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State of the Art in the Heuristically Based Generalized Perturbation Theory (**)

Abstract - In design and operation studies relevant to complex systems, perturbation, or sensitivity analysis have always played an important role. This stems from the interest of evaluating the changes of significant responses (relevant to performance, safety, etc.) following alterations of system parameters (such as physical constants and design specifications). In many cases the sensitivity coefficients required are obtained by direct calculational runs at perturbed and unperturbed conditions. If a large number of parameters are to be considered, this may become a heavy calculational burden, and cost. Moreover, the effect often consisting of a small difference between two large numbers, the result so obtained may be significantly affected by numerical errors. These difficulties may be overcome by the heuristically-based generalized perturbation theory (HGPT) method described in the present article. In fact, with it the sensitivity coefficients entering into the perturbation expressions are obtained by simple integration operations in terms of functions calculated at unperturbed system conditions. No significant numerical inaccuracies are so introduced, and, moreover, particular perturbation effects may be singled out for a deeper insight into the system behaviour. A distinctive feature of this method consists in the systematic use of conservation concepts relevant to the importance function. As well known, its use leads to fundamental reciprocity relationships from which perturbation, or sensitivity expressions can be derived to first and higher order. The state of the art of the HGPT methodology is here illustrated. Its application to a number of specific nonlinear fields relevant to nuclear reactor physics is commented, with particular emphasis to problems implying an intensive system control variable.

Riassunto - Negli studi di progetto e di operazione di sistemi complessi le analisi perturbative, o di sensitività, hanno sempre giocato un ruolo importante. Questo è dovuto all'interesse di valutare i cambiamenti di risposte significative (relative alle prestazioni, alla sicurezza, ecc.) a seguito di alterazioni di parametri del sistema (quali le costanti fisiche e le specifiche di progetto). In molti casi i coefficienti di sensitività richiesti sono ottenuti attraverso calcoli diretti in condizioni perturbate e imperturbate. Nel caso si debba considerare un gran numero di parametri, questo può comportare un carico di calcolo, e costi, notevoli. Inoltre, poiché in molti casi la quantità cercata è data da una piccola differenza di grandi numeri, il risultato così ottenuto può essere significativamente affetto da

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errori numerici. Queste difficoltà possono essere superate con il metodo euristico basato sulla teoria perturbativa generalizzata (HGPT), discusso in questo articolo. Infatti, con esso i coefficienti di sensitività che entrano nelle espressioni perturbative sono ottenuti attraverso semplici operazioni di integrazione in cui compaiono funzioni calcolate in condizioni di sistema imperturbato. Non vengono così introdotti errori numerici e, inoltre, effetti particolari della perturbazione possono essere isolati per una più profonda comprensione del funzionamento del sistema. Una peculiarità di questo metodo è l'uso sistematico di concetti di conservazione relativi alla funzione importanza. Come ben noto, il suo uso conduce a relazioni fondamentali di reciprocità da cui possono essere ricavate le espressioni perturbative, o di sensitività, al primo o più elevato ordine. Lo stato dell'arte della metodologia HGPT è qui illustrata. La sua applicazione ad alcuni specifici campi non lineari relativi alla fisica dei reattori nucleari è commentata, con particolare enfasi ai problemi che implicano una variabile intensiva di controllo.

1. INTRODUCTION

Since the beginning of nuclear reactor physics studies, perturbation theory has played an important role. As well known, it was first proposed by Wigner [1] as early as 1945 to study fundamental quantities such as the reactivity worths of different materials in the reactor core. It is also well known that this first formulation, today widely used by reactor analysis, makes a consistent use of the adjoint flux concept.

The advantage of using perturbation theory lies in the fact that instead of making a new, often lengthy direct calculation of the eigenvalue (and then of the real flux) for every perturbed system configuration, a simple integration operation is required in terms of unperturbed quantities.

It is interesting that as early as 1948 Soodak [2] associated to the adjoint flux the concept of importance, viewing it as proportional to the contribution of a neutron inserted in a given point of a critical system, to the asymptotic power.

Along with the introduction of the concept of importance and, parallel to it, along with the development of calculational methods and machines, from the early 60' a flourishing of perturbation methods, at first in the linear domain and then in the nonlinear one, have been proposed for the analysis of reactor core, shielding, nuclide evolution, thermohydraulics, as well as other fields.

The perturbation formulations proposed by various authors may be subdivided into three main categories, according to the approach followed in their derivation:

1. The heuristic approach, making exclusive use of importance conservation concepts, adopted first by Usachev [3] and then extensively developed by Gandini [4-7]. It will be referred to, in the following, as heuristic generalized perturbation theory (HGPT) method.
2. The variational approach adopted, in particular, by Lewins [8], Pomraning [9], Stacey [10], Harris and Becker [11] and Williams [12].

3. The differential method, proposed by Oblov [13] and extensively developed by Cacuci [14], based on a formal differentiation of the response considered.

Each of the above methods has its own merit, although all of them can be shown equivalent to each other [15].

Basing on a long experience, it is our belief that the HGPT approach can be easily grasped by the reactor engineers, due to the inherent simplicity and elegance of the heuristic derivation.

As mentioned above, a distinctive feature of heuristically based HGPT methodology consists in the systematic use of importance conservation concepts. As well known, this use leads to fundamental reciprocity relationships. Instead, the variational and the differential derivations make a consistent use of the properties of the adjoint function. The equivalence between the importance and the adjoint functions have been demonstrated in most cases of interest. There are some instances, however, in which the commonly known operator reversal rules to determine the operator governing the adjoint function are not adequate. In this paper a generalisation of these rules, as adopted with the HGPT methodology, is commented in relation to a number of significant cases.

2. THE HGPT METHOD

In the HGPT method the importance function is uniquely defined in relation to a given system response, for example, a neutron dose, the quantity of plutonium in the core at end of cycle, the temperature of the outlet coolant.

The HGPT method was first derived in relation to the linear neutron density field. Then it was extended to other linear ones. For all these fields the equation governing the importance function was obtained directly by imposing that on average the contribution to the chosen response from a particle [a neutron, or a nuclide, or an energy carrier] introduced at a given time in a given phase space point of the system is conserved through time (importance conservation principle). Obviously such importance will result generally dependent on the time, position, and, when the case, energy and direction, of the inserted particle.

Consider a linear particle field density represented by vector f (e.g., the multigroup neutron density field) and a response Q of the type¹

¹ Expression (1) is also representative of more general responses, of the type

$$Q = \langle\langle L(f) \rangle\rangle,$$

L being a given function of f . In fact, if we extend f to the field $\hat{f} = \begin{bmatrix} f \\ y \end{bmatrix}$, where $y = L(f)$, Q reduces to the form of Eq. (1), i.e.,

$$Q = \langle\langle s^*, \hat{f} \rangle\rangle,$$

having set $s^* = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$.

$$Q = \int_{t_0}^{t_f} \langle s^*, f \rangle dt = \langle\langle s^*, f \rangle\rangle, \quad (1)$$

where s^* is an assigned vector function and where brackets $\langle \rangle$ indicate integration over the phase space. Weighting all the particles inserted into the system, let's assume a source s , with the corresponding importance (f^*) will obviously give the response itself, i.e.,

$$\langle\langle f^*, s \rangle\rangle = Q = \langle\langle s^*, f \rangle\rangle, \quad (2)$$

which represents an important reciprocity relationship.

From the first derivations mentioned above the rules for determining the equation governing the importance function f^* were learned (see Appendix A). They imply, in relation to the equation governing f^* :

- change of sign of the odd derivatives,
- transposing matrix elements,
- reversing the order of operators,
- substitution of the source s with s^* .

The first three rules will be generally called "operator reversal" rules.

The HGPT method was then extended to any field governed by linear operators for which the rules for their reversal were known. In particular, it was extended to the derivative fields, obtained from expanding to first order, around a given starting solution, a number of important nonlinear equations as those governing:

- the coupled neutron/nuclide field, relevant to core evolution and control problems,
- the temperature field, relevant to thermohydraulics.

2.1 General Formulation

Consider a generic physical model defined by a number of parameters p_i ($i = 1, 2, \dots, J$) and described by an N -component vector field f obeying equation

$$m(f | p) = 0. \quad (3)$$

Vector $f(q, t)$ generally depends on the phase space coordinates q and time t . Vector p represents the set of independent parameters p_i ($i = 1, 2, \dots$) fully describing the system and entering into equation (3). Their value generally

determines physical constants, initial conditions, source terms, etc. Equation (3) can be viewed as an equation comprising linear, as well as nonlinear, operators and is assumed to be derivable with respect to parameters p_i and (in the Frechet sense) component functions f_n ($n = 1, 2, \dots, N$).

Consider now a response of interest, or functional Q given by Eq. (1). In the following, we shall look for an expression giving perturbatively the change δQ of the response Q in terms of perturbations δp_i of the system parameters. In particular, expressions giving the sensitivity coefficients relevant to each parameter p_i will be obtained.

