

## **VARIATIONAL REACTIVITY ESTIMATES: NEW ANALYSES AND NEW RESULTS**

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### **ABSTRACT**

A modified form of the variational estimate of the reactivity worth of a perturbation was previously developed to extend the range of applicability of variational perturbation theory for perturbations leading to negative reactivity worths. Recent numerical results challenged the assumptions behind the modified form. In this paper, more results are obtained, leading to the conclusion that sometimes the modified form extends the range of applicability of variational perturbation theory for positive reactivity worths as well, and sometimes the standard variational form is more accurate for negative-reactivity perturbations. In addition, this paper proves that using the exact generalized adjoint function would lead to an inaccurate variational reactivity estimate when the error in the first-order estimate is large; the standard generalized adjoint function, an approximation to the exact one, leads to more accurate results. This conclusion is also demonstrated numerically. Transport calculations use the PARTISN multigroup discrete ordinates code.

*Key Words:* Variational perturbation theory, transport theory

### **1. INTRODUCTION**

In previous work [1-3], it was found that the variational estimate of a quantity of interest associated with a perturbation leading to a negative change was less accurate than the variational estimate of the quantity of interest associated with a similarly sized perturbation leading to a positive change. In other words, the range of applicability of the variational estimate was more limited on the negative side than the positive side. This phenomenon was observed in a sodium slab inhomogeneous source problem with transport theory (using an unknown number of energy groups), shown in Fig. 1 [1]; a 24-group fast spherical reactor with diffusion theory [2]; and a two-group thermal slab reactor with diffusion theory, shown in Fig. 2 [3]. In Ref. 1, the quantity of interest was the flux exiting the slab; in Refs. 2 and 3, the quantity of interest was the reactivity worth of the perturbation. Figures 1 and 2 show the characteristic quadratic shape of the variational (second-order) estimate.

Over a decade ago, an attempt to extend the range of applicability of the variational reactivity estimate resulted in the development of a modified form [4]. Positive reactivities were to be estimated using the standard form, but negative reactivities were to be estimated using the modified form. This development resulted in more accurate negative-reactivity estimates [4] for the 24-group fast spherical reactor with diffusion theory and the two-group thermal slab reactor with diffusion theory.

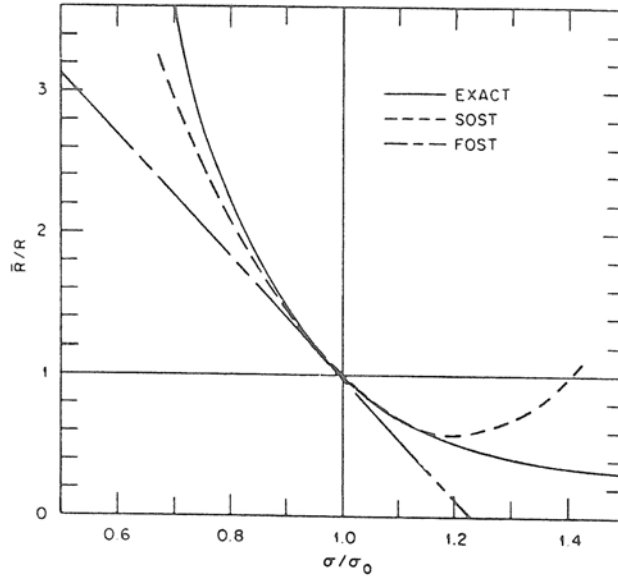


FIGURE 20. Relative flux change vs. relative change in 297-keV cross section minimum in sodium.

Figure 1. Fig. 20 from Ref. 1. FOST = first-order sensitivity theory; SOST = second-order sensitivity theory. Reprinted with permission of the author.

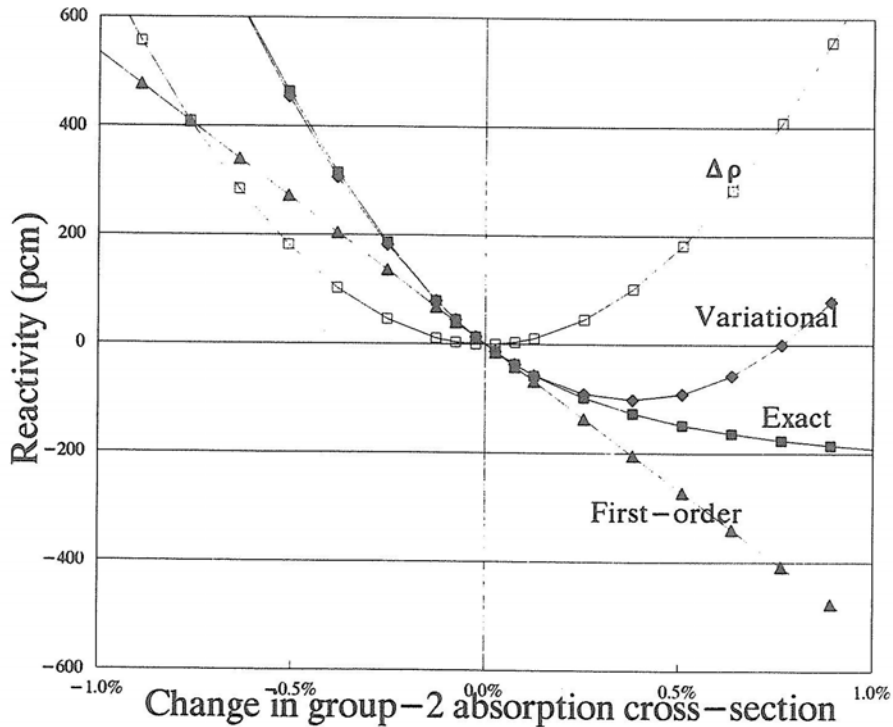


Fig. 5. Results from static reactivity calculations for the 240-cm core.

Figure 2. Fig. 5 from Ref. 3.  $\Delta\rho = -f_2\rho_0$ . © 1995 by the American Nuclear Society, La Grange Park, Illinois.

Last year, surprising results were obtained for a 47-group thermal spherical reflected reactor with transport theory [5]. The modified form of the variational reactivity estimate was more accurate than the regular form for some negative reactivity worths.

