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Angélique Ponçot, Jean-Philippe Argaud, Bertrand Bouriquet, Patrick Erhard, Serge Gratton, et al.. Variational assimilation for xenon dynamical forecasts in neutronic using advanced background error covariance matrix modelling. *Annals of Nuclear Energy*, 2013, vol. 60, pp. 39-50. 10.1016/j.anucene.2013.04.026 . hal-00832455

**HAL Id: hal-00832455**

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URL : <http://dx.doi.org/10.1016/j.anucene.2013.04.026>

**To cite this version:**

Ponçot, Angélique and Argaud, Jean-Philippe and Bouriquet, Bertrand and Erhard, Patrick and Gratton, Serge and Thual, Olivier *Variational assimilation for xenon dynamical forecasts in neutronic using advanced background error covariance matrix modelling*. (2013) *Annals of Nuclear Energy*, vol. 60. pp. 39-50. ISSN 0306-4549

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# Variational assimilation for xenon dynamical forecasts in neutronic using advanced background error covariance matrix modelling

Angélique Ponçot<sup>a,\*</sup>, Jean-Philippe Argaud<sup>a</sup>, Bertrand Bouriquet<sup>a</sup>, Patrick Erhard<sup>a</sup>, Serge Gratton<sup>c,b</sup>, Olivier Thual<sup>c,b</sup>

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## A B S T R A C T

Data assimilation method consists in combining all available pieces of information about a system to obtain optimal estimates of initial states. The different sources of information are weighted according to their accuracy by the means of error covariance matrices. Our purpose here is to evaluate the efficiency of variational data assimilation for the xenon induced oscillations forecasts in nuclear cores. In this paper we focus on the comparison between 3DVAR schemes with optimised background error covariance matrix **B** and a 4DVAR scheme. Tests were made in twin experiments using a simulation code which implements a mono-dimensional coupled model of xenon dynamics, thermal, and thermal-hydraulic processes. We enlighten the very good efficiency of the 4DVAR scheme as well as good results with the 3DVAR one using a careful multivariate modelling of **B**.

## Keywords:

Xenon dynamics

Variational data assimilation

Background error covariance matrix

## 1. Introduction

In this article we aim to evaluate the efficiency of variational data assimilation methods known as 3DVAR and 4DVAR methods in the forecasting of Xenon-135 oscillations.

Xenon-135 is known to be at the origin of axial power oscillations of about one day period in pressurised water reactors (PWRs)(Canosa and Brooks, 1966). These oscillations do not change the overall power produced by the nuclear plant but they are undesirable from a safety point of view. As soon as oscillations are detected, they are damped using appropriate control rod movements inside the core. Detection as well as prediction of xenon induced oscillations are an important part in the operation of a nuclear power plant.

No direct measurement of the concentration of xenon in the reactor core is available, and the simulation of the nonlinear xenon dynamics still represents a challenge for real time applications such as system monitoring. Several models have been proposed for the real time estimation of xenon concentration. They include flux and iodine-135 dynamics modelling. Some of them require an estimation of parameters such as presented in Onega and Kisner (1978). This approach is a first step in improving the state estimation but it does not take into account errors in the measurements used to adjust the model parameters: therefore bad measurements

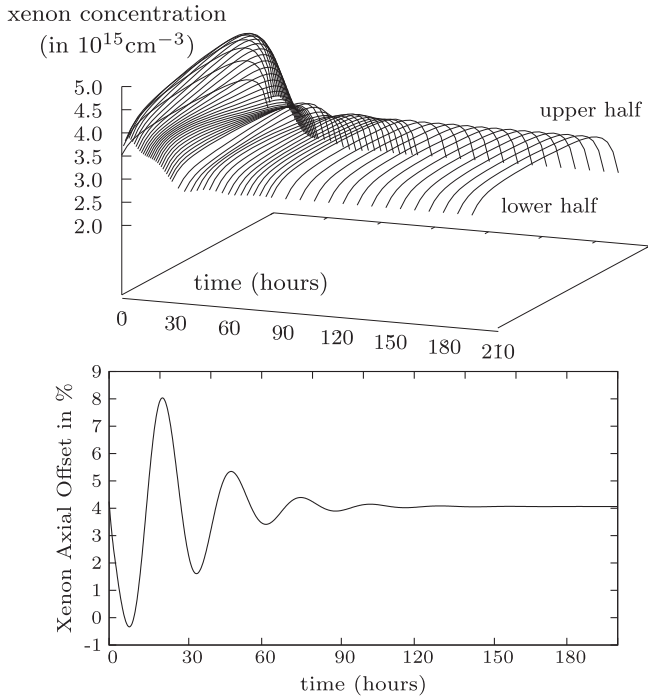
can affect adversely the quality of the computed state. In addition, it does not allow to correct initial conditions of the coupled flux-iodine-xenon dynamical system. Most of these models assume equilibrium concentrations, though the initial distributions of iodine and xenon have a significant impact on the power transient.

Song et al. (1996) determined an analytic initialisation of iodine and xenon of an out-of-equilibrium state which consists in adding a corrective term with a sinus shape to the 1D equilibrium concentrations. The amplitude of the sinus is fitted with axial offset power measurements. These measurements are considered to be perfect, in the same way as the xenon dynamics model is considered exact. This approach is based on analytical developments which limit the pattern of the added correction and still does not take into account the errors in the measurements.

