$$\frac{a}{1+a \sum_{(j)} \frac{A_j S_j}{s-S_j}} = \frac{1}{s \sum_{(j)} \frac{A_j}{s-S_j}} \text{ and } \sum_{(j)} \frac{A_j}{s-S_j} = \frac{\sum_{j=0}^{j_{\max}} \left[ A_j \prod_{(i \neq j)} (s-S_i) \right]}{\prod_{j=0}^{j_{\max}} (s-S_j)}.$$

Therefore,

$$\frac{1}{s \sum_{(j)} \frac{A_j}{s-S_j}} = \frac{\prod_{j=0}^{j_{\max}} (s-S_j)}{\sum_{j=0}^{j_{\max}} \left[ A_j \prod_{(i \neq j)} (s-S_i) \right]} = \frac{\prod_{j=1}^{j_{\max}} (s-S_j)}{\sum_{j=0}^{j_{\max}} \left[ A_j \prod_{(i \neq j)} (s-S_i) \right]},$$

and

$$\frac{Y(s)}{s} = \frac{\prod_{j=1}^{j_{\max}} (s - s_j)}{s \sum_{j=0}^{j_{\max}} \left[ A_j \prod_{i \neq j} (s - s_i) \right]} \cdot \int_0^{\infty} e^{-st} n(t) dt.$$

The quotient of polynomials in  $s$  may be written as a partial fraction expansion:

$$\frac{\prod_{j=1}^{j_{\max}} (s - s_j)}{s \sum_{j=0}^{j_{\max}} \left[ A_j \prod_{i \neq j} (s - s_i) \right]} = \sum_{j=0}^{j_{\max}} \frac{R_j}{s - s_j^*},$$

where the  $S^*$ 's are the roots of the denominator and the  $R$ 's are constants. Obviously,  $S_0^* = 0$ . A method of determining the  $R$ 's and a discussion of the signs and magnitudes of the  $R$ 's and  $S^*$ 's will be given later on.

Let  $Q$  be the function such that

$$\int_0^{\infty} e^{-st} Q(t) dt = \sum_{j=0}^{j_{\max}} \frac{R_j}{s - s_j^*}.$$

Then

$$Q(t) = \sum_{j=0}^{j_{\max}} R_j e^{s_j^* t}, \quad t \geq 0.$$

Therefore,

$$\frac{Y(s)}{s} = \left[ \int_0^\infty e^{-st} Q(t) dt \right] \left[ \int_0^\infty e^{-st} n'(t) dt \right].$$

Using the Convolution Theorem again:

$$\frac{Y(s)}{s} = \int_0^\infty e^{-st} \left[ \int_0^t n'(u) Q(t-u) du \right] dt,$$

and, since

$$\frac{Y(s)}{s} = \int_0^\infty e^{-st} \left[ \int_0^t y(u) du \right] dt$$

and since two different functions cannot have the same Laplace transform,

$$\int_0^t y(u) du = \int_0^t n'(u) Q(t-u) du, \quad t \geq 0.$$

Differentiating both sides with respect to  $t$  yields

$$y(t) = n'(t)Q(0) + \int_0^t n'(u)Q'(t-u) du. \quad (3)$$

Since

$$Q'(t) = \sum_{j=0}^{j_{\max}} R_j S_j^* e^{S_j^* t}, \quad Q(0) = \sum_{j=0}^{j_{\max}} R_j, \quad \text{and} \quad y(t) = n(t)D(t),$$
$$t \geq 0,$$

substitution in equation (3) yields

$$D(t) = \left( \sum_{j=0}^{j_{\max}} R_j \right) \frac{n'(t)}{n(t)} + \frac{1}{n(t)} \int_0^t n'(u) \left[ \sum_{j=0}^{j_{\max}} R_j S_j^* e^{S_j^*(t-u)} \right] du,$$

or

$$D(t) = \left( \sum_{j=0}^{j_{\max}} R_j \right) \frac{n'(t)}{n(t)} + \frac{1}{n(t)} \sum_{j=1}^{j_{\max}} R_j S_j^* e^{S_j^* t} \int_0^t n'(u) e^{-S_j^* u} du, \quad (4)$$