In this paper, several perturbations of the thermal problem used in Ref. 5 are considered. The simple algorithm for choosing the modified variational form over the standard variational form is shown to be inadequate. Unfortunately, the correct algorithm, if one exists, is elusive. Note that the goal is to *extend* the range of accuracy of the variational perturbation theory; its range of accuracy is already much greater than that of the standard perturbation theory.

## 2. BACKGROUND

The exact reactivity worth of a perturbation,  $\rho_{ex}$ , is

$$\rho_{ex} = -\Delta\lambda = \frac{\langle \psi_0^*, (\lambda_0 \Delta F - \Delta A) \psi' \rangle}{\langle \psi_0^*, F' \psi' \rangle}. \quad (1)$$

Primes indicate perturbed quantities, subscript 0 indicates unperturbed quantities, and the perturbation in quantity  $X$  is  $\Delta X = X' - X_0$ . The standard first-order reactivity estimate is obtained by using the unperturbed flux  $\psi_0^g(r, \hat{\Omega})$  instead of the perturbed flux  $\psi'^g(r, \hat{\Omega})$  in Eq. (1):

$$\rho_0 = \frac{\langle \psi_0^*, (\lambda_0 \Delta F - \Delta A) \psi_0 \rangle}{\langle \psi_0^*, F' \psi_0 \rangle}. \quad (2)$$

The standard variational reactivity estimate,  $\rho_v$ , can be written

$$\rho_v = \rho_0(1 - f_v), \quad (3)$$

where

$$f_v = \langle \Gamma_{\Delta}^*, (\Delta A - \lambda_0 \Delta F - \Delta \lambda \Delta F) \psi_0 \rangle \quad (4)$$

is a flux correction factor that accounts for the effect of fundamental-mode flux shifts on the perturbation [4].  $\Gamma_{\Delta}^{*g}(r, \hat{\Omega})$  is a generalized adjoint function satisfying

$$(A_0^* - \lambda_0 F_0^*) \Gamma_{\Delta}^{*g}(r, \hat{\Omega}) = \frac{(\Delta A^* - \lambda_0 \Delta F^*) \psi_0^{*g}(r, \hat{\Omega})}{\langle \psi_0^*, (\Delta A - \lambda_0 \Delta F) \psi_0 \rangle} - \frac{F_0^* \psi_0^{*g}(r, \hat{\Omega})}{\langle \psi_0^*, F_0 \psi_0 \rangle}, \quad (5)$$

which only approximates the equation satisfied by the exact generalized adjoint function  $\Gamma_s^{*g}(r, \hat{\Omega})$ :

$$(A'^* - \lambda' F'^*) \Gamma_s^{*g}(r, \hat{\Omega}) = \frac{(\Delta A^* - \lambda_0 \Delta F^*) \psi_0^{*g}(r, \hat{\Omega})}{\langle \psi_0^*, (\Delta A - \lambda_0 \Delta F) \psi' \rangle} - \frac{F'^* \psi_0^{*g}(r, \hat{\Omega})}{\langle \psi_0^*, F' \psi' \rangle}. \quad (6)$$

Since the exact value of  $\Delta\lambda$  is unavailable, some estimate must be used if the second-order term  $\Delta\lambda\Delta F\psi_0$  is used in Eq. (4) (often, it isn't). One obvious choice is  $-\rho_0$ . Another possibility is to use  $-\rho_0$  as an initial guess, compute  $\rho_v$  using Eq. (3), then iterate with  $-\rho_v$ .

An exact value of  $f, f_{ex}$ , was defined [4] by writing, in analogy with Eq. (3),

$$\rho_{ex} = \rho_0(1 - f_{ex}). \quad (7)$$

A third value of  $f$  is  $f_s$ , the value that would be obtained using  $\Gamma_s^{*g}(r, \hat{\Omega})$  instead of  $\Gamma_\Delta^{*g}(r, \hat{\Omega})$  in Eq. (4):

$$f_s = \langle \Gamma_s^*, (\Delta A - \Delta(\lambda F)) \psi_0 \rangle. \quad (8)$$

[ $\Gamma_\Delta^{*g}(r, \hat{\Omega})$  of Eq. (5) has associated with it the biorthogonality relation  $\langle \Gamma_\Delta^*, F_0 \psi_0 \rangle = 0$ , which is why there is no  $\lambda_0 F_0 \psi_0$  term in Eq. (4).] It has been shown [4, 6] that

$$f_s = - \frac{\langle \psi_0^*, (\Delta A - \Delta(\lambda F)) \Delta \psi \rangle}{\langle \psi_0^*, (\Delta A - \lambda_0 \Delta F) \psi' \rangle}. \quad (9)$$

Previous analyses have pointed out that Eq. (9) means that the factor  $f$  is an attempt to account for the effect of the flux shift  $\Delta\psi / \psi'$  on the perturbation. Rearranging the right side of Eq. (9) and using Eqs. (1) and (2) results in

$$f_s = \frac{\langle \psi_0^*, F' \psi_0 \rangle}{\langle \psi_0^*, F' \psi' \rangle} \left( \frac{\rho_0 - \rho_{ex}}{\rho_{ex}} \right), \quad (10)$$

and using Eq. (7) results in

$$f_s = \frac{\langle \psi_0^*, F' \psi_0 \rangle}{\langle \psi_0^*, F' \psi' \rangle} \left( \frac{f_{ex}}{1 - f_{ex}} \right). \quad (11)$$

Rearranging Eq. (11) yields

$$f_{ex} = \frac{f_s}{1 + f_s - \frac{\langle \psi_0^*, F' \Delta \psi \rangle}{\langle \psi_0^*, F' \psi' \rangle}}. \quad (12)$$

Ignoring the ratio of adjoint-weighted fission sources in the denominator of Eq. (12) suggested the following modified form of the variational reactivity estimate [4]:

$$\rho_{v,mod.} = \rho_0 \left( 1 - \frac{f_v}{1 + f_v} \right). \quad (13)$$

Essentially, the modification attempts a better estimate of the flux correction factor  $f$ . In Ref. 4 it was recommended that  $\rho_{v,mod.}$  be used where  $\rho_0$  is negative and the standard  $\rho_v$  of Eq. (3) be used where  $\rho_0$  is positive. The result was a variational reactivity curve that much more closely followed the exact reactivity curve on the right side of Fig. 2.