Here we aim to improve the Xenon-135 concentration forecast by finding alternative and more accurate solutions using variational data assimilation techniques. Such techniques find their root in earth science and are used daily in weather forecast. Data assimilation is nowadays more and more used in the nuclear science community for the improvement of the nuclear core activity determination (Bouriquet et al., 2011; Bouriquet et al., 2011) as well as for the nuclear accident model parameter determination (Cacuci and Ionescu-Bujor, 2010; Petrucci et al., 2010). Thus it is challenging to apply such a technique to xenon oscillation forecast even if other attempts have been made through genetic algorithm (Marseguerra et al., 2003) or optimal control (Shumazu, 2007).

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**Fig. 1.** Xenon dynamics simulation on a time range of 200 h. The map of the first figure represents the evolution of the monodimensional xenon vector with respect to the time ( $x$ -axis). The  $y$ -coordinate corresponds to the position in core and the vertical coordinate gives the xenon level. The second plot gives the xenon axial offset with respect to the time, i.e. the power difference between the half top and bottom parts of the core.

Even if the problem we deal with can be seen as very well adapted to the Kalman method as it has been shown in Lin and Lin (1994), we choose to use the variational one instead. This choice has been done as on long term plan we expect to use some high resolution models, hopefully together with their adjoint. Thus it is important to already test variational techniques that are the only one available when the control space is too large.

Two data assimilation methods, the 3DVAR and the 4DVAR, will be used here. The main difference between those methods is that the 4DVAR takes into account the dynamic of the process. This is a tremendous improvement as it has been proven in weather forecast. But such a method needs the adjoint that is costly to develop in an industrial context. To overcome this difficulty a specific model (CIREP1D) compatible with automatic differentiation has been developed.

In a first part (Section 2) we describe the model, CIREP1D, a mono-dimensional xenon dynamics model which includes neutron and thermal-hydraulic processes. Then we give a brief overview of variational data assimilation methods in Section 3. The setting of the data assimilation method is presented in Section 4. In Section 5 we propose three background error covariance matrix modellings (two univariate modellings and a last multivariate modelling). Finally in Section 6, we compare the quality of the 3DVAR estimates to a 4DVAR estimate.

## 2. The CIREP1D model

Since 3D operational industrial codes are time consuming, we use a monodimensional axial xenon/iodine dynamics model coupled with a monodimensional neutronic/thermal/thermal-hydraulic model, named CIREP1D. It simulates axial xenon dynamics according to the overall power and the control rod insertion records in a given time window. CIREP1D takes a few seconds to simulate a xenon oscillation of a one-week time range but contrary to

simpler models, it gives access to quantities measured in core: axial power, axial xenon, axial iodine, axial flux and boron concentration. The agreement between 1D and 3D models for axial xenon dynamics is good and has been studied in detail in Ponçot (2008).

Globally speaking, CIREP1D solves a nonlinear system of ordinary differential equations given by an operator  $\mathcal{G}$ :

$$\frac{\partial(C_{Xe}, C_I)}{\partial t}(z, t) = \mathcal{G}(C_{Xe}, C_I)(z, t), \quad (1)$$

by using an implicit Euler scheme.  $C_{Xe}(z, t)$  and  $C_I(z, t)$  represent the axial concentration of xenon and iodine respectively. Each time step requires a critical boron concentration computation corresponding to the assumption that neutron and thermal-hydraulic effects may be treated with stationary coupled equations. The xenon dynamics can be initialised by either a given xenon and iodine concentrations or by equilibrium concentrations. Hereafter we give CIREP 1D equations in detail.

### 2.1. Iodine and xenon equations

Iodine and xenon balance equations are differential equations on the variables  $z, t$ :

$$\begin{cases} \frac{\partial C_I}{\partial t} = \gamma_I \Sigma_f \Phi - \lambda_I C_I, \\ \frac{\partial C_{Xe}}{\partial t} = \gamma_{Xe} \Sigma_f \Phi + \lambda_I C_I - (\lambda_{Xe} + \sigma_{Xe} \Phi) C_{Xe}, \end{cases} \quad (2)$$

$\Sigma_f$  is the fission cross-section of the fuel and  $\sigma_{Xe}$  the absorption cross-section of xenon-135. These variables depend on  $z$  and  $t$ . The  $z$ -coordinate is measured from the bottom of the 1D reactor.  $\gamma_I$  and  $\gamma_{Xe}$  are the fractional fission yield of iodine and xenon. Finally,  $\lambda_I$  and  $\lambda_{Xe}$  are decay constants of iodine and xenon.