since  $S_0^* = 0$ . If one includes the source term  $\Omega_0'$  as defined by Keppin [(1) p. 672], the comparable result is

$$D(t) = \left( \sum_{j=0}^{j_{\max}} R_j \right) \frac{n'(t) - \Omega_0'(0)}{n(t)} + \frac{1}{n(t)} \sum_{j=1}^{j_{\max}} R_j S_j^* e^{S_j^* t} \int_0^t [n'(u) - \Omega_0'(u)] e^{-S_j^* u} du. \quad (4')$$

There are some facts about the  $R$ 's and  $S^*$ 's which are easy to obtain without numerical procedures and which are of interest.

First, the sum of the  $R$ 's is the reciprocal of the sum of the  $A$ 's in the original equations. To obtain this relationship set  $t = 0$  in equation (2) and in equation (4).

From (2),  $n(0)D(0) = \frac{1}{\sum_j A_j} \cdot n'(0)$ , and from (4),

$$D(0) = \left[ \sum_j R_j \right] \frac{n'(0)}{n(0)}.$$

Thus

$$\frac{1}{\sum A_j} = \sum (j) R_j.$$

Second, the  $S^*$ 's are all negative, except for  $S_0^*$ , which is zero, and they interlace the  $S$ 's in the original equations according to the inequality  $0 > S_1^* > S_1 > S_2^* > S_2 > S_3^* > S_3 > \dots > S_{j_{\max}}^* > S_{j_{\max}}$ . This fact can be shown fairly easily. The  $S^*$ 's, for  $j \geq 1$ , are the roots of the polynomial

$$Q(s) = \sum_{j=0}^{j_{\max}} \left[ A_j \prod_{i \neq j} (s - S_i) \right],$$

which can be written as

$$\left[ \prod_{j=0}^{j_{\max}} (s - S_j) \right] \left( \frac{A_0}{s} + \frac{A_1}{s - S_1} + \frac{A_2}{s - S_2} + \dots + \frac{A_{j_{\max}}}{s - S_{j_{\max}}} \right)$$

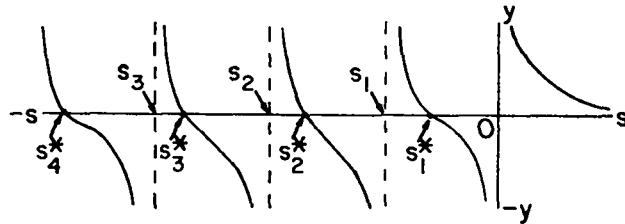
for  $s \neq S_i$ ,  $i = 0, 1, 2, \dots, j_{\max}$ .

The first factor is not zero except at the  $S_i$ 's, so the second factor must be zero at the roots,  $S_i^*$ . All the  $A_i$ 's are positive and all the  $S_i$ 's are negative. Therefore, there are no non-negative  $S_i^*$ 's. From continuity considerations and the fact that  $s - S_i > 0$ ,  $i = 1, 2, \dots, j_{\max}$ ,

when  $0 > s > S_1$ , it is obvious that  $s$  may be taken close enough to zero so that  $\frac{A_0}{s}$  exactly cancels the sum of the other items. Similarly, when  $S_1 > s > S_2$ ,  $s$  and  $s-S_1$  are negative, and  $s-S_2$ ,  $s-S_3$ , etc., are all positive, and  $s$  may be taken close enough to (or far enough from)  $S_1$  so that  $\frac{A_0}{s} + \frac{A_1}{s-S_1}$  exactly cancels the sum of the rest of the terms.

Pictorially, the situation is described below, where

$$y(s) = \frac{A_0}{s} + \frac{A_1}{s-S_1} + \dots + \frac{A_{j_{\max}}}{s-S_{j_{\max}}}.$$



I have not been able to find any simple way to relate the  $S^*$ 's to the  $A$ 's and  $S$ 's and presume that they have to be calculated by using a polynomial solver on  $Q$  or by using some approximation method on the  $y$  pictured above.