### 3. USING THE EXACT GENERALIZED ADJOINT FUNCTION $\Gamma_s^{*g}(r, \hat{\Omega})$

Using Eq. (11),  $f_s$  can be calculated for any perturbed configuration without having to calculate  $\Gamma_s^{*g}(r, \hat{\Omega})$  of Eq. (6). This fact will be used to gain insight into the behavior of the variational reactivity estimate in this paper. What is needed is the  $\psi'^g(r, \hat{\Omega})$  that is calculated along with the exact reactivity (for testing purposes) anyway. A particular normalization [6] of  $\psi'^g(r, \hat{\Omega})$  is a requirement for the existence of a solution to Eq. (6):

$$\langle \psi_0^*, F_0 \Delta \psi \rangle = 0 \Rightarrow \langle \psi_0^*, F_0 \psi' \rangle = \langle \psi_0^*, F_0 \psi_0 \rangle. \quad (14)$$

Care must be taken to apply Eq. (14) before using  $\psi'^g(r, \hat{\Omega})$  in Eq. (11).

In analogy with Eqs. (3) and (7), define

$$\rho_s \equiv \rho_0(1 - f_s). \quad (15)$$

It is generally assumed that using the exact generalized adjoint function and therefore  $f_s$  would lead to more accurate variational reactivity estimates. This assumption may be true when  $\rho_0$  is accurate to within ~20%, but for large perturbations for which  $\rho_0$  is really inaccurate it is untrue. The reason is that Eq. (11) can be rewritten

$$f_s = \left( 1 - \frac{\langle \psi_0^*, F' \Delta \psi \rangle}{\langle \psi_0^*, F' \psi' \rangle} \right) \left( \frac{f_{ex}}{1 - f_{ex}} \right) = \left( 1 - \frac{\langle \psi_0^*, F' \Delta \psi \rangle}{\langle \psi_0^*, F' \psi' \rangle} \right) (f_{ex} + f_{ex}^2 + f_{ex}^3 + f_{ex}^4 + \dots) \quad (16)$$

for  $|f_{ex}| < 1$ . Thus, the accuracy of  $\rho_s$  [Eq. (15)] with respect to  $\rho_{ex}$  [Eq. (7)] depends on the magnitude of  $f_{ex}$  and on the flux shift induced by the perturbation (in the perturbed fission region). Generally, only for very small values (magnitudes) of  $f_{ex}$  and small flux shifts will  $\rho_s \approx \rho_{ex}$  (in addition to the occasional occurrence of  $\langle \psi_0^*, F' \Delta \psi \rangle \approx f_{ex} \langle \psi_0^*, F' \psi' \rangle$ ). Of course, small values of  $f_{ex}$  also imply  $\rho_0 \approx \rho_{ex}$  [Eq. (7)].

Thus, in situations where we intend to realize big gains from using the variational reactivity estimate – that is, when the first-order estimate  $\rho_0$  is substantially different from  $\rho_{ex}$ , the exact reactivity –  $\rho_s$  will also be substantially different from  $\rho_{ex}$ . This conclusion is one of the main new results of this paper.

For perturbations that do not affect the fission operator,  $\langle \psi_0^*, F' \Delta \psi \rangle = \langle \psi_0^*, F_0 \Delta \psi \rangle = 0$  in Eq. (16) [because of Eq. (14)], and  $f_s$  is guaranteed to be in poor agreement with  $f_{ex}$ , except for very small magnitudes of  $f_{ex}$ . In fact in this case the relative error in  $f_s$  is  $(f_s - f_{ex}) / f_{ex} = f_s$ .

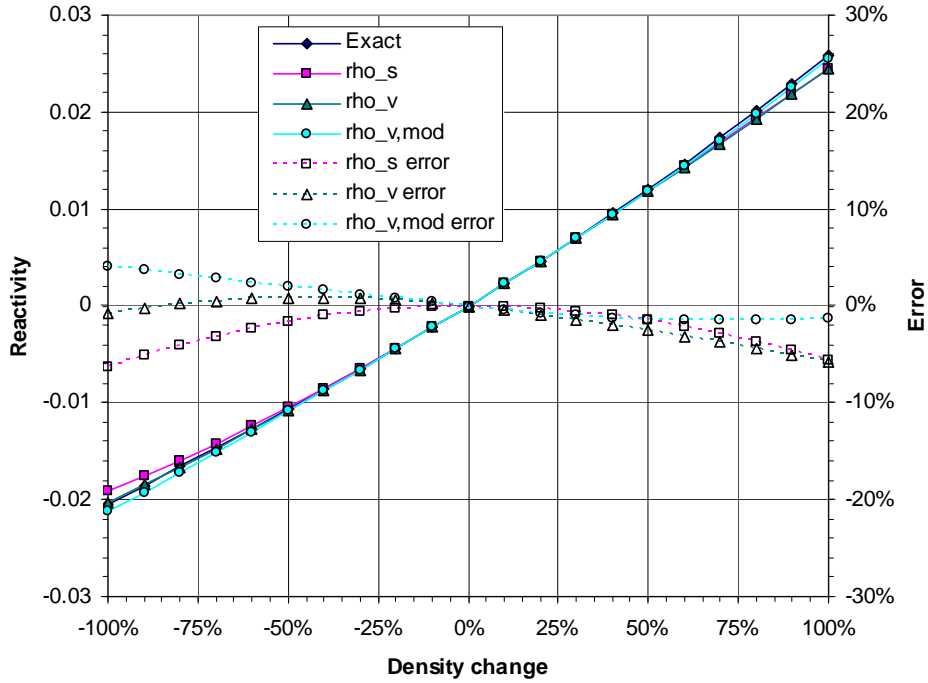
Given the above demonstrated inaccuracy of  $f_s$ , it is counterintuitive that the use of  $\Gamma_{\Delta}^{*g}(r, \hat{\Omega})$  of Eq. (5) as an approximation for  $\Gamma_s^{*g}(r, \hat{\Omega})$  of Eq. (6) should improve matters – i.e., that  $\rho_v$  or even  $\rho_{v,mod}$  should be more accurate than  $\rho_s$ . Nevertheless, that is very frequently the case, as the test results below will show.