### 2.2. Neutronic model

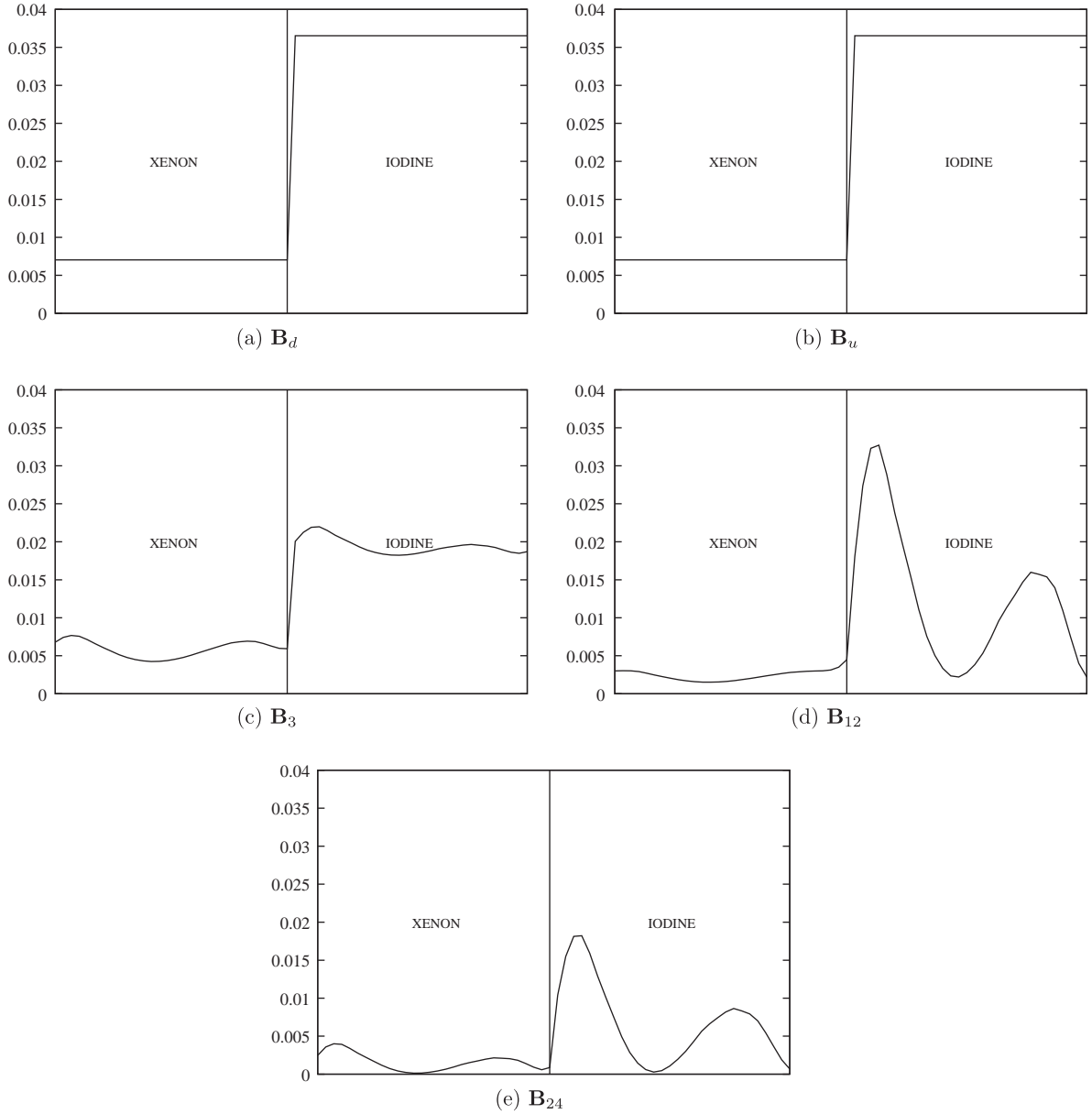
The neutronic flux  $\Phi = (\Phi_1, \Phi_2)$  is identified by solving two-group diffusion equations with no-upscattering. We assume that the time step of flux simulation (a few seconds) is shorter than the xenon oscillations. As a consequence, at each time step for the resolution of xenon equation, the flux can be computed using the stationary diffusion equations:

$$\begin{cases} -\partial_z D_1 \partial_z \Phi_1 + [\Sigma_{a1} + \Sigma_r] \Phi_1 = \frac{1}{k} \nu \Sigma_f \Phi, \\ -\partial_z D_2 \partial_z \Phi_2 + \Sigma_{a2} \Phi_2 - \Sigma_r \Phi_1 = 0, \\ \text{with } \nu \Sigma_f \Phi = \nu_1 \Sigma_{f1} \Phi_1 + \nu_2 \Sigma_{f2} \Phi_2, \end{cases} \quad (3)$$

where  $\Phi_1$  and  $\Phi_2$  are groupwise neutron axial flux distribution,  $\Sigma_r$  is the scattering cross-section and  $\Sigma_{ag}, D_g$  and  $\nu_g \Sigma_{fg}$  are the absorption cross-section, the diffusion coefficient, and the neutron emitted by fission. All these variables depend on the  $z$  variable. The system is closed by using albedo boundary condition. The balance is obtained by looking for boron concentration such that the eigenvalue  $k$  is equal to one (this is critical boron concentration computation). The boron influence does not appear explicitly in the previous equations but is linked to cross-section values through the feedback model. The feedback model changes the cross-sections according to the state of the core (temperature, boron concentration and so on).