Expanding equation (3) around a reference solution gives, setting $f_{ij} = \frac{df}{dp_i}$,

$$\sum_{j=1}^J \delta p_j (H f_{ij} + m_j) + O_2 = 0, \quad (4)$$

where O_2 is a second, or higher order term, and where $m_j = \frac{\partial m}{\partial p_j}$.

The (Jacobian) operator H is given by the expression

$$H = \begin{pmatrix} \frac{\partial m_1}{\partial f_1} & \frac{\partial m_1}{\partial f_2} & \dots & \frac{\partial m_1}{\partial f_N} \\ \frac{\partial m_2}{\partial f_1} & \frac{\partial m_2}{\partial f_2} & \dots & \frac{\partial m_2}{\partial f_N} \\ \dots & \dots & \dots & \dots \\ \frac{\partial m_N}{\partial f_1} & \frac{\partial m_N}{\partial f_2} & \dots & \frac{\partial m_N}{\partial f_N} \end{pmatrix}$$

where by $\frac{\partial}{\partial f_n}$ we have indicated a Frechet derivative.²

² We shall give in the following the definition of the Frechet derivative (see Ref. [16]). Given an f -dependent expression $m(f)$ and an increment d of f , such that we can write

$$m(f+d) - m(f) = F(d, f) + w(d, f),$$

where $F(d, f)$ is linear with d and

$$\lim_{\|d\| \rightarrow 0} \frac{\|w(d, f)\|}{\|d\|} = 0,$$

$F(d, f)$ is called the Frechet differential and the (linear) operator $F[(-), f]$ the Frechet derivative

Since parameters p_j and then their changes δp_j , have been assumed to be independent from each other, it must follow

$$Hf_j + m_j = 0, \quad (6)$$

which represents the (linear) equation governing the derivative functions f_j . The source term m_j is here intended to account also, via appropriate delta functions, for the initial and, if the case, boundary conditions.¹

Consider now functional

$$Q_j = \langle\langle h^*, f_j \rangle\rangle. \quad (7)$$

Introducing the importance (f^*) associated with field f_j , if we use it as weight of the source term m_j and integrate space- and time-wise, according to the source reciprocity relationship, Eq. (2), the resulting quantity will be equivalent to functional Q_j , i.e.,

(denoted above by the symbol $\frac{\partial m}{\partial t}$).

For example:

if $m(t) = \alpha t$, then $\frac{\partial m}{\partial t} = \alpha$ (here coinciding with a normal derivative)

if $m(t) = \frac{\partial f}{\partial x}$, then $\frac{\partial m}{\partial t} = \frac{\partial}{\partial x}$

if $m(t) = \int dx K(x) f(x)$, then $\frac{\partial m}{\partial t} = \int dx K(x) f(x)$.

To note that a Frechet derivative corresponds always to an operator,

¹ For example, consider an equation of the type

$$\frac{\partial n}{\partial t} = Bn. \quad (a)$$

An initial time condition at t_0 may be accounted for if we rewrite Eq. (a) in the form

$$\frac{\partial n}{\partial t} = Bn + s_0 \delta(t - t_0). \quad (b)$$

with $s_0 = n(t_0)$. In fact, let us integrate Eq. (b), between $t - \epsilon$ and $t + \epsilon$, ϵ being an arbitrarily small positive quantity. It immediately results

$$n(t_0 + \epsilon) - n(t_0 - \epsilon) = s_0 + o(\epsilon),$$

$o(\epsilon)$ being a vector with components of the order of ϵ . Considering that $n(t_0 - \epsilon) = 0$ (no neutron sources being assumed prior to t_0), if we make $\epsilon \rightarrow 0$, it is $n(t_0) = s_0$, as we wanted to demonstrate.

$$Q_j = \langle\langle f^*, m_j \rangle\rangle, \quad (8)$$

where the importance f^* obeys the (index-independent) equation

$$H^* f^* + h^* = 0, \quad (9)$$

H^* being obtained by reversing operator H . As said above, this implies transposing matrix elements, changing sign of the odd derivatives, inverting the order of operators.

We can easily see that the sensitivities s_j ($j = 1, 2, \dots, J$) of system parameters can be written

$$s_j = \frac{dQ}{dp_j} = \langle\langle \frac{\partial h^*}{\partial p_j}, f \rangle\rangle + \langle\langle f^*, \frac{\partial m}{\partial p_j} \rangle\rangle, \quad (10)$$

where the first term at the right-hand side represents the so called, easy to calculate, direct term.

The overall change δQ due to perturbations δp_j ($j = 1, 2, \dots, J$) of system parameters can be written, at first order,

$$\delta Q = \sum_{j=1}^J \delta p_j [\langle\langle \frac{\partial h^*}{\partial p_j}, f \rangle\rangle + \langle\langle f^*, \frac{\partial m}{\partial p_j} \rangle\rangle]. \quad (11)$$

Higher order expression may be obtained making explicit use of the derivative functions described above [7].

3. NUCLIDE/NEUTRON FIELDS

Two main areas of interest for application of the HGPT methodology may be mentioned: the fuel cycle analysis during burnup, in which optimal fuel shuffling strategies are of interest (with a time scale of the order of months, or years), and the reactor operation, in which optimal control strategies are sought (in a time scale of the order of hours, or days).

3.1 Fuel Cycle

An HGPT related perturbation methodology relevant to the (heavy) nuclide density evolution has been first developed in 1975 [17]. Kallifeltz et al. [18] coupled it with the HGPT methodology relevant to the neutron field to account for nonlinear effects inherent to burnup problems. Other efforts in the nonlinear

domain have been made by Harris and Becker [11], who arrived at a still crude formulation, and, successively, by Williams [12] and Gandini [6, 7].

Williams used variational techniques starting from the time-wise discretized neutron and nuclide density equations, along with the quasi-static approximation.

Gandini used the heuristically based HGPT method after having formally extended the neutron and nuclide densities to a control (intensive) variable. The equations obtained governing the corresponding (time-wise continuous) importance functions are relevant to the physical solution. Different schemes of integration can then be defined [19].

Typical quantities which can be analysed with this methodology are:

- the amount of a material specified in a given region at the end of the reactor life cycle;
- the d.p.a. of a specific material and at a given position;
- the residual reactivity at the end of the reactor life cycle. The analysis of this quantity may be of particular interest in studies aiming at extending the reactor life cycle.

In Appendix B the derivation of the governing equations is illustrated.

3.2. Reactor Operation

In power reactor systems (in particular, in PWRs) the following significant responses, can be on-line monitored:

- the reactivity;
- the axial offset;
- the assembly outlet temperature;
- the local power.

Constraints over these responses enter into the safe/reliable operation of the reactor. It appears then of great interest the possibility of an on-line, anticipated appraisal by the operator, via a sensitivity methodology, of these main physical responses when the reactor is subject to alterations relevant to normal exploitation, e.g., control rod movement, and/or soluble boron concentration changes to be introduced for power level variations induced by electrical network demands. In view of this application, an intense R & D effort is underway to set up a fast response system for operator's support in PWR normal operation [20].

A fundamental role is played here by the so called "control variable option" [21], which consists in the fact that the importance functions calculated at unperturbed conditions, stored in order to be used for system analysis along with the HGPT methodology, need not reflect an "a priori" control strategy to be adopted at a given time by the reactor operator, but may be "a posteriori" transformed by a simple filtering operation, consistently with the particular control strategy being

APPENDIX A. *The importance function in the neutron density field*

Let us consider in the time interval (t_0, t_p) the neutron density field $n(\mathbf{r}, E, \Omega, t)$, function of position (\mathbf{r}), energy (E), angle (Ω) and time (t), relevant to a given fission, or external-source driven system. Having assumed this system isolated, we shall include into it also external sources and detection devices.

Let us assume that the system considered is fully described by parameters p_j ($j = 1, 2, \dots, J$). Besides describing the medium in which the density field diffuses, these parameters will include also initial conditions, source terms, etc.

As well known, the density field (n) is governed by the Boltzmann operator B_T given by the general expression

$$\begin{aligned} B_T = & [-\Omega \cdot \text{grad } v(\cdot) - \Sigma_t(E) v \\ & + \int_0^\infty dE' \int_{4\pi} d\Omega' \Sigma_s(E' \rightarrow E; \Omega' \rightarrow \Omega) v(E')(\cdot) \\ & + \frac{\chi(E)}{4\pi} \int_0^\infty dE' \int_{4\pi} d\Omega' v \Sigma_f(E') v(E')(\cdot)] , \end{aligned} \quad (\text{A. 1})$$

where (\cdot) is a position symbol, v the neutron velocity corresponding to energy E , $\chi(E)$ the fission neutron spectrum, $\Sigma_s(E)$ the total macroscopic cross-section, $\Sigma_s(E' \rightarrow E; \Omega' \rightarrow \Omega)$ the macroscopic (elastic and inelastic) scattering cross-section kernel and $v \Sigma_f$ the macroscopic fission cross-section multiplied by the number of secondaries per fission. The neutron density field, having assumed for the present that all neutrons are born prompt, obeys then, in general, the differential equation

$$\frac{\partial n}{\partial t} = B_T n + s \quad (\text{A. 2})$$

where s is an external source term. Since operator B_T contains macroscopic (cross-sections) quantities, it is clearly dependent on the material densities c_m ($m = 1, 2, \dots, M$ (number of materials)) which, through irradiation and transmutations processes, change with time. In other words, the real problem is evidently a nonlinear one. Here we shall neglect the evolution process, so that operator B_T will result linear.