#### 4. RECENT RESULTS, NOW WITH $\rho_s$

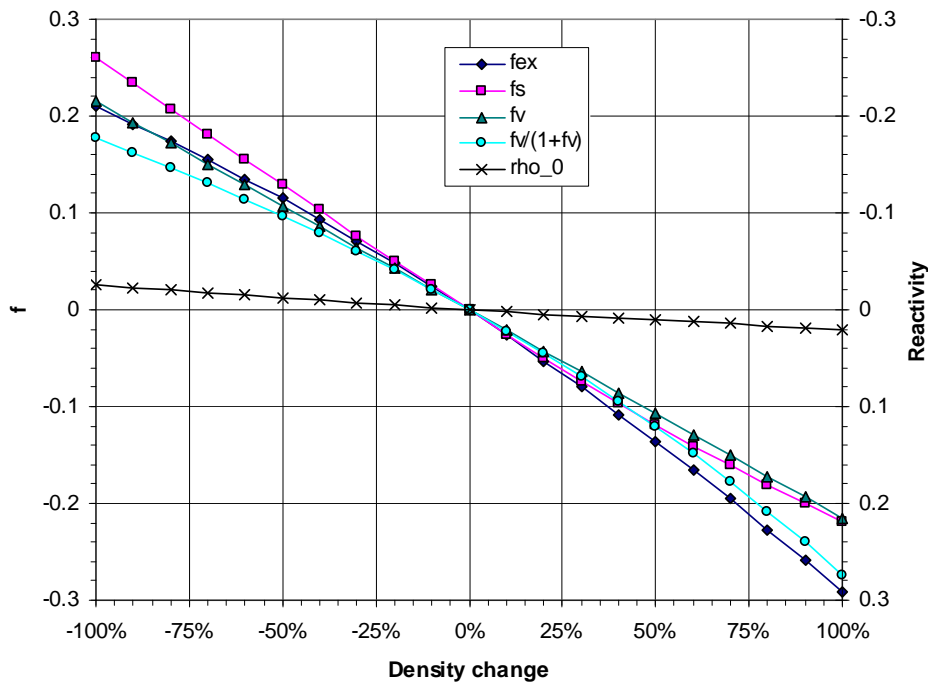
Recently [5], a 47-group thermal spherical reactor problem was run in which the modified variational reactivity estimate  $\rho_{v,mod}$  was surprisingly more accurate than  $\rho_v$  for positive-reactivity perturbations and less accurate for negative-reactivity perturbations. The perturbation was a density change in the inner third (by radius) of an enriched uranium oxyfluoride solution with an infinite water reflector [7]. Results are shown in Fig. 3, where “rho\_v” is from Eq. (3), “rho\_v,mod” is from Eq. (13), and “rho\_s” is from Eq. (15). This figure was presented differently, and without  $\rho_s$ , in Ref. 5 (where it was Fig. 1).

In Fig. 3,  $\rho_s$  is very accurate for density changes between –30% and +50%. Outside that range, to the right (positive reactivity),  $\rho_{v,mod}$  is the most accurate, and to the left (negative reactivity),  $\rho_v$  is the most accurate. This is the opposite of what was expected from the development of  $\rho_{v,mod}$  in Ref. 4. [In Fig. 3 the second-order term  $\Delta \lambda \Delta F \psi_0$  was ignored in Eq. (4).]

The flux correction factors  $f$  and first-order reactivity worth  $\rho_0$  for this problem are plotted in Fig. 4. (Note that the reactivity is plotted in reverse order, with negative values above the x-axis.) The first-order reactivity is not compared with the others in Fig. 3 because it is so much worse and Fig. 4 has enough curves on it. However, in realistic analyses, the only information available will be  $f_v$  and  $\rho_0$ . From these values it is hoped that a decision can be made on whether  $\rho_v$  or  $\rho_{v,mod}$  is expected to be more accurate.



**Figure 3. The reactivity worth associated with changing the density of the inner region of a spherical uranium oxyfluoride solution (without conserving the mass). Solid symbols are reactivity.**



**Figure 4. The flux correction factors and first-order reactivity worth corresponding to Fig. 3.**

In Fig. 4,  $|f_v| < 0.21$  and  $\rho_0 / f_v \approx -1/10$  for the entire range of perturbations. In Fig. 3, for positive reactivities  $\rho_{v,mod.}$  is the one to use but for negative reactivities  $\rho_v$  is the one to use.

## 5. NEW RESULTS

Using the uranium oxyfluoride model, a perturbation was found whose results resemble those of Figs. 1 and 2. As in Ref. 5, the PARTISN multigroup discrete-ordinates code [8] was used with the 47-group BUGLE cross-section library [9], which was not corrected for self-shielding, and  $S_{32}$  quadrature was used with  $P_3$  scattering. A standard production version of PARTISN was used with a special-purpose wrapper code [5] to compute  $\Gamma_{\Delta}^{*g}(r, \hat{\Omega})$ .

A perturbation of the group-40 capture cross section of the entire volume of fuel is shown in Fig. 5 as a function of the change in the total cross section (the unperturbed capture cross section is not known but  $\Delta\Sigma_t^{40} = \Delta\Sigma_c^{40}$ ). The variational reactivity curves have the obvious quadratic shape seen in Figs. 1 and 2. The variational reactivity  $\rho_v$  is quadratic with the perturbation  $p$  because  $f_v$  is linear with  $p$  and  $\rho_0$  is approximately linear with  $p$  (exactly linear if the perturbation does not affect the fission operator, as in this problem). As expected based on previous experience [4],  $\rho_{v,mod.}$  was much more accurate than  $\rho_v$  for negative-reactivity perturbations. Surprisingly, however, for this problem  $\rho_{v,mod.}$  turned out to be more accurate than  $\rho_v$  for positive-reactivity perturbations also.