### 2.3. Feedback model

Thermal effects are not lumped in a power feedback parameter as done in some other cases (Onega and Kisner, 1978). The developed feedback model is a linear interpolation model relying on assumption that the cross-sections depend on six quantities: fuel irradiation, xenon concentration  $C_{Xe}$ , boron concentration  $C_B$ , moderator density  $\rho_{mod}$ , moderator temperature  $T_{mod}$  and fuel



**Fig. 2.** Diagonal terms of  $\mathbf{B}$  matrices for univariate and multivariate modelling, that is to say background error variances with respect to the node of the spatial mesh.

temperature  $T_f$ . Therefore, CIREP1D includes a thermal/thermal-hydraulic model, as described below.

#### 2.4. Thermal-hydraulic model

Since the speed of the water flowing upwards through the reactor is high, we can assume that the thermal-hydraulic problem is an axial monodimensional problem for the slow transients which are common in the normal operational mode. The moderator temperature  $T_{mod}$  is then described by the following equation:

$$Q \partial_z T_{mod}(z, t) = \frac{1}{\rho_{mod} c_{mod}} \left[ P_f^{lin}(z, t) + P_{mod}^{lin}(z, t) \right], \quad (4)$$

where  $Q$ ,  $c_{mod}$  and  $\rho_{mod}$  respectively represent the volume flow rate, the moderator specific heat capacity and the moderator density. Lineic power  $P_f$  and  $P_{mod}$  released in both fuel and moderator are computed from the known two-group flux  $\Phi$ .

#### 2.5. Thermal fuel model

Contrary to the thermal-hydraulic model, we employ a radial model for the thermal fuel model. Thus, a radial description of the fuel is required. We neglect the axial conduction in fuel pin and assume rotational symmetry of the problem. Under these assumptions, the thermal problem can be described by a monodimensional model in the radial variable  $r$ :

$$-\frac{1}{r} \lambda_f \partial_r T_f(r, z) - \lambda_f \partial_r^2 T_f(r, z) = P_f(z)/\mathcal{A}. \quad (5)$$

The variable  $\lambda_f$  represents the fuel thermal conductivity and  $\mathcal{A}$  corresponds to the pin section. This equation is coupled with the neutron equation through the lineic power  $P_f$  and to the thermal-hydraulic problem through the boundary condition expressed on edge  $\Gamma$ :

$$\forall r \in \Gamma, \quad \lambda_f \partial_r T_f(r, z) = h_{tot}(z)[T_f(r, z) - T_{mod}(z)], \quad (6)$$