It is also well known that the external boundary conditions relevant to the density $n(\mathbf{r}, E, \Omega, t)$ is (assuming that the system considered comprehends also its inhomogeneous sources and, for simplicity, that it is limited by a convex surface)

$$n(\mathbf{r}, E, \Omega, t) = 0 \quad (\text{for } \mathbf{r} \text{ belonging to outer boundary and inward } \Omega \text{ directions}). \quad (\text{A. 3})$$

Let us consider now a response linear with the neutron density, i.e., of the generic form

$$Q = \int_{t_0}^{t_f} dt \int_{\text{sys}} d\mathbf{r} \int_0^\infty dE \int_{4\pi} d\Omega s^+ (\mathbf{r}, E, \Omega, t) n (\mathbf{r}, E, \Omega, t) \\ = \int_{t_0}^{t_f} \langle s^+ n \rangle dt, \quad (\text{A. 4})$$

where s^+ is an assigned function and where brackets $\langle \rangle$ indicate integration over space, angle and energy.

According to the response under consideration s^+ may assume a variety of expressions. If, for example, Q represents the amount of activated nuclei of a given sample at t_f , then (assuming constant sample material density)

$$s^+ = \Sigma_a e^{-\lambda (t_f - t)} v(E) \xi(\mathbf{r}) \quad (\text{A. 5})$$

where Σ_a represents the macroscopic activation cross-section, λ the time constant of the activated nuclei, and $\xi(\mathbf{r})$ a function equal to unity within the sample, and zero outside.

Another response of interest is the reaction rate of a given material at some time t_f and specified point \mathbf{r}_0 . In this case

$$s^+ = \Sigma_x(E) v(E) \delta(\mathbf{r} - \mathbf{r}_0) \delta(t - t_f) \quad (\text{A. 6})$$

Σ_x being the particular reaction cross-section considered.

We shall now introduce the "physical" concept of importance. A few important properties relevant to it will then be derived.

The neutron processes will be intended here as average ones, random events not being the object of the present study.

Let us assume that we are interested in the analysis of a response Q , as expressed by Eq. (A. 4). Let us then suppose we introduce one neutron at time t in position \mathbf{r} , direction Ω , and energy E . From this neutron an (average) increase Δn of the neutron density will subsequently result and, correspondingly, a change ΔQ of the response Q under consideration. This increase may be produced either directly by this same neutron or, in presence of a multiplying system, through its progeny. Such increase ΔQ will correspond to the importance of such neutron, along with its definition in Section 2. We shall denote it by $n^+(\mathbf{r}, E, \Omega, t)$, i.e., as a function dependent on time, space, angle, and energy coordinates, corresponding to those of the neutron to which it is associated.⁴

⁴ As it is defined, and recalling that systems considered here are linear, the importance of a

After a time Δt a fraction $(1 - v\Sigma_s\Delta t)$ of this neutron reaches a position $\mathbf{r} + v\Delta t\Omega$. Of the remaining fraction, a fraction Σ_s/Σ_t undergoes (elastic and inelastic) scattering and a fraction Σ_f/Σ_t is subject to fission. Of the fraction undergoing scattering, a fraction

$$\frac{\Sigma_s(E \rightarrow E'; \Omega \rightarrow \Omega')}{\Sigma_s} dE' d\Omega'$$

is scattered from energy E into energy interval dE' and from direction Ω into solid angle $d\Omega'$ around Ω' . Taking the product of these fractions, we obtain the fraction

$$v\Sigma_s(E \rightarrow E'; \Omega \rightarrow \Omega') dE' d\Omega' \Delta t$$

undergoing (elastic and inelastic) scattering from E into dE' and from $d\Omega$ into $d\Omega'$.

Quite analogously, in relation to the fission process, we obtain the fraction

$$v \frac{\chi(E')}{4\pi} v\Sigma_f(E) dE' d\Omega' \Delta t$$

of fission neutrons born into dE' and $d\Omega'$.

A fraction of the original neutron has also contributed during the interval Δt to the response Q by the (average) amount

$$s^*(\mathbf{r}, E, \Omega, \bar{t}) \Delta t,$$

\bar{t} being a time between t and $t + \Delta t$.

Recalling that the importance of this neutron has to be conserved, we can write a balance equation in which the importance of the original neutron at point \mathbf{r} , direction Ω and time t is set equal to that associated to the fraction reaching point $\mathbf{r} + v\Delta t\Omega$, plus that associated with the fraction emerging from scattering and fission processes, plus the contribution to Q , i.e.,

$$\begin{aligned} n^*(\mathbf{r}, E, \Omega, t) &= n^*(\mathbf{r} + v\Delta t\Omega, E, \Omega, t + \Delta t) (1 - v\Sigma_t\Delta t) \\ &+ \Delta t v \int_0^\infty dE' \int_{4\pi} d\Omega' \Sigma_s(E \rightarrow E'; \Omega \rightarrow \Omega') n^*(\mathbf{r}, E', \Omega, \bar{t}) \\ &+ \Delta t v \int_0^\infty dE' \int_{4\pi} d\Omega' \Sigma_f(E \rightarrow E'; \Omega \rightarrow \Omega') n^*(\mathbf{r}, E', \Omega, \bar{t}) \\ &+ s^*(\mathbf{r}, E, \Omega, \bar{t}) \Delta t \end{aligned}$$

neutron added at a given time with given phase-space coordinates (which might be distinguished as *marginal importance*) coincides with the average importance of neutrons already existing within the system at the same time and with same coordinates (which might be distinguished as *mean importance*). Obviously these two importances do not coincide in nonlinear systems. Since in the HGPT methodology problems relevant to nonlinear systems are transformed into linear ones, we need not distinguish between these two importances. The simple term «importance» will only be maintained in the text.

$$\begin{aligned}
 & + \Delta t \, v \frac{\nu \Sigma_f(E)}{4\pi} \int_0^\infty dE' \int_{4\pi} d\Omega' \chi(E') n^*(r, E', \Omega', t) \\
 & + s^*(r, E, \Omega, t) \Delta t.
 \end{aligned} \tag{A. 7}$$

Subtracting from both sides the term $n^*(r, E, \Omega, t + \Delta t)$, dividing by Δt and making $\Delta t \rightarrow 0$, we easily obtain

$$\begin{aligned}
 -\frac{\partial n^*}{\partial t} &= v \Omega \cdot \text{grad } n^* - v \Sigma_t n^* \\
 &+ v \int_0^\infty dE' \int_{4\pi} d\Omega' \Sigma_s(E \rightarrow E'; \Omega \rightarrow \Omega') n^*(r, E', \Omega', t) \\
 &+ v \frac{\nu \Sigma_f(E)}{4\pi} \int_0^\infty dE' \int_{4\pi} d\Omega' \chi(E') n^*(r, E', \Omega', t) \\
 &+ s^*(r, E, \Omega, t).
 \end{aligned} \tag{A. 8}$$

If we define the operator

$$\begin{aligned}
 B_T^* &= v \Omega \cdot \text{grad } v(\cdot) - v \Sigma_t \\
 &+ v \int_0^\infty dE' \int_{4\pi} d\Omega' \Sigma_s(E \rightarrow E'; \Omega \rightarrow \Omega') (\cdot) \\
 &+ v \frac{\nu \Sigma_f(E)}{4\pi} \int_0^\infty dE' \int_{4\pi} d\Omega' \chi(E') (\cdot),
 \end{aligned} \tag{A. 9}$$

Eq. (A. 8) may be written

$$-\frac{\partial n^*}{\partial t} = B_T^* n^* + s^* \tag{A. 10}$$

Comparing Eq. (A. 10) with Eq. (A. 2), we observe that the former one could have been obtained from that relevant to the neutron density by changing the sign of the time derivative, substituting the source term s with s^* , and making changes in operator B_T which we shall identify as "reversal" operations. These reversal operations imply changing sign of the space (odd) derivatives (as is likewise done with the derivative operator with respect to time), reversing the sense of energy and angle transfer in the scattering kernel, etc.

Consider, for instance, the scattering operator. This can be interpreted as the product of two operations, i.e.,

$$\begin{aligned} & \int_0^\infty dE' \int_{4\pi} d\Omega' \Sigma_s(E' \rightarrow E; \Omega' \rightarrow \Omega) v(E') (-) \\ & = \left[\int_0^\infty dE' \int_{4\pi} d\Omega' \Sigma_s(E' \rightarrow E; \Omega' \rightarrow \Omega) (-) \right] [v] . \end{aligned} \quad (\text{A. 11})$$

Its reversal will imply reversing both the sequence of the operations and, when the case, each single operator. Doing so, we obtain

$$v(E) \int_0^\infty dE' \int_{4\pi} d\Omega' \Sigma_s(E \rightarrow E'; \Omega \rightarrow \Omega') (-) \quad (\text{A. 12})$$

consistently with the scattering term in Eq. (A. 8).