Third, the  $R$ 's are given explicitly from a theorem which states that if  $P$  and  $Q$  are polynomials, and the roots of  $Q$  are distinct,  $P$  is of degree less than  $Q$ , and  $\frac{P(s)}{Q(s)} = \sum (j) \frac{R_j}{s-S_j}$ , where the  $S_j$ 's are the roots of  $Q$ ; then  $R_j = \frac{P(S_j)}{Q'(S_j)}$ ,  $j = 0, 1, 2, \dots$ . For the present problem,

$$P(s) = \prod_{j=1}^{j_{\max}} (s - S_i) \text{ and } Q(s) = s \sum_{j=0}^{j_{\max}} A_j \prod_{i \neq j} (s - S_i).$$

The polynomial

$$\frac{Q(s)}{s} = \sum_{j=0}^{j_{\max}} \left[ A_j \prod_{i \neq j} (s - S_i) \right]$$

is the sum of  $j_{\max} + 1$  polynomials, each of degree  $j_{\max}$  and with leading coefficients  $A_0, A_1, A_2, \dots$  etc. The sum polynomial thus has leading coefficient  $\sum_{j=0}^{j_{\max}} A_j$  and can be written

$$\frac{Q(s)}{s} = \left[ \sum_{(j)} A_j \right] \prod_{i=1}^{j_{\max}} (s - S_i^*)$$

by the factorization theorem.

Since  $S_0^* = 0$ ,

$$Q(s) = \left[ \sum_{(j)} A_j \right] \prod_{i=0}^{j_{\max}} (s - S_i^*),$$

and

$$Q'(s) = \left[ \sum_{(j)} A_j \right] \left\{ \sum_{j=0}^{j_{\max}} \left[ \prod_{(L \neq j)} (s - S_L^*) \right] \right\}.$$

By the theorem cited:

$$R_i = \frac{P(S_i^*)}{Q'(S_i^*)} = \frac{\prod_{j=1}^{j_{\max}} (S_i^* - S_j)}{\left[ \sum_{(j)} A_j \right] \left\{ \sum_{j=0}^{j_{\max}} \left[ \prod_{(L \neq j)} (S_i^* - S_L^*) \right] \right\}}, \quad i = 0, 1, 2, \dots, j_{\max}.$$

For a given  $i$ , the only product which does not drop out in the sum of partial products in the denominator is the one for which  $j = i$ .

Thus,

$$R_i = \frac{1}{\sum_{(j)} A_j} \cdot \frac{\prod_{j=1}^{j_{\max}} (S_i^* - S_j)}{\prod_{(j \neq i)} (S_i^* - S_j^*)}, \quad i = 0, 1, 2, \dots, j_{\max}. \quad (5)$$

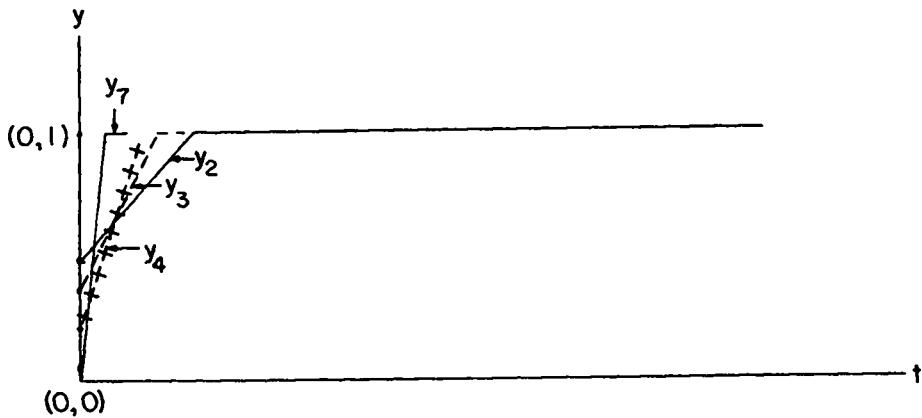
$$R_0 = \frac{1}{\sum_{(j)} A_j} \cdot \frac{\prod_{j=1}^{j_{\max}} |S_j|}{\prod_{j=1}^{j_{\max}} |S_j^*|} > 0.$$

A little analysis of the ordering of the  $S$ 's and  $S^*$ 's shows that  $R_i < 0$  for  $i > 0$ .