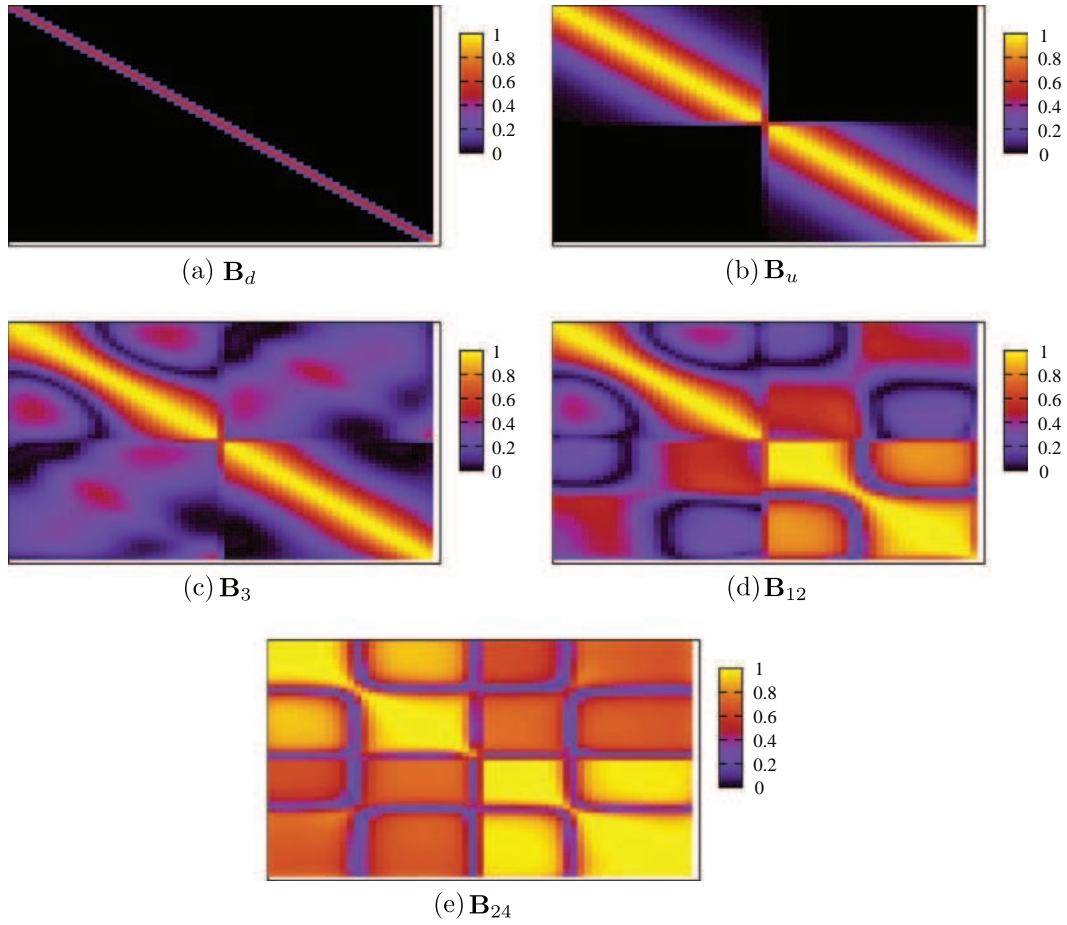


Fig. 3. Absolute values of the components of the correlations related to the matrices  $\mathbf{B}$  for univariate and multivariate modelling with respect to the nodes of the spatial mesh.

where  $h_{tot}$  is the thermal exchange parameter. The thermal and thermal-hydraulic parameters  $\rho_{mod}$ ,  $c_{mod}$ ,  $\lambda_f$  and  $h_{tot}$  depend on moderator and fuel temperatures. Therefore, the coupled thermal/thermal-hydraulic problem is nonlinear.

### 2.6. Xenon transient simulation

As an example of CIREP1D simulation, we present results from a computation with the following characteristics: time range of 200 h, load following during 30 min and, then until the end of simulation, no further rod movement and no power change. The simulated core is in the middle of a burnup cycle and then is moderately irradiated. Fig. 1 shows a xenon oscillation which disappears without any external intervention after 100 h.

## 3. A brief overview of data assimilation techniques

Introducing data assimilation method in operational simulation has been an important step to improve forecasts as for example weather in meteorology. The aim is to provide a satisfactory estimation of the unknown true state of a dynamical system by combining all pieces of information about the system. This information, obtained from measurements (called observations) and simulation, is weighted according to its reliability expressed in terms of error covariance matrices. In practice, the model gives a simulated state called the background state. The purpose of data assimilation is to determine a state, called the analysis state, which is closer to the

true state than the one described solely by the observations or the model. Thus, the analysis state can be used for forecasting.

### 3.1. Concepts and definitions

We now introduce some concepts and definitions. A discrete model for the evolution of physical system from time  $t_i$  to time  $t_{i+1}$  is described by:

$$\mathbf{X}(t_{i+1}) = \mathcal{M}_{i+1,i}(\mathbf{X}(t_i)),$$

where  $\mathbf{X}$  and  $\mathcal{M}$  are respectively the model's state vector and its corresponding dynamics operator. The dynamics  $\mathcal{M}$  of the model evolution is commonly nonlinear. We note respectively  $\mathbf{M}_{i,j}$  and  $\mathbf{M}_{i,j}^T$  the linear tangent and the adjoint operators with respect to the vector  $\mathbf{X}_j$  associated with the dynamics model  $\mathcal{M}$  between  $t_j$  and  $t_i$ . The state vector  $\mathbf{X}$  is usually obtained by discretisation of physical fields on a grid. Its dimension is denoted by  $n$ . The aim is to evaluate the best estimate of the unknown *true state*, denoted  $\mathbf{X}^*$  which is defined by the best possible representation of reality as a state vector at an initial time  $t_0$ . The best estimate that we are looking for in the data assimilation process is called *analysis* and is denoted by  $\mathbf{X}^a$ .

The information about the system that can be used to produce the analysis is listed below:

**Measurements** in the core gathered into an *observation vector*  $\mathbf{Y}^o$ . Its dimension is  $p$ .

**The observation operator.** The key to data analysis is to take advantages of the discrepancy between observations and state