Quite analogously, the reversal of the fission operator

$$\frac{\chi(E)}{4\pi} \int_0^\infty dE' \int_{4\pi} d\Omega' v \Sigma_f(E') v(E') (-) \quad (\text{A. 13})$$

leads to

$$v \frac{v \Sigma_f(E)}{4\pi} \int_0^\infty dE' \int_{4\pi} d\Omega' \chi(E') (-) . \quad (\text{A. 14})$$

We observe that these "reversal" operations coincide with those adopted to transform an operator into its adjoint.

To obtain the boundary conditions for n^* , consider that, on (assumed) convex surfaces delimiting the whole system (inclusive also of the regions in which the source s^* is defined), the contribution to response Q by a neutron going out of the system will be zero, so that we can write:

$$n^*(r, E, \Omega, t) = 0 \quad (\text{for } r \text{ belonging to outer boundary and outward } \Omega \text{ directions}). \quad (\text{A. 15})$$

The Adjoint Flux

As a particular case, consider now a (supposed linear) multiplying system at critical conditions during the time interval (t_0, t_f) and a response

$$Q = \langle s_0^* n(t_f) \rangle , \quad (\text{A. 16})$$

with s_0^* given. Setting

$$s^*(r, E, \Omega, t) = s_0^*(r, E, \Omega) \delta(t - t_p), \quad (\text{A. 17})$$

we can write

$$Q = \int_{t_0}^{t_p} \langle s^* n \rangle dt, \quad (\text{A. 18})$$

It is easy to verify that the importance function n^* , corresponding to this response, obeys equation

$$-\frac{\partial n^*}{\partial t} = B_T^* n^* \quad (\text{A. 19})$$

with "final" condition $n^*(t_p) = s_0^*$. If t_p assumes asymptotically large values, the importance function n^* at finite times tends to be time independent. In fact, recalling its physical meaning, the contribution to a response Q , defined at an asymptotically large time t_p , from a neutron inserted at a finite time t into a (critical) system will be only through the change of the flux level, i.e.,

$$\delta Q = \varepsilon \langle s_0^* n \rangle \quad (\text{A. 20})$$

ε being a quantity depending on the position, energy, and direction of the initial neutron. This value will tend to be not different if the neutron, rather than at t , is inserted at $t + \delta t$ with the same position, energy, and direction coordinates. So, the time derivative vanishing, Eq. (A. 19) is shown to asymptotically coincide with the equation relevant to the so called adjoint flux, ϕ^* , i.e.,

$$B_T^* \phi^* = 0 \quad (\text{A. 21})$$

Vice versa, the conventional adjoint flux ϕ^* is proved to be proportional to the importance function relevant to a response (the reactor power, or any other) defined at an asymptotic time, as anticipated by Soodak [2].

APPENDIX B. Cycle analysis

To the neutron and fuel nuclide densities, represented by vectors $\mathbf{n}(\mathbf{r}, t)$ and $\mathbf{c}_f(\mathbf{r}, t)$, respectively, defined in the reactor cycle interval (t_0, t_f) , a specified intensive control variable, $\rho(t)$, is associated so that the assigned, overall power history $W(t)$ is maintained. Vector \mathbf{n} represents the space- and time-dependent neutron density in a multigroup energy form, whereas vector \mathbf{c}_f the space- and time-dependent density of the various fuel nuclide species. The intensive, time-dependent, control variable $\rho(t)$ may represent, for instance, the overall control rod bank penetration into the core (not their relative movement, which is generally described by parameters p_j), or the average neutron poison material density. The nonlinear governing equations can then be written formally as

$$m_{(n)}(\mathbf{n}, \mathbf{c}_f, \rho | \mathbf{p}) = - \frac{\partial \mathbf{n}}{\partial t} + B\mathbf{n} + \mathbf{s}_n = 0 \quad (\text{B. 1})$$

$$m_{(c)}(\mathbf{n}, \mathbf{c}_f | \mathbf{p}) = - \frac{\partial \mathbf{c}_f}{\partial t} + E\mathbf{c}_f + \mathbf{s}_c = 0 \quad (\text{B. 2})$$

$$m_{(p)}(\mathbf{n}, \mathbf{c}_f | \mathbf{p}) = \langle \mathbf{c}_f, S\mathbf{n} \rangle - W = 0, \quad (\text{B. 3})$$

where B is the neutron diffusion, or transport, matrix operator (depending on \mathbf{c}_f and ρ), E the nuclide evolution matrix (depending on \mathbf{n}), \mathbf{s}_n and \mathbf{s}_c are given source terms,³ while

$$S = \gamma \begin{vmatrix} \sigma_{f1}^1 & \sigma_{f2}^1 & \dots & \sigma_{fg}^1 \\ \sigma_{f1}^2 & \sigma_{f2}^2 & \dots & \sigma_{fg}^2 \\ \dots & \dots & \dots & \dots \\ \sigma_{f1}^M & \sigma_{f2}^M & \dots & \sigma_{fg}^M \end{vmatrix} V, \quad (\text{B. 4})$$

γ being the amount of energy per fission, and σ_{fg}^m the microscopic g 'th group fission cross-section of the m 'th heavy isotope. V is the diagonal neutron velocity matrix. Quantities γ , V , W and σ_{fg}^m may be considered generally represented by (or function of) system parameters p_j . Source terms \mathbf{s}_n and \mathbf{s}_c are also parameter dependent.

³ \mathbf{s}_n is generally assumed zero during burnup, except a delta-like source at t_0 to represent initial conditions (usually considered at steady state), whereas \mathbf{s}_c is generally given by a sum of delta functions defined at t_0 and at given times to account for fuel feed and shuffling operations [6].

In quasi-static problems, as those of interest here, the derivative $\frac{\partial n}{\partial t}$ is negligible. If we introduce the field

$$f(r, t) = \begin{vmatrix} n(r, t) \\ c_f(r, t) \\ \rho(t) \end{vmatrix} \quad (B. 5)$$

the system of Eqs. (B. 1), (B. 2) and (B. 3) may be represented in the compact symbolic form, Eq. (3), and the HGPT methodology described above applied.

Consider a functional

$$Q = \int_{t_0}^{t_f} \left\langle \begin{vmatrix} s_n^+ & s_c^+ & s_p^+ \end{vmatrix} \begin{vmatrix} n(r, t) \\ c_f(r, t) \\ \rho(t) \end{vmatrix} \right\rangle dt \quad (B. 6)$$

Q may represent, for instance, the amount of a given nuclide built up at time t_f [in this case $s_n^+ = 0$, $s_p^+ = 0$ and s_c^+ includes a delta function $\delta(t - t_f)$], or the fluence at a specific point \bar{r} [in this case $s_n^+ = 0$, $s_p^+ = 0$ and s_c^+ includes a delta function $\delta(r - \bar{r})$]. The importance function

$$f^+(r, t) = \begin{vmatrix} n^+(r, t) \\ c_f^+(r, t) \\ \rho^+(t) \end{vmatrix} \quad (B. 7)$$

can then be defined, and results governed by Eq. (9), with H^* and h^* given by expression:

$$H^* = \begin{vmatrix} \left(\frac{\partial}{\partial t} + B^* \right) & \Omega_c^* & S^* c_f \\ \Omega_n^* & \left(\frac{\partial}{\partial t} + E^* \right) & S n \\ \langle n, \left(\frac{\partial B}{\partial \rho} \right)^* (\cdot) \rangle & 0 & 0 \end{vmatrix} \quad (B. 8)$$

$$h^+ = \begin{vmatrix} s_n^+ \\ s_c^+ \\ s_p^+ \end{vmatrix} \quad (B. 9)$$

Ω_c^* and Ω_n^* being operators adjoint of Ω_c [$= \frac{\partial}{\partial n}(E c_f)$] and Ω_n [$= \frac{\partial}{\partial c_f}(B n)$], respectively.

The equation relevant to function ρ^* corresponds to a relationship between n^* and n , i.e.,

$$\langle \mathbf{n}, \left(\frac{\partial B^*}{\partial \mathbf{p}} \right) \mathbf{n}^* \rangle = s_p^* \quad (\text{B. 10})$$

In case $s_p^* = 0$, Eq. (B. 10) corresponds to an orthogonality relationship.

To solve the equations relevant to \mathbf{n}^* and \mathbf{c}_i^* different resolution recurrent schemes may be considered, starting from the 'final' time t_f and proceeding backward, along with the same time discretisation adopted in the forward reference calculation.

It can be shown [7] that, at quasi static conditions, the equations to be solved reduce to the types:

$$B^* \mathbf{n}^* + \mathbf{h}_n^* = 0 \quad (\text{B. 11})$$

$$-\frac{\partial \mathbf{c}_i^*}{\partial t} = E^T \mathbf{c}_i^* + \mathbf{h}_c^* \quad (\text{B. 12})$$

where \mathbf{h}_n^* and \mathbf{h}_c^* correspond to known source terms determined during the recurrent calculational procedure. Therefore, existing, well established codes can be used for their solution.