In Fig. 5,  $\rho_v \approx \rho_s$  for the entire range of perturbations. This result contradicts expectations but can be explained. For this problem we have  $f_v / (1 + f_v) \approx f_{ex}$  (i.e.,  $\rho_{v,mod.} \approx \rho_{ex}$ , as the graph shows), or  $f_v \approx f_{ex} / (1 - f_{ex}) = f_s$  from Eq. (16), or  $\rho_v \approx \rho_s$ .

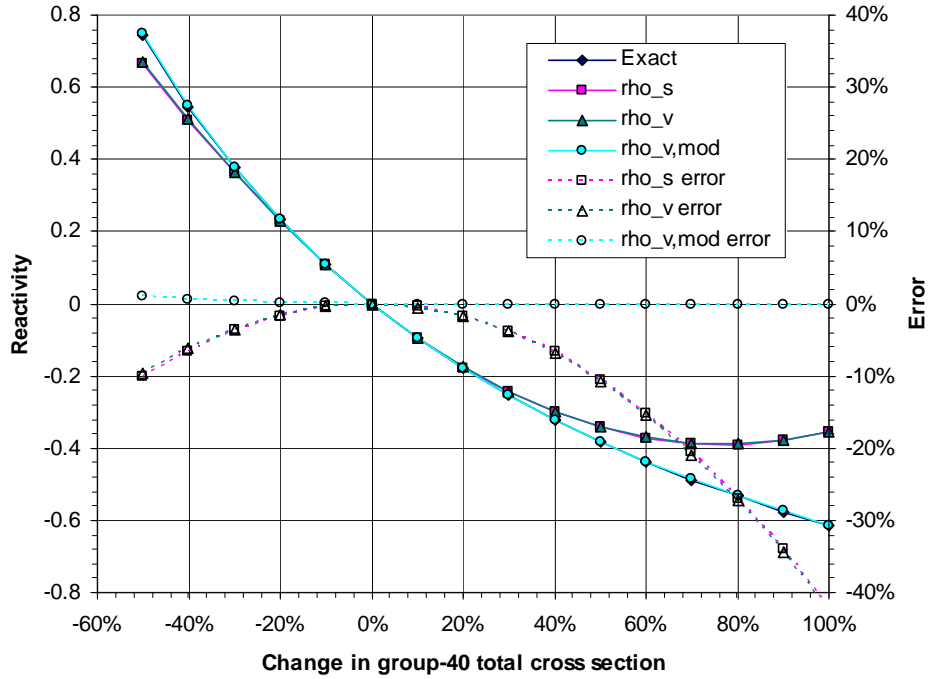
The second-order term  $\Delta\lambda\Delta F\psi_0$  in the variational estimate is zero for this problem since the fission source is unperturbed.

The flux correction factors  $f$  and first-order reactivity worth  $\rho_0$  for this problem are plotted in Fig. 6. (Note that the reactivity is plotted in reverse order, with negative values above the  $x$ -axis.)

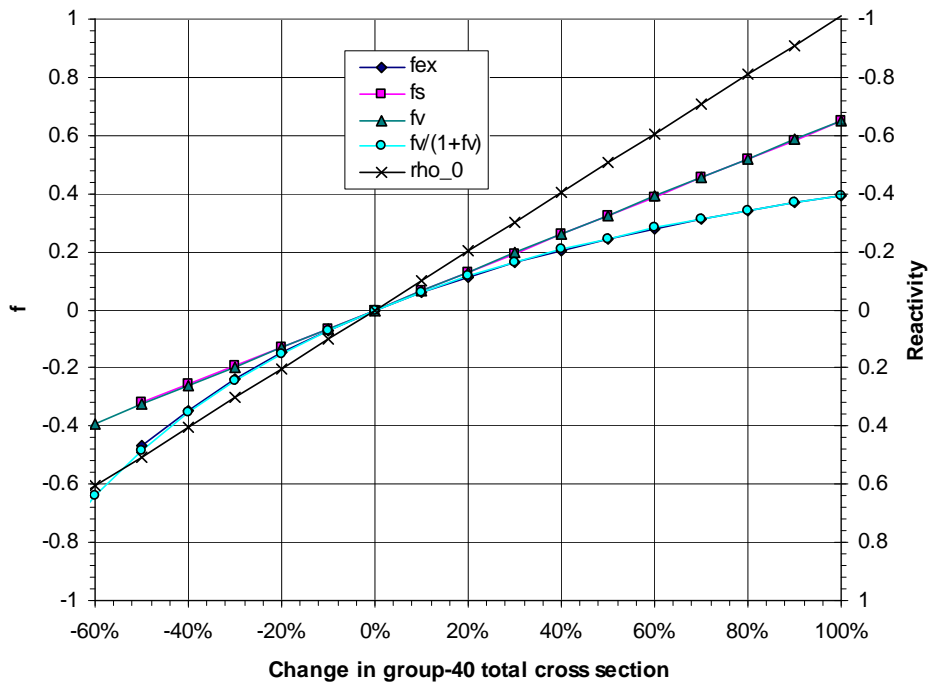
In Fig. 6,  $-0.40 < f_v < 0.62$ . Interestingly, for this range,  $-0.62 < f_v / (1 + f_v) < 0.40$ . Because both  $\rho_0$  and  $f_v$  are linear with the perturbation for this problem, the ratio  $\rho_0 / f_v$  is a constant, in this case equal to  $-1.55$ . In Fig. 5, for both positive and negative reactivities  $\rho_{v,mod.}$  is the one to use.

Note that for this problem both the magnitude of the perturbation and its reactivity worth are huge, far outside the ranges normally associated with perturbation theory applications. The goal of the variational reactivity estimate is to extend the range of applicability of perturbation theory, and  $\rho_v$  succeeds. For perturbations of  $\pm 20\%$ , the standard variational reactivity estimate is in error by only  $\sim -1.8\%$ , while the first-order reactivity estimate is in error by  $\pm 13\%$ . The goal of  $\rho_{v,mod.}$  is to extend the range of applicability of perturbation theory even further. In fact for this





**Figure 5. The reactivity worth associated with changing the group-40 capture cross section of the uranium oxyfluoride solution. Solid symbols are reactivity.**



**Figure 6. The flux correction factors and first-order reactivity worth corresponding to Fig. 5.**

problem  $\rho_{v,mod}$  is more accurate both at the extreme ranges of the perturbation and in the middle; for perturbations of  $\pm 20\%$ ,  $\rho_{v,mod}$  is in error by only  $\sim \mp 0.20\%$ .