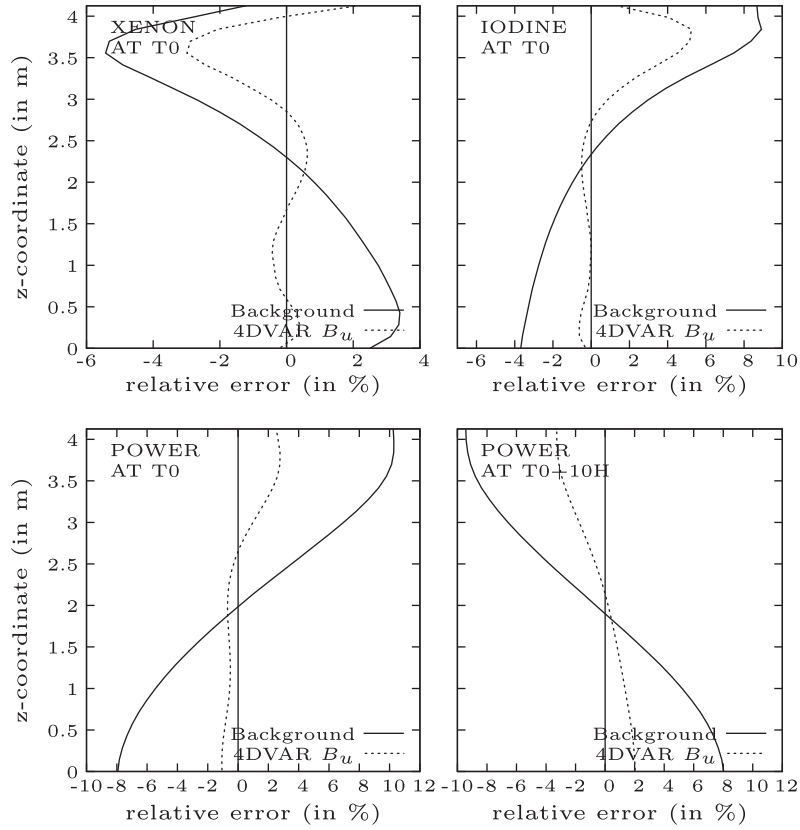


Fig. 4. Relative errors on xenon, iodine at  $t_0$  and on power at  $t_0$  and  $t_0 + 10h$  for the background state and the 4DVAR analysis state.

vector. Usually observation vector and state vector are not defined in the same space. They can be compared through the use of a function from model state space to observation space called *observation operator* and denoted  $\mathcal{H}$ . The operator  $\mathcal{H}$  can be nonlinear.

**An a priori estimate of the true state** before the analysis is carried out. This estimate is called *background state* and is denoted  $\mathbf{X}^b$ . In most cases, the analysis problem is under-determined because observations are sparse and only indirectly related to the model variables. The use of this background information helps to make it a well-posed problem and to introduce some physical knowledge. Usually, this background state is generated from the output of a previous analysis.

**Uncertainties** in the previous data. Background and observation errors are defined by:

$$\epsilon^b = \mathbf{X}^b - \mathbf{X}^t \quad \text{and} \quad \epsilon_i^o = \mathbf{Y}_i^o - \mathcal{H}(\mathcal{M}_{i,0}(\mathbf{X}^t)).$$

The covariance matrices of these errors are denoted by  $\mathbf{B}$  and  $\mathbf{R}$  respectively. Error modelling is a difficult task, mostly because true state  $\mathbf{X}^t$  is unknown and the knowledge of the error covariances is approximative. But it is a very important step which influences the quality of the analysis. The basic modelling consists in setting up diagonal matrices where the diagonal elements correspond to the variances of the errors on the background or observation vector. When different fields are involved in the state or observation vector, it is then possible to choose between an univariate or multivariate modelling. In the former, the errors between the different fields are assumed to be uncorrelated whereas in the multivariate modelling, the errors are assumed to be correlated. Usually errors between the different kinds of observation are assumed to be independent and then the covariance matrix  $\mathbf{R}$  is diagonal. It is more common to assume correlations for the background part but the evaluation of these is also difficult.

In the same way, the analysis state  $\mathbf{X}^a$  is associated to an analysis error defined by:  $\epsilon^a = \mathbf{X}^a - \mathbf{X}^t$ . And its covariance matrix denoted by  $\mathbf{A}$  is estimated during the assimilation process or as a post-processing procedure.

Basically, two families of data assimilation methods exist: stochastic and variational methods. The most famous stochastic method is probably the Kalman filter. This method is still considered as a reference but its application for real data assimilation problems is limited to problems of small to medium size due to its huge computational cost involved in matrix computation. Several variants of this method have been developed either to reduce its computational cost or to remove the assumption on linearity of the used operators. Variational methods are based on the minimisation of a cost function (Talagrand, 1997). These methods, 3DVAR and 4DVAR, that can be adapted to nonlinear cases and problems of large size, are mainly used in operational meteorology and oceanography since the 1990s. Each variational method is equivalent to a stochastic filter method under linear assumptions.