The sensitivity coefficient $\frac{dQ}{dp_i}$ with respect to a given parameter p_i may then be obtained from Eq. (10), with vector \mathbf{m} made of components $\mathbf{m}_{(n)}$, $\mathbf{m}_{(c)}$ and $\mathbf{m}_{(p)}$ defined in Eqs. (B. 1), (B. 2) and (B. 3), respectively.

A general problem we are faced with is the following: how does the control criticality reset (p) strategy affect the sensitivity analysis results? To answer this question, let us consider Eq. (B. 1) governing \mathbf{n} . We note that, given a particular solution $\mathbf{n}_{\text{part}}^*$, the general one may be written as

$$\mathbf{n}^* = \mathbf{n}_{\text{part}}^* + \alpha \phi^* \quad (\text{B. 13})$$

where α is an arbitrary coefficient and ϕ^* the conventional adjoint function obeying the homogeneous equation

$$B^* \phi^* = 0. \quad (\text{B. 14})$$

Once a solution $\mathbf{n}_{\text{part}}^*$ has been obtained, the solution desired can then be derived by proper filtering from the fundamental mode, i.e., it will be given by Eq. (B. 13), with coefficient α determined by imposing condition (B. 10). Assuming $s_p^* = 0$, we shall have

$$\mathbf{n}^* = \mathbf{n}_{\text{part}}^* - \frac{\langle \mathbf{n}_{\text{part}}^*, \frac{\partial B}{\partial \mathbf{p}} \mathbf{n} \rangle}{\langle \phi^*, \frac{\partial B}{\partial \mathbf{p}} \mathbf{n} \rangle} \phi^*. \quad (\text{B. 15})$$

The dependence of the importance function n^* on the control mode adopted is evident.

When calculating the sensitivity coefficient of a response Q with respect to a given parameter p_i (or its change δQ with respect to parameter alterations δp_i), the filtering of the importance function as shown in Eq. (B. 15) corresponds to *implicitly* account for the p -mode control reset of the criticality (in the following we shall refer to it simply as p -mode reset) [7].

The above result may have important implications, in the sense that in many circumstances, prior to a sensitivity study, it may be necessary to consider the proper reactivity control mode to be adopted. On the other hand, within many existing codes used with the HGPT methodology, the fictitious " λ -mode" reset control is implicitly assumed, i.e., related to the coefficient (eigenvalue) λ multiplying the fission source term ($F n$) in the Boltzmann (or diffusion) equation. In this circumstance expression (B. 15) for the importance n^* will result, recalling that in this case $\frac{\partial B}{\partial \lambda} = F$,

$$n^* = n_{part}^* - \frac{\langle n_{part}^*, F n \rangle}{\langle \phi^*, F n \rangle} \phi^*. \quad (B. 16)$$

Using this λ -mode filtering, rather than the correct p -mode one, may lead to erroneous results.

Consider, for instance, the case of a sensitivity analysis with respect to core breeding, or conversion ratio, a quantity clearly dependent on the neutron energy spectrum. Assuming that the reactivity compensation, corresponding to a system parameter (for instance, the initial fuel enrichment) change, is effected, as it may very well be the case for a thermal reactor, by an alteration of the average (boron) poison concentration in the coolant, the correct choice of the control mode reset would clearly have the effect of hardening (if boron is added), or softening (if boron is subtracted) the neutron spectrum. Instead, if a λ -mode reset would have been implicitly adopted (as is often done with existing codes), no significant neutron energy shift would have been taken into account, and, consequently, an erroneous sensitivity coefficient would result.

It is also true that in principle one could calculate separately the amount of control poison (referring to the above example) to reset the criticality and consider the overall parameter plus control change along with the λ -mode methodology. But this would imply a reactivity reset calculation to be performed for each parameter considered. On the other hand, the correct fundamental p -mode filtering may be a quite straightforward procedure. In fact, it can be effected "*a posteriori*" adopting expression (B. 15) in which n_{part}^* would correspond to a preliminary λ -mode calculation with an existing code.

APPENDIX C. Reactor operation control

The general equations governing the neutron density n and the poison (vector) concentration density c_p may be written (assuming all neutrons are born prompt, which is an acceptable assumption in quasi-static problems)

$$m_{(n)}(n, c_p, \rho | p) = -\frac{\partial n}{\partial t} + Bn = 0 \quad (C. 1)$$

$$m_{(p)}(n, c_p, \rho | p) = -\frac{\partial c_p}{\partial t} + Ec_p + Pn = 0 \quad (C. 2)$$

$$m_{(p)}(n | p) = \langle c_f, Sn \rangle - W = 0, \quad (C. 3)$$

where the term Pn accounts for the poison production due to fission, whereas Ec_p accounts for the poison removal by neutron absorption, or decay. Operator B ($= A + F$, F being the fission matrix and A that relevant to absorption, scattering and leakage) depends on density c_p and on an (intensive) control variable p . It depends also on the fuel isotope concentrations c_f , which here, according to the short time scale considered, is assumed constant (and then a parameter). Evolution matrix E depends on the neutron density n . Eq. (C. 3) corresponds to a constraint over the power history W , while S is given by Eq. (B. 4).

In quasi-static problems, as those of interest here, the derivative $\frac{\partial n}{\partial t}$ is negligible.

Any physical "observable", or response, of interest for operation control, can be represented by a functional expression (for simplicity, assumed linear)

$$Q = \int_{t_0}^{t_f} (\langle h_n^*, n \rangle + \langle h_c^*, c_p \rangle) dt \quad (C. 4)$$

(t_0, t_f) being an assigned time interval.

The importance functions n^* , c_p^* and ρ^* relevant to this response are defined, along with a procedure similar to that followed in Appendix B, by a system of (linear) equations:

$$-\frac{\partial n^*}{\partial t} = B^* n^* + (\Omega_c^* + P^*) c_p^* + S^T c_f \rho^* + h_n^* \quad (C. 5)$$

$$-\frac{\partial c_p^*}{\partial t} = E^* c_p^* + \Omega_p^* n^* + S n \rho^* + h_c^* \quad (C. 6)$$

$$\langle \mathbf{n}^*, \frac{\partial B}{\partial p} \mathbf{n} \rangle = 0, \quad (C. 7)$$

Ω_c^* and Ω_n^* being coupling operators defined with Eq. (B. 8).

Having assumed $h_p^* = 0$ for $t < t_0$, Eq. (C. 7) implies an orthogonality condition on \mathbf{n}^* . The solution of Eqs. (C. 5) and (C. 6) is clearly dependent on the specific definition of the p -control mode.

The sensitivity coefficient relevant to the j 'th parameter can then be written as

$$s_j = \frac{dQ}{dp_j} = \frac{\partial Q}{\partial p_j} + \int_{t_0}^{t_f} [\langle \mathbf{n}^*, \frac{\partial B}{\partial p_j} \mathbf{n} \rangle + \langle \mathbf{e}^*, (\frac{\partial E}{\partial p_j} \mathbf{e}_p + \frac{\partial P}{\partial p_j} \mathbf{n}) \rangle] dt + \rho^* \frac{\partial}{\partial p_j} (\langle \mathbf{e}, S \mathbf{n} \rangle - W) dt. \quad (C. 8)$$

To notice how function ρ^* corresponds to the importance associated to the system power.

For xenon poisoning problems, implying significant offset effects on the axial power distribution, first order HGPT methodology may not be adequate. Second order terms might be required in the perturbation expansion, this implying the use of derivative functions $\mathbf{n}_{/j} (= \frac{\partial \mathbf{n}}{\partial p_j})$ and $\rho_{/j} (= \frac{\partial \rho}{\partial p_j})$ [7]. The second order perturbative expression will then read, assuming only operator B is perturbed,

$$\delta Q = \sum_{j=1}^I \delta p_j \int_{t_0}^{t_f} \langle \mathbf{n}^*, \frac{\partial B}{\partial p_j} \mathbf{n} \rangle dt + \sum_{i,j=1}^I \delta p_i \delta p_j \int_{t_0}^{t_f} [\langle \mathbf{n}^*, (\frac{\partial B}{\partial p_i} + \rho_{/j} \frac{\partial B}{\partial \rho}) \mathbf{n}_{/j} \rangle + \frac{1}{2} \langle \mathbf{n}^*, \frac{\partial^2 B}{\partial p_i \partial p_j} \mathbf{n} \rangle + \rho_{/i} \langle \mathbf{n}^*, \frac{\partial^2 B}{\partial p_j \partial \rho} \mathbf{n} \rangle] dt. \quad (C. 9)$$

Criticality can be theoretically restored in three different ways: by changing the fuel enrichment (at all impractical in real cases), by varying the soluble boron concentration in the primary system, by moving control devices.