#### AN APPLICATION

Equation (4) may be applied conveniently to determine the inverse,  $D$ , when  $n$  is specified to be the step function  $\begin{cases} n(0) = 0 \\ n(t) = 1, \quad t > 0 \end{cases}$ . This problem is approached most easily by treating a sequence of continuous functions whose limit is the step function above. For each positive integer  $m > 1$  let

$$y_m(t) = \begin{cases} \frac{1}{m} \text{ when } t = 0 \\ \frac{1}{m} + mt \text{ when } 0 < t \leq \frac{1}{m} \left(1 - \frac{1}{m}\right) \\ 1 \text{ when } t > \left(1 - \frac{1}{m}\right) \frac{1}{m} \end{cases}$$



For each positive integer  $m > 1$ ,

$$D_m(t) = \sum_{j=1}^{j_{\max}} R_j S_j^* \int_0^{\frac{1}{m}(1-\frac{1}{m})} m e^{\frac{1}{m}(1-\frac{1}{m})u} S_j^*(t-u) du,$$

since, for  $t > \frac{1}{m}(1-m)$ ,  $y_m'(t) = 0$ , and, for  $0 \leq t < \frac{1}{m}(1-m)$ ,  $y_m'(t) = m$ .

(The break in the graph of  $y_m'$  at  $t = \frac{1}{m}(1-m)$  may be ignored since  $y_m'$  is bounded.)

$$\begin{aligned}
 D_m(t) &= m \sum_{j=1}^{j_{\max}} R_j S_j^* e^{S_j^* t} \int_0^m \left(1 - \frac{1}{m}\right) e^{-S_j^* u} du \\
 &= m \sum_{j=1}^{j_{\max}} R_j S_j^* e^{S_j^* t} \left[ \frac{1}{S_j^*} - \frac{e^{-S_j^* \left(1 - \frac{1}{m}\right) m}}{S_j^*} \right]
 \end{aligned}$$

or

$$D_m(t) = m \sum_{j=1}^{j_{\max}} R_j \left[ 1 - e^{-\frac{S_j^*}{m} \left(1 - \frac{1}{m}\right)} \right] e^{S_j^* t}, \quad t > \frac{1}{m} \left(1 - \frac{1}{m}\right).$$

In order to find  $\lim_{m \rightarrow \infty} D_m(t)$ , it is necessary to evaluate

$$\lim_{m \rightarrow \infty} m \left[ 1 - e^{-\frac{S_j^*}{m} \left(1 - \frac{1}{m}\right)} \right].$$

Thus,

$$m \left[ 1 - e^{-\frac{S_j^*}{m} \left(1 - \frac{1}{m}\right)} \right] = -\frac{1 - e^{-\frac{S_j^*}{m} \left(1 - \frac{1}{m}\right)}}{0 - \frac{1}{m}} = -\frac{e^0 - e^{-\frac{S_j^*}{m} \left(1 - \frac{1}{m}\right)}}{0 - \frac{1}{m}}.$$

Therefore, the limit above is

$$\frac{d}{dx} \left[ -e^{-S_j^* x (1-x)} \right]_{x=0} = \left[ S_j^* (1-2x) e^{-S_j^* x (1-x)} \right]_{x=0} = S_j^*.$$

Therefore,

$$\lim_{m \rightarrow \infty} D_m(t) = \sum_{j=1}^{J_{\max}} R_j S_j^* e^{S_j^* t}, \quad t > 0.$$

Consequently, the required reactivity is a sum of negative exponentials.

#### REFERENCE

1. G. R. Keepin and C. W. Cox, "General Solution of the Reactor Kinetic Equations," *Nucl. Sci. Eng.* 8, 670-690 (1960).