### 3.2. Variational methods

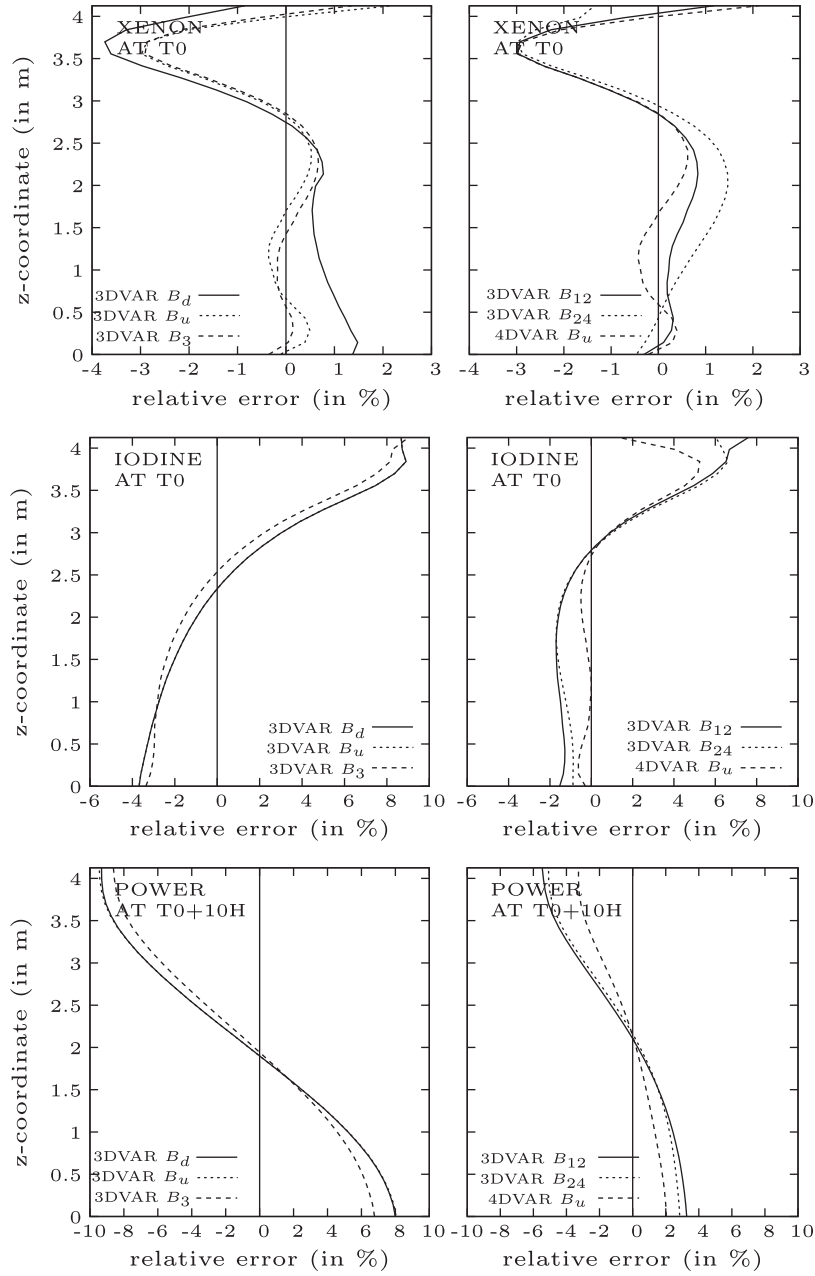
We now give here some elements on variational methods. The 4DVAR cost function measures the weighted sum of the square of distances  $\mathcal{J}^b$  to background state  $\mathbf{X}^b$  and  $\mathcal{J}^o$  to the observations  $\mathbf{Y}^o$  over a time interval  $[t_0, t_n]$ :

$$\mathcal{J}_{4DVAR}(\mathbf{X}(t_0)) = \mathcal{J}^b(\mathbf{X}(t_0)) + \mathcal{J}^o_{4DVAR}(\mathbf{X}(t_0)) \quad (7)$$

with

$$\mathcal{J}^b(\mathbf{X}) = \frac{1}{2} [\mathbf{X} - \mathbf{X}^b]^T \mathbf{B}^{-1} [\mathbf{X} - \mathbf{X}^b],$$

$$\mathcal{J}^o_{4DVAR}(\mathbf{X}) = \frac{1}{2} \sum_{i=0}^n [\mathbf{Y}_i^o - \mathcal{H}(\mathcal{M}_{i,0}(\mathbf{X}))]^T \mathbf{R}_i^{-1} [\mathbf{Y}_i^o - \mathcal{H}(\mathcal{M}_{i,0}(\mathbf{X}))],$$



**Fig. 5.** Relative errors on xenon, iodine at  $t_0$  and on power at  $t_0 + 10h$ . At  $t_0$  3DVAR iodine analysis and background are mistaken. At  $t_0 + 10h$ , 3DVAR and background predicted axial power shapes are mistaken.

where weight matrices  $\mathbf{B}^{-1}$  and  $\mathbf{R}_i^{-1}$  are the inverse of the background and observation error covariance matrices at time  $t_i$ . Minimisation of (7) is done with respect to initial state  $\mathbf{X}(t_0)$ . In practice, the starting point of the minimisation algorithm is taken equal to the background  $\mathbf{X}^b$ . Evaluations of gradient of  $\mathcal{J}_{4DVAR}$ :

$$\nabla \mathcal{J}_{4DVAR}(\mathbf{X}(t_0)) = \nabla \mathcal{J}^b(\mathbf{X}(t_0)) + \nabla \mathcal{J}_{4DVAR}^o(\mathbf{X}(t_0))$$

with

$$\nabla \mathcal{J}^b(\mathbf{X}) = \mathbf{B}^{-1}[\mathbf{X} - \mathbf{X}^b],$$

$$\nabla \mathcal{J}_{4DVAR}^o(\mathbf{X}) = -\sum_{i=0}^n \mathbf{M}_{i,0}^T \mathbf{H}^T \mathbf{R}_i^{-1} [\mathbf{Y}_i^o - \mathcal{H}(\mathcal{M}_{i,0}(\mathbf{X}))],$$

are required by most minimisation methods which implies that the adjoint operator  $\mathbf{M}_{i,0}^T$  and  $\mathbf{H}^T$  have to be evaluated. 3DVAR method is a cheaper alternative to 4DVAR because it does not require the evaluation of the model evolution and its adjoint. The 3DVAR cost

function is very close to the 4DVAR one, except for the time sum that disappears:

$$\mathcal{J}_{3DVAR}(\mathbf{X}(t_0)) = \mathcal{J}^b(\mathbf{X}(t_0)) + \mathcal{J}_{3DVAR}^o(\mathbf{X}(t_0)),$$

$$\text{with } \mathcal{J}_{3DVAR}^o(\mathbf{X}) = \frac{1}{2} [\mathbf{Y}^o - \mathcal{H}(\mathbf{X})]^T \mathbf{R}^{-1} [\mathbf{Y}^o - \mathcal{H}(\mathbf{X})].$$