The first control strategy may be simplified by considering variations of a coefficient (λ) multiplying the fission matrix F . In this case coefficient λ will play the role of the control variable.

In the case the second control strategy is adopted we may correspondingly write the portion of operator B dependent on the soluble boron density as ρB_{sol} , ρ being the control variable. Disregarding effects of the boron concentration different from absorption, we can write (recalling that the boron is dissolved only within the coolant)

$$B_{sol} = -\xi_{sol} \text{diag} \{ \Sigma_{B,1}^{sol}, \Sigma_{B,2}^{sol}, \dots, \Sigma_{B,G}^{sol} \} V, \quad (C. 10)$$

where ξ_{sol} is a coefficient equal to unity within the boron solution and zero outside, G is the number of energy groups and V is the diagonal neutron velocity matrix. In this case, the impact on responses of interest consequent to different control rod (clusters) movements (defined parametrically) can be analysed. A parameter involved could be, for instance, the r 'th rod (cluster) depth, given by the value, z_r , of the (axial) penetration of the control rod (assuming its insertion measured from above). We shall then write the portion of B dependent on parameter z_r as

$$\pi_r h(z - z_r) B_{bor}^r \quad (C. 11)$$

where $h(z - z_r)$ is the Heaviside function [equal to unity in points along z corresponding to the rod insertion, and equal to zero elsewhere], π_r a function equal to unity in points in the plane (x, y) within the r 'th rod and zero otherwise, while B_{bor}^r corresponds to the part of B which depends on the r 'th control rod density. Again disregarding effects other than absorption, it can be given by the diagonal matrix

$$B_{bor}^r = -\text{diag} \{ \Sigma_{B,1}^r, \Sigma_{B,2}^r, \dots, \Sigma_{B,G}^r \} V. \quad (C. 12)$$

Recalling that the derivative of an Heaviside function is a Dirac function, matrix $\frac{\partial B}{\partial z_r}$ appearing in the source term of the equations governing the derivative functions n_{ij} , and then in the perturbative expression, Eq. (C. 9), will assume the form

$$\begin{aligned} \frac{\partial B}{\partial z_r} &= \frac{\partial}{\partial z_r} [\pi_r h(z - z_r) B_{bor}^r] \\ &= \delta(z - z_r) \pi_r \text{diag} \{ \Sigma_{B,1}^r, \Sigma_{B,2}^r, \dots, \Sigma_{B,G}^r \} V. \end{aligned} \quad (C. 13)$$

In the third case the criticality reset is made by adjusting the depth of a control rod (cluster), assuming this depth as given by $(z_k + \rho H)$ [k being the index of the k 'th rod within the control cluster, with reference positions corresponding to $\rho = 0$], with similar notation as used above, we may indicate that portion of B dependent on variable ρ as

$$\pi_k h(z - z_k - \rho H) B_{bor}^k, \quad (C. 14)$$

where H represents a scale parameter, for instance, the core height.

Matrix $\frac{\partial B}{\partial \rho}$ [appearing in the constraint, Eq. (7)] will then be (assuming $\rho = 0$ at unperturbed conditions)

$$\begin{aligned} \frac{\partial B}{\partial p} &= \frac{\partial}{\partial p} \sum_{k=1}^K [\pi_k h (z - z_k - p H) B_{\text{hor}}^k] \\ &= \sum_{k=1}^K H \delta (z - z_k) \pi_k \text{diag} \{ \Sigma_{B,1}^z, \Sigma_{B,2}^z, \dots, \Sigma_{B,G}^z \} V \quad (C. 15) \end{aligned}$$

Also in this case it is easy to verify that the general solution of Eq. (C. 5) is $\mathbf{n}^* = \mathbf{n}_{\text{part}}^* + \alpha \phi^*$, $\mathbf{n}_{\text{part}}^*$ being a particular solution, ϕ^* the standard adjoint flux and α an arbitrary constant, determined by imposing the orthogonality relation, Eq. (C. 7). It results, for this case,

$$\mathbf{n}^* = \mathbf{n}_{\text{part}}^* - \frac{\sum_{k=1}^K \mathbf{n}_{\text{part}}^{*kT} \text{diag} \{ \Sigma_{B,1}^k, \Sigma_{B,2}^k, \dots, \Sigma_{B,G}^k \} V \cdot \mathbf{n}^k}{\sum_{k=1}^K \phi^{*kT} \text{diag} \{ \Sigma_{B,1}^k, \Sigma_{B,2}^k, \dots, \Sigma_{B,G}^k \} V \cdot \mathbf{n}^k} \phi^* \quad (C. 16)$$

where $\mathbf{n}_{\text{part}}^{*k}$, \mathbf{n}^k and ϕ^{*k} are values averaged in the plane (x, y) within π_k .

APPENDIX D. Source driven systems

The methodologies described above in Appendices B and C for long term nuclide/neutron core cycle evolution and short term control analysis may be very well applied to source driven, subcritical systems.

One of the advantages often claimed for the subcritical source driven power systems is associated to the fact that the power level may be basically controlled by the source strength (via the regulation of the accelerator current). So, no control, or regulating elements would be necessary, if a sufficient breeding is available (and/or an appropriate core burnable poison distribution is provided at the beginning of cycle) in the core for compensating the reactivity loss during burnup. To represent this, we shall rewrite Eqs. (B. 1), (B. 2) and (B. 3) in the form

$$m_{(n)}(n, c_f, \rho | p) = - \frac{\partial n}{\partial t} + Bn + \rho s_n = 0 \quad (D. 1)$$

$$m_{(c)}(n, c_f | p) = - \frac{\partial c}{\partial t} + Ec_f + s_c = 0 \quad (D. 2)$$

$$m_{(\rho)}(n, c_f | p) = c_f S n - W = 0, \quad (D. 3)$$

where B and E depend on densities c_f and n , respectively.

Since we generally consider systems at quasi-static, i.e., stationary conditions, the time derivative at the second member of Eq. (D. 1) may be neglected in the course of the integration process.

Any response, functional of variables n , c_f , and ρ , could be considered for analysis. We think instructive to limit consideration to the response defined by the expression

$$Q = \rho(t_f) = \int_{t_0}^{t_f} \delta(t - t_f) \rho(t) dt, \quad (D. 4)$$

which corresponds to the relative source strength required at t_f to assure the power level imposed. We may assume that, at unperturbed conditions, $\rho(t) = 1$ in the interval (t_0, t_f) . If some system parameter (for instance, the initial enrichment, or some other material density) is altered, as in an optimization search analysis, it may be of interest to evaluate the corresponding change of ρ at the end of cycle, to make sure that given upper limit specifications of the source strength are non exceeded.

Along with the HGPT methodology, the equations for the corresponding importance functions result

$$- \frac{\partial n^*}{\partial t} = B^* n^* + \Omega_c^* c_f^* + S^* c_f p^* \quad (D. 5)$$

$$-\frac{\partial \mathbf{c}_f^*}{\partial t} = E^* \mathbf{c}_f^* + \Omega_n^* \mathbf{n}^* + S n p^* \quad (\text{D. 6})$$

$$\langle \mathbf{n}^*, \mathbf{s}_n \rangle + \delta(t - t_p) = 0 \quad (\text{D. 7})$$

with Ω_c^* and Ω_n^* again being the coupling operators defined with Eq. (B. 8).

Eq. (D. 7) corresponds to an orthonormal condition for \mathbf{n}^* .

In order to determine the 'final' value $\mathbf{n}^*(t_p)$ required for starting the integration of Eq. (D. 5), in consideration of the nature of the above governing equations, we shall first write \mathbf{n}^* and ρ^* in the form⁶

$$\mathbf{n}^*(\mathbf{r}, t) = \mathbf{n}_p^*(\mathbf{r}) \delta(t - t_p) + \tilde{\mathbf{n}}^*(\mathbf{r}, t) \quad (\text{D. 8})$$

$$\rho^*(t) = \rho_p^* \delta(t - t_p) + \tilde{\rho}^*(t) \quad (\text{D. 9})$$

with $\tilde{\mathbf{n}}^*(\mathbf{r}, t)$ and $\tilde{\rho}^*(t)$ being finite functions, vanishing at t_p .