Figure 7 shows the results of another problem with unexpected results. The number of neutrons per fission,  $\nu$ , in every group was perturbed in the outer third (by radius) of the fuel solution. The standard variational estimate  $\rho_v$  was more accurate than the modified estimate  $\rho_{v,mod}$  for negative-reactivity perturbations, as in Fig. 3. However, this time the standard variational estimate  $\rho_v$  was also more accurate than the modified estimate  $\rho_{v,mod}$  for positive-reactivity perturbations.

The range of applicability of the variational reactivity estimate is limited in this problem, but more so on the positive-reactivity side than the negative. This result defies previous experience.

For positive-reactivity perturbations,  $\rho_s$  was more accurate than the variational estimates. For negative-reactivity perturbations, however,  $\rho_v$  was much more accurate than  $\rho_s$ .

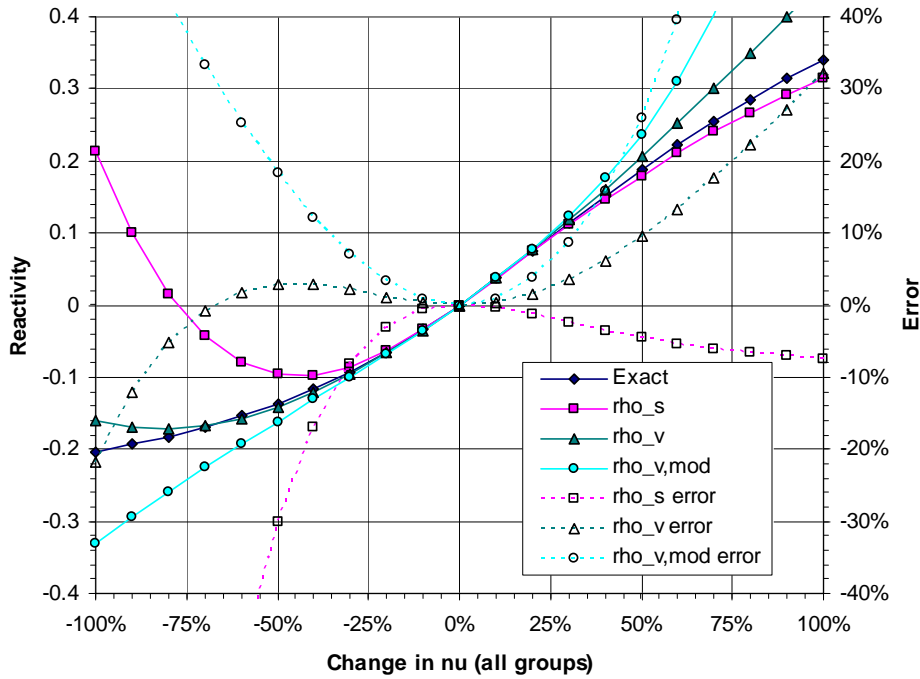
The results of Fig. 7 ignore the second-order term  $\Delta\lambda\Delta F\psi_0$  in the variational estimate. However, an interesting result is obtained and shown in Fig. 8 if that term is included and  $\Delta\lambda$  is converged to  $-\rho_v$  as described above. The variational estimate should become more accurate with the inclusion of this term. Figure 8 shows that in this case,  $\rho_v$  does indeed become more accurate, but only for positive perturbations  $p$  and small ( $|p| < 30\%$ ) negative perturbations. (For variety, Fig. 8 also shows  $\rho_0$  instead of  $\rho_s$ .)

The flux correction factors  $f$  and first-order reactivity worth  $\rho_0$  for this problem are plotted in Fig. 9 for the case when the second-order term  $\Delta\lambda\Delta F\psi_0$  is ignored in  $\rho_v$ . (Note that the reactivity is plotted in reverse order, with negative values above the  $x$ -axis.)

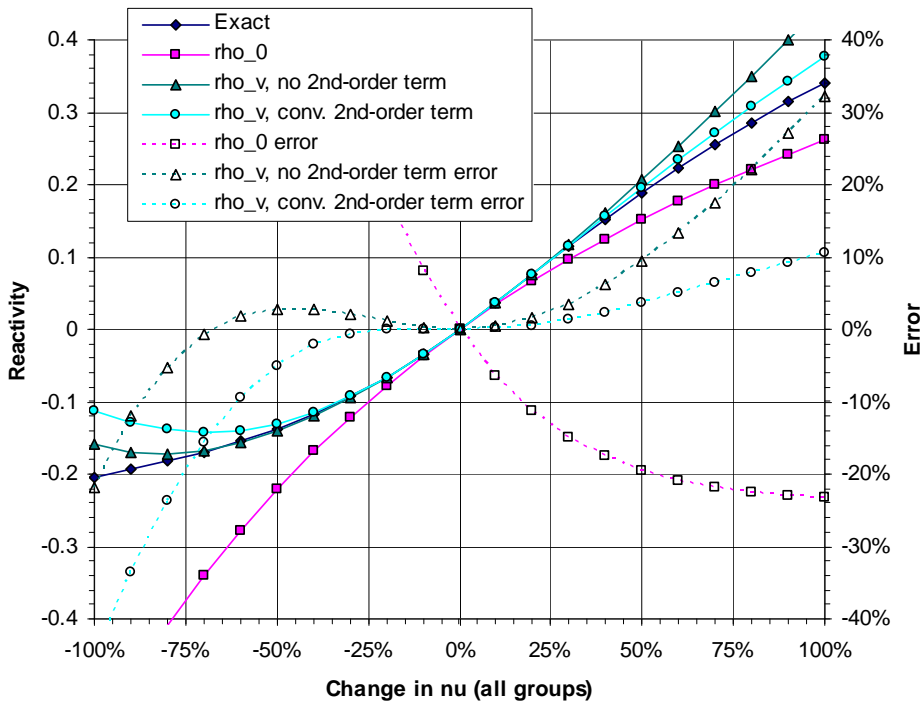
In Fig. 9,  $|f_v| < 0.72$ . Except for the very largest negative perturbations,  $\rho_0 \approx f_v / (1 + f_v)$  for  $\rho_0 < 0$ . For  $\rho_0 > 0$ ,  $\rho_0 / f_v$  varies from  $\sim -1/2$  to  $\sim -1/3$ . In Fig. 7, for both positive and negative reactivities  $\rho_v$  is the one to use, although its accuracy is limited on the positive-reactivity side. This can be improved by including the second-order term  $\Delta\lambda\Delta F\psi_0$  in  $\rho_v$  (Fig. 8), but then that hurts the estimates on the negative-reactivity side.