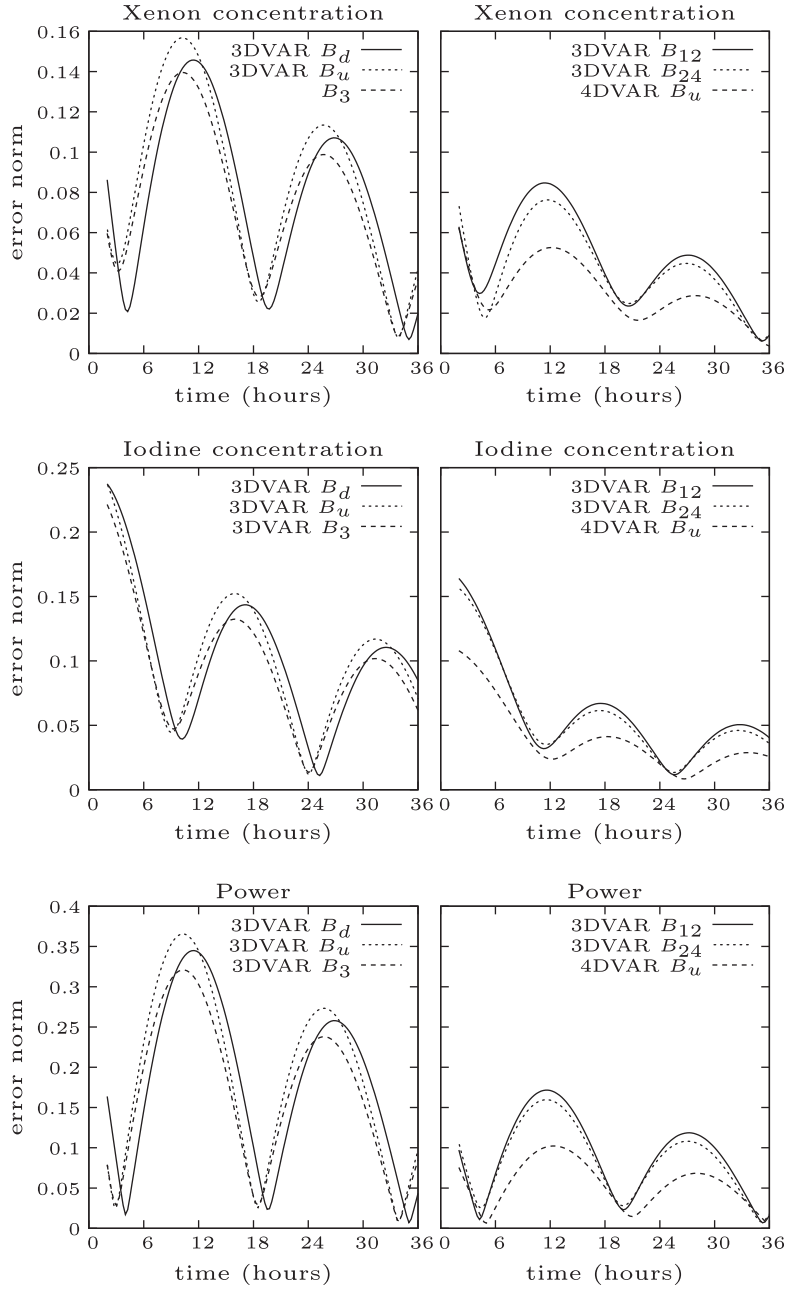
In a variational assimilation process, the error covariances of the analysis can be deduced from the Hessian of the cost function  $\mathcal{J}_{3DVAR}$  or  $\mathcal{J}_{4DVAR}$  (Bouttier and Courtier, 1999):

$$\mathbf{A}_{4DVAR}^{-1} = \mathbf{B}^{-1} + \sum_{i=0}^n (\mathbf{H}\mathbf{M}_{i,0})_{|\mathcal{X}_{4DVAR}^o}^T \mathbf{R}^{-1} (\mathbf{H}\mathbf{M}_{i,0})_{|\mathcal{X}_{4DVAR}^o}.$$

### 3.3. Twin experiment frame

To validate assimilation schemes independently of the model, one performs twin experiments. In twin experiments, the initial true state  $\mathbf{X}^t(0)$  is chosen and the true trajectory for any time is





**Fig. 6.** Relative  $L^2$ -norm errors on monodimensional xenon and iodine fields with respect to time for 3DVAR and 4DVAR schemes based on various background matrices.

known. It is a simulated state usually obtained by the model used for assimilation. Twin experiments also offer the opportunity to compare the analysis to the true state. The true state can be used to build background state, for example by adding a noise to  $\mathbf{X}^t$ . It can also be used to build synthetic observations by applying observation operator  $\mathcal{H}$  to  $\mathbf{X}^t$  and noise afterwards.