Replacing into Eq. (D. 5), integrating in the interval $(t_p - \varepsilon, t_p + \varepsilon)$, and then making $\varepsilon \rightarrow 0$, we obtain the equation

$$B^* \mathbf{n}_p^* + S^T \mathbf{c}_f(t_p) \rho_p^* = 0 \quad (\text{D. 10})$$

Let us now define $\hat{\mathbf{n}}_p^*$ as obeying equation

$$B^* \hat{\mathbf{n}}_p^* + S^T \mathbf{c}_f(t_p) = 0, \quad (\text{D. 11})$$

We note that $\hat{\mathbf{n}}_p^*$ corresponds to the importance relevant to functional $\langle \mathbf{c}_f(t_p), S \mathbf{n}(t_p) \rangle$, i.e., to the system power W . From the source reciprocity relationship (Section 2), we may write

$$\langle \mathbf{c}_f(t_p), S \mathbf{n}(t_p) \rangle = \langle \hat{\mathbf{n}}_p^*, \mathbf{s}_n \rangle = W, \quad (\text{D. 12})$$

⁶ The diverging of $\mathbf{n}^*(\mathbf{r}, t)$ at t_p may be explained on physical grounds recalling the meaning of importance (in this case, the contribution to the given response by a neutron with the same space/time coordinates) and considering that the response here is $\rho(t_p)$, i.e., the control assumed to maintain the power at a prefixed level. A neutron introduced at t_p into the system would in fact produce a (delta-like) impulse of control ρ to balance its effect on the power level. Then, the importance associated to such neutron would be characterized by a similar delta-like behaviour. A quite similar reasoning applies in relation to the diverging of importance $\rho^*(t)$ at t_p , considering that its physical meaning corresponds to the contribution to the response $[\rho(t_p)]$ due to a unit energy insertion at t_p or, which is the same, to an overall power pulse $\delta(t - t_p)$.

From constraint, Eq. (D. 7), we easily obtain

$$\rho_f^* = - \frac{1}{\langle \hat{n}_f^*, s_n \rangle} = - \frac{1}{W} \quad (D. 13)$$

and then

$$\mathbf{n}_f^* = \hat{n}_f^* \rho_f^* = - \frac{\hat{n}_f^*}{W}. \quad (D. 14)$$

From this 'final' value, a recurrent calculational scheme may be defined starting from t_f and proceeding backward.

The sensitivity coefficient relevant to the j 'th parameter p_j can then be defined as

$$\begin{aligned} \frac{d\rho(t_f)}{dp_j} &= \rho_f^* \left[\langle \hat{n}_f^*, \frac{\partial}{\partial p_j} (B\mathbf{n} + s_n) \rangle + \frac{\partial}{\partial p_j} (\langle c_f, S\mathbf{n} \rangle - W) \right]_{t_f} \\ &+ \int_{t_0}^{t_f} \left[\langle \hat{n}^*, \frac{\partial}{\partial p_j} (B\mathbf{n} + s_n) \rangle + \langle c^*, \frac{\partial E}{\partial p_j} c_f \rangle + \hat{p}^* \frac{\partial}{\partial p_j} (\langle c_f, S\mathbf{n} \rangle - W) \right] dt. \end{aligned} \quad (D. 15)$$

with ρ_f^* given by Eq. (D. 13). The first term at right side accounts for effects on ρ (t_f) due to parameter changes at t_f , in particular, if $p_j = W$, it gives the (trivial) result

$$\frac{d\rho(t_f)}{dW} = \frac{1}{W}.$$

The second, integral term accounts for analogous effects on $\rho(t_f)$ produced by parameter changes at times $t < t_f$.

Rather than on the source term, a control on the neutron absorption in the multiplying region could be of interest. In this case, the (intensive) control variable p would represent the average penetration of the control elements, or the average density of the soluble boron in the coolant, and then would enter into the (transport, or diffusion) operator B . The orthonormal condition for the neutron importance \hat{n}^* would now be, rather than Eq. (D. 7),

$$\langle \hat{n}^*, \frac{\partial B}{\partial p} \mathbf{n} \rangle + \delta(t - t_f) = 0. \quad (D. 16)$$

In this case, the sensitivity coefficient with respect to a given parameter p_j would always be given by Eq. (D. 15), with \hat{n}_f^* obeying Eq. (D. 11), but with

$$\rho_f^* = - \frac{1}{\langle \hat{n}_f^*, \frac{\partial B}{\partial p} \mathbf{n} \rangle}. \quad (D. 17)$$

In general, a control strategy, by which an automatic resetting of the imposed overall power is actuated, might imply a control intervention on both the neutron source strength and the absorbing elements within the multiplying region. In this case, ρ (which remains a unique, intensive control variable) would affect both operator B and the neutron source [in this latter case, via an appropriate ρ - and parameter dependent coefficient $\alpha(\rho|p)$, assumed unity at unperturbed conditions]. The distribution between these two control mechanisms could be described by appropriate parameters (subject to perturbation analysis). The sensitivity coefficient, in this case, with respect to a given parameter p_j would always be given by Eq. (D. 15), with \hat{n}_0^* obeying Eq. (D. 11), but with

$$\rho_j^* = - \frac{1}{\langle \hat{n}_0^* | \left(\frac{\partial B}{\partial \rho} n + \frac{\partial \alpha}{\partial \rho} s_n \right) \rangle} \quad (D. 18)$$

Stationary Case

To study a given subcritical system at the beginning of its cycle life, we may consider the corresponding stationary case, i.e., that same system in which the neutron source and the nuclide density are assumed time-independent during an arbitrary time interval (t_0, t_b) . We assume that at t_0 the neutron density (n_0), as well as the control (ρ_0) have already reached stationary conditions. So, also these two quantities are time-independent in the same time interval. Their governing equations can then be written, in case the power level is controlled by the source strength,

$$Bn_0 + \rho_0 s_{n0} = 0 \quad (D. 19)$$

$$\langle c_{i0}, s_{n0} \rangle - W_0 = 0 \quad (D. 20)$$

Also here we shall assume that at unperturbed conditions $\rho_0=1$.

The same equations derived previously are applicable to this case, with the advertence of replacing t_r with with t_b and setting the coupling operators Ω_c^* and Ω_n^* appearing in Eqs. (D. 5) and (D. 6) equal to zero. The sensitivity coefficient of the response $\rho(t_b)$ [$=\rho(t)=\rho_0$, i.e., constant in the whole interval (t_0, t_b)] relevant to the j 'th parameter p_j can then be obtained. Since in this case c^* , as well as \hat{n}^* and $\hat{\rho}^*$, vanish, recalling Eq. (D. 15), we obtain

$$\frac{d\rho_0}{dp_j} = \rho_0^* \left[\langle \hat{n}_0^* | \frac{\partial}{\partial p_j} (Bn_0 + s_{n0}) \rangle + \frac{\partial}{\partial p_j} (\langle c_{i0}, s_{n0} \rangle - W_0) \right] \quad (D. 21)$$

where

$$\rho_0^* = - \frac{1}{W_0} \quad (D. 22)$$

and n_0^* obeys equation

$$B^* n_0^* + S^T c_{to} = 0. \quad (D. 23)$$

If, rather than via the source strength, the power level reset control is assumed to be regulated via neutron absorption, so that the control ρ_0 would enter into operator B , the sensitivity coefficient would be given always by Eq. (D. 21), but with

$$\rho_0^* = - \frac{1}{\langle n_0^*, \frac{\partial B}{\partial \rho_0} n_0 \rangle}. \quad (D. 24)$$

We might as well consider a (fictitious) control mechanism affecting the fission source, rather than the neutron absorption, i.e., we might choose as control a coefficient multiplying the fission matrix (F) and, therefore, entering into the Boltzmann, or diffusion, operator B ($= A + \rho_0 F$). The sensitivity coefficient would be given again by Eq. (D. 21), but with

$$\rho_0^* = - \frac{1}{\langle n_0^*, F n_0 \rangle}. \quad (D. 25)$$

Reactivity of Subcritical Systems

For resetting the power level, we have considered above different control mechanisms to which the following types of equations governing the neutron density may be associated:

$$B(p) n_0 + \rho_0 s_{to}(p) = 0 \quad (\text{source control}) \quad (D. 26)$$

$$B(\rho_0 | p) n_0 + s_{to}(p) = 0 \quad (\text{neutron absorption, or fission control}) \quad (D. 27)$$

$$B(\rho_0 | p) n_0 + \alpha(\rho_0 | p) s_{to}(p) = 0 \quad (\text{mixed control})^7 \quad (D. 28)$$

⁷ A mixed control strategy may be considered also using Eq. (D. 26), or Eq. (D. 27). Adopting, for instance, Eq. (D. 26), relevant to the neutron source control, part of the power level would be taken care of parametrically (e.g., by properly changing the control rod position, or the soluble boron density). The remaining reset would be taken care of intrinsically, by the ρ -control chosen.

where the control and parameter dependence is indicated. Coefficient α is given and reflects the mixed strategy chosen. Eqs. (D. 26), (D. 27) and (D. 28) may be generally represented by equation

$$\mathbf{m}_{(n, o)}(n_o, \rho_o | \mathbf{p}) = 0. \quad (\text{D. 29})$$

The sensitivity expression (D. 21) may then be generalized so that

$$\frac{d\rho_o}{d\mathbf{p}_j} = - \frac{\langle \mathbf{n}_o^* \frac{\partial \mathbf{m}_{(n, o)}}{\partial \mathbf{p}_j} \rangle + \frac{\partial}{\partial \mathbf{p}_j} (\langle \mathbf{c}_{fo}^T, \delta \mathbf{n}_o \rangle - W_o)}{\langle \mathbf{n}_o^* \frac{\partial \mathbf{m}_{(n, o)}}{\partial \rho_o} \rangle}, \quad (\text{D. 30})$$

with \mathbf{n}_o^* obeying Eq. (D. 23).