In Ref. 4 it was suggested that the magnitude of the flux correction factor may be a good indicator of the accuracy of the variational reactivity estimate. In this problem, at a perturbation of  $+50\%$ , where  $\rho_v$  has reached an error of  $9.5\%$ ,  $f_v = -0.36$  and  $f_v / (1 + f_v) = -0.56$ , which are much smaller in magnitude than the value of  $-1.3$  that was associated with inaccuracy (for positive reactivities) in Ref. 4.

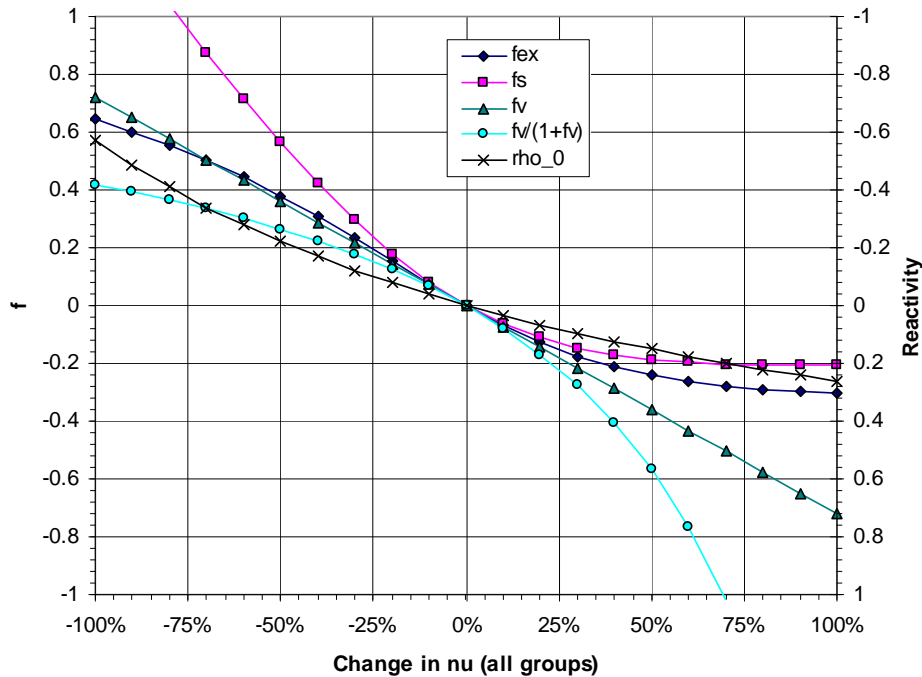
Examining the exact reactivity worths of Figs. 5 and 7 is interesting. In Fig. 5, adding more and more to the group-40 capture cross section has less and less effect, but taking more and more from it has greater and greater effect. The negative-reactivity effect tends to saturate. This is also true for the  $\nu$  perturbation of Fig. 7, but there is also a downward concavity suggesting a



**Figure 7.** The reactivity worth associated with changing  $\nu$  for all groups in the outer third of the uranium oxyfluoride solution. Solid symbols are reactivity.



**Figure 8.** The reactivity worth associated with changing  $\nu$  for all groups in the outer third of the uranium oxyfluoride solution. Solid symbols are reactivity.



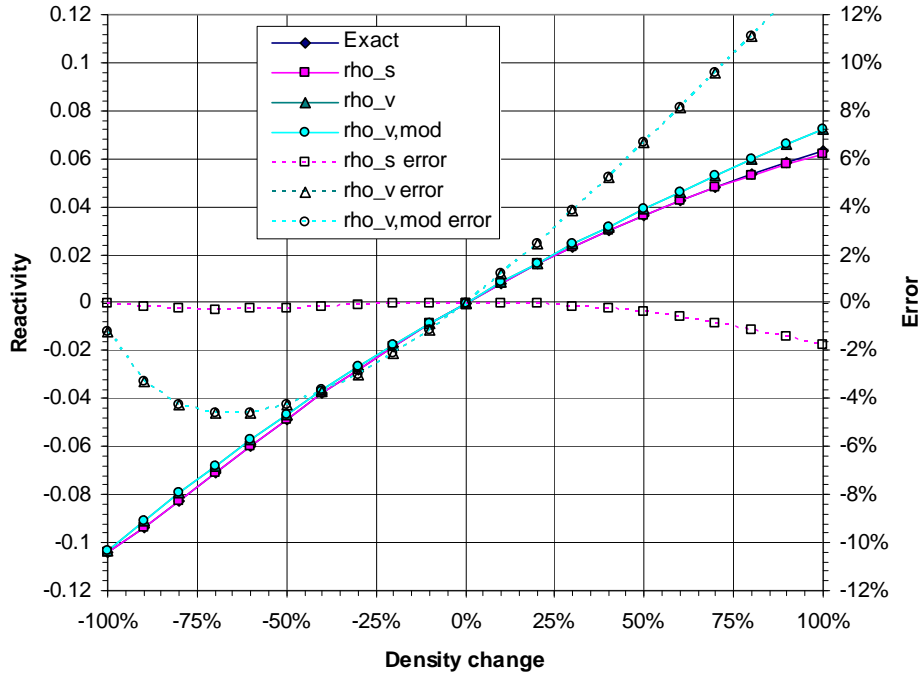
**Figure 9. The flux correction factors and first-order reactivity worth corresponding to Fig. 7.**

saturation on the positive-reactivity side as well. This is an effect that the variational estimate misses.