A corresponding perturbation expression may now be obtained. Assuming that the power W_o appearing in Eq. (D. 30) is not subject to perturbation, we may write:

$$\delta \rho_o = - \frac{\langle \mathbf{n}_o^* \delta \mathbf{m}_{(n, o)} \rangle + \langle \mathbf{n}_o^* \delta (S^T \mathbf{c}_{fo}) \rangle}{\langle \mathbf{n}_o^* \frac{\partial \mathbf{m}_{(n, o)}}{\partial \rho_o} \rangle}, \quad (\text{D. 31})$$

$$\text{where } \delta \mathbf{m}_{(n, o)} = \sum_j \delta \mathbf{p}_j \frac{\partial \mathbf{m}_{(n, o)}}{\partial \mathbf{p}_j} \text{ and } \delta (S^T \mathbf{c}_{fo}) = \sum_j \delta \mathbf{p}_j \frac{\partial (S^T \mathbf{c}_{fo})}{\partial \mathbf{p}_j}.$$

As said previously, $\delta \rho_o$ corresponds to the control change necessary to reestablish the power level existing before the perturbation $\delta \mathbf{m}_{(n, o)}$. We may as well say that the perturbation $\delta \mathbf{m}_{(n, o)}$ [and $\delta (S^T \mathbf{c}_{fo})$] would produce a power level change equivalent to that produced by a control change δK_p given by the equation

$$\delta K_p = \frac{\langle \mathbf{n}_o^* \delta \mathbf{m}_{(n, o)} \rangle + \langle \mathbf{n}_o^* \delta (S^T \mathbf{c}_{fo}) \rangle}{\langle \mathbf{n}_o^* \frac{\partial \mathbf{m}_{(n, o)}}{\partial \rho_o} \rangle}. \quad (\text{D. 32})$$

In the case of the (fictitious) control on the neutron fission, setting λ in place of ρ to distinguish this peculiar case, we may explicitly write

$$\delta K_\lambda = \frac{\langle \mathbf{n}_o^* \delta B \mathbf{n}_o \rangle}{\langle \mathbf{n}_o^* F \mathbf{n}_o \rangle} + \frac{\langle \mathbf{n}_o^* \delta s_{po} \rangle}{\langle \mathbf{n}_o^* F \mathbf{n}_o \rangle} + \frac{\langle \mathbf{n}_o^* \delta (S^T \mathbf{c}_{fo}) \rangle}{\langle \mathbf{n}_o^* F \mathbf{n}_o \rangle}. \quad (\text{D. 33})$$

The first term at the right side closely resembles the reactivity expression for

critical systems.⁸ So, we shall call a quantity δK_λ as given expression (D. 33) a 'generalized reactivity'. To account for a generic ρ -mode control mechanism, we shall extend this definition to δK_ρ , similarly defined by Eq. (D. 32), i.e.,

$$\delta K_\rho = \frac{\langle n_{cr}^* \delta \beta n_0 \rangle}{\langle n_{cr}^* \frac{\partial m_{(n,0)}}{\partial \rho_0} \rangle} + \frac{\langle n_{cr}^* \delta s_{n0} \rangle}{\langle n_{cr}^* \frac{\partial m_{(n,0)}}{\partial \rho_0} \rangle} + \frac{\langle n_{cr}^* \delta (S^c e_{(0)}) \rangle}{\langle n_{cr}^* \frac{\partial m_{(n,0)}}{\partial \rho_0} \rangle} \quad (D. 34)$$

and call it generalized ρ -mode reactivity.⁹ We may as well define a (generalized) reactivity coefficient, as given by the expression

$$\frac{\partial K_\rho}{\partial \rho_1} = \frac{\langle n_{cr}^* \frac{\partial \beta}{\partial \rho_1} n_0 \rangle}{\langle n_{cr}^* \frac{\partial m_{(n,0)}}{\partial \rho_0} \rangle} + \frac{\langle n_{cr}^* \frac{\partial s_{n0}}{\partial \rho_1} \rangle}{\langle n_{cr}^* \frac{\partial m_{(n,0)}}{\partial \rho_0} \rangle} + \frac{\langle n_{cr}^* \frac{\partial (S^c e_{(0)})}{\partial \rho_1} \rangle}{\langle n_{cr}^* \frac{\partial m_{(n,0)}}{\partial \rho_0} \rangle} \quad (D. 35)$$

⁸ Eq. (D. 33) can be demonstrated to formally approach the standard reactivity expression as the (reference) system considered gets close to criticality conditions, the λ control coefficient (at reference conditions) approaching its critical value λ_c [for example, consequent to assuming the (reference) neutron source term, defined as $s_{n0} = \zeta \hat{s}_{n0}$, with (positive) coefficient ζ approaching zero, while maintaining unaltered the power level W_d]. To show this, let us consider (arbitrarily normalized) functions \bar{n}_0 and $\hat{\phi}_0^*$ relevant to the associated critical system, obeying equations

$$A \bar{n}_0 + \lambda_c F \bar{n}_0 = 0 \quad ; \quad A^* \hat{\phi}_0^* + \lambda_c F^* \hat{\phi}_0^* = 0$$

Clearly, functions n_0 and n_{cr}^* obeying heterogeneous equations (D. 27) (with source term $s_{n0} = \zeta \hat{s}_{n0}$, and with $\rho = \lambda$) and (D. 23), respectively, for $\lambda \rightarrow \lambda_c$ (corresponding to $\zeta \rightarrow 0$) approach limiting values, i.e.,

$$n_0 \rightarrow \alpha_1 \bar{n}_0 \quad ; \quad n_{cr}^* \rightarrow \alpha_2 \hat{\phi}_0^*$$

where α_1 is a finite (positive) coefficient while α_2 diverges. Correspondingly, the third term at the right side of Eq. (D. 33) tends to vanish. Eq. (D. 33) then approaches the asymptotic expression,

$$\delta K_\lambda^{as} = \frac{\langle \phi_{cr}^* \delta \beta \bar{n}_0 \rangle}{\langle \phi_{cr}^* F \bar{n}_0 \rangle} + \frac{\langle \hat{\phi}_0^* \delta s_{n0} \rangle}{\langle \hat{\phi}_0^* F \bar{n}_0 \rangle}$$

The first term at right side formally coincides with the reactivity expression for critical systems. The sum of the first and second term may be viewed as a generalization of the traditional reactivity expression. The second term would allow to account for the possibility of introducing into a critical system a neutron source s_{n0}^* ($= \delta s_{n0}$), viewed as a perturbation. The quantity $-\delta K_\lambda^{as}$ would in this latter case correspond to the control (λ) change associated with δs_{n0} , so that in the altered system (subcritical, after the control reset) the previous power level is maintained. This possibility is not of particular interest in critical system studies, so that reactivity expressions containing only the first term at right side have been so far considered.

⁹ In the following, if no ambiguity occurs, we shall call it simply 'reactivity'.

Expressions (D. 34) and (D. 35) can be useful in the analysis and exploitation of measurements on subcritical experimental facilities, as well as for analytical studies of power source driven reactors (for example, for optimal configuration searches).

In relation to the application of above formulations to experimental facility analysis, a (measurable) change of the flux level produced by a perturbation of a parameter (such as a material density, the neutron source intensity, etc.) would be associated to the corresponding 'reactivity' δK_p^{ex} where apex 'ex' indicates that it would correspond to a measured quantity. The determination of δK_p^{ex} could be effected either directly, by resetting the initial flux level conditions via the specific p-mode control chosen (for instance, as is the case for an experimental facility, through a regulatory rod movement), or indirectly, through its previous calibration vs. neutron flux level.

Calculating value δK_p^{cal} of the same 'reactivity' from Eq. (D. 34), would enable a comparison between experimental and calculational results, in view, for instance, of data adjustments exercises via statistical fitting methods [27]. The data to be adjusted could be differential quantities (e.g., cross-sections), as well as neutron source parameters (e.g., related to the energy distribution and intensity) to which 'a priori' uncertainties have been associated.

A measurement of the power level change consequent to a perturbation of system parameters could be also used directly in an 'unconstrained' system, i.e., in a system in which no reset mechanism is considered (which may be the case for an experimental subcritical facility). In this case, the neutron density n_0 at unperturbed conditions would obey equation

$$Bn_0 + s_{n0} = 0. \quad (D. 36)$$

Considering the importance n_0^* governed by Eq. (D. 23), relevant to the system power $W_0 = \langle c_{l0}, Sn_0 \rangle$, along with the HGPT methodology [7] we would obtain the perturbation expression (inclusive also of the so called 'direct effect' term)

$$\delta W_0 = \langle n_0^*, \delta B n_0 \rangle + \langle n_0^*, \delta s_{n0} \rangle + \langle n_0^*, \delta (S^T c_{l0}) \rangle. \quad (D. 37)$$

This expression could also be used for experimental data analysis.

In certain circumstances, Eq. (D. 37) could as well be adopted for system analysis and optimization searches, even though in this case no direct appreciation would be obtained on the 'reactivity' δK_p associated with the control mode selected.

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