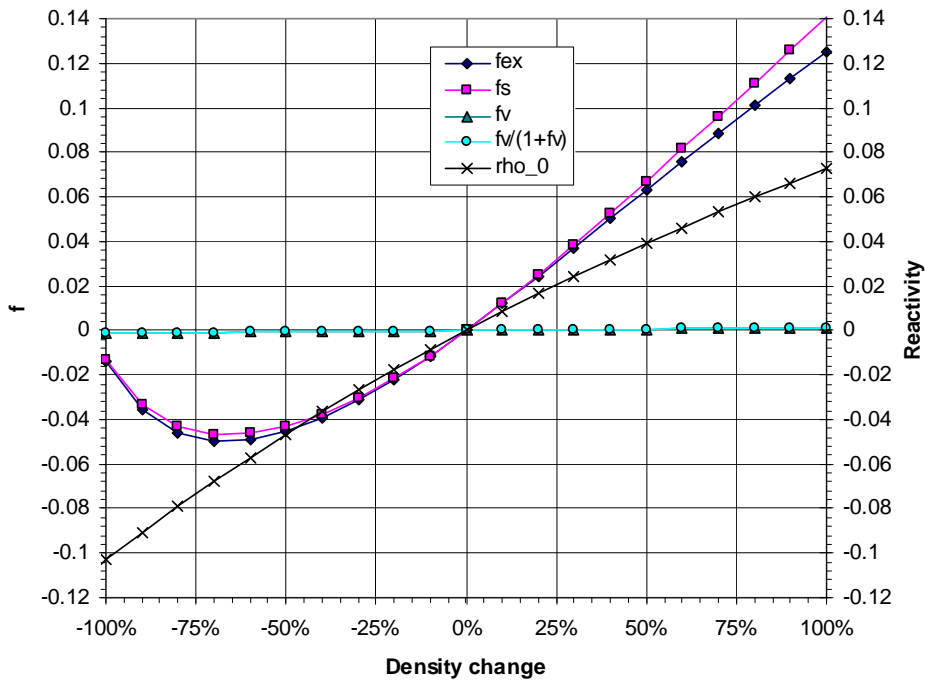
Results for a final problem are shown in Fig. 10. The perturbation was a density change in the outer 20% (by radius) of the uranium oxyfluoride solution. In this case,  $\rho_0$  (not shown on Fig. 10) is fairly accurate, being in error by only  $-1.35\%$  for  $p = -100\%$  and  $14.3\%$  for  $p = +100\%$ .  $\rho_v$  and  $\rho_{v,mod.}$  are essentially equal and a bit better than  $\rho_0$ . This problem is noteworthy in that  $\rho_s$  is extremely accurate over the entire range of perturbations. The conclusion is that the variational estimate does not buy very much for this problem;  $f_v$  is too small to make a difference.

In Fig. 10 the second-order term  $\Delta\lambda\Delta F\psi_0$  was ignored in Eq. (4).

The flux correction factors  $f$  and first-order reactivity worth  $\rho_0$  for this problem are plotted in Fig. 11. Although it is difficult to see in Fig. 11, another noteworthy feature of this problem is that  $f_v$  and  $\rho_0$  have the same sign, contrary to a conclusion reached in Ref. 4. However,  $f_v$  is very small in magnitude. The ratio  $\rho_0 / f_v$  varies from 83 to 58.  $f_v$  is so small that it doesn't matter whether  $\rho_v$  or  $\rho_{v,mod.}$  is used in Fig. 10; both are only very slight improvements on  $\rho_0$ .



**Figure 10. The reactivity worth associated with changing the density of the outer region of a spherical uranium oxyfluoride solution (without conserving the mass). Solid symbols are reactivity.**



**Figure 11. The flux correction factors and first-order reactivity worth corresponding to Fig. 10.**

## 6. SUMMARY AND CONCLUSIONS

Several anomalous conclusions have been reached in this paper. First, using the “exact” generalized adjoint function  $\Gamma_s^{*g}(r, \hat{\Omega})$  about which the variational reactivity functional is stationary leads to a reactivity estimate  $\rho_s$  that has been shown to be inaccurate because of the difference between the flux correction factor  $f_s$  and the true flux correction factor  $f_{ex}$  [Eq. (16)]. Somehow, the use of two approximate trial functions [ $\Gamma_{\Delta}^{*g}(r, \hat{\Omega})$  and  $\psi_0^g(r, \hat{\Omega})$  for  $\Gamma_s^{*g}(r, \hat{\Omega})$  and  $\psi'^g(r, \hat{\Omega})$ , respectively] is an improvement over the use of one approximate trial function [ $\psi_0^g(r, \hat{\Omega})$  for  $\psi'^g(r, \hat{\Omega})$ ]. This conclusion was verified in numerical test problems in which  $\rho_v$  was more accurate, in some cases much more so, than  $\rho_s$ . However, when the flux correction factor is small,  $\rho_s$  can be more accurate. This paper may be the first in which calculations of  $\rho_s$  were made.

The second conclusion is that there is as yet no simple way to tell which variational reactivity estimate should be preferred in a given situation. The simple algorithm previously suggested [4] (use  $\rho_v$  when  $\rho_0 > 0$ ,  $\rho_{v,mod}$  when  $\rho_0 < 0$ ) has been shown to be not always optimum.

A third conclusion is that the variational reactivity estimate can sometimes, but not always, be improved by including the second-order  $\Delta\lambda\Delta F\psi_0$  term and iterating until  $\Delta\lambda \rightarrow -\rho_v$ .

None of these conclusions should cause any doubt about the efficacy of the variational reactivity estimate as an improvement over the first-order reactivity estimate. The goal of this work is merely to extend the range of applicability of perturbation theory even further.

We suggest that other workers collaborate in this effort by reporting values of  $f_v$  and  $\rho_{v,mod}$  whenever values of  $\rho_v$  are reported and especially when those values are compared with exact results.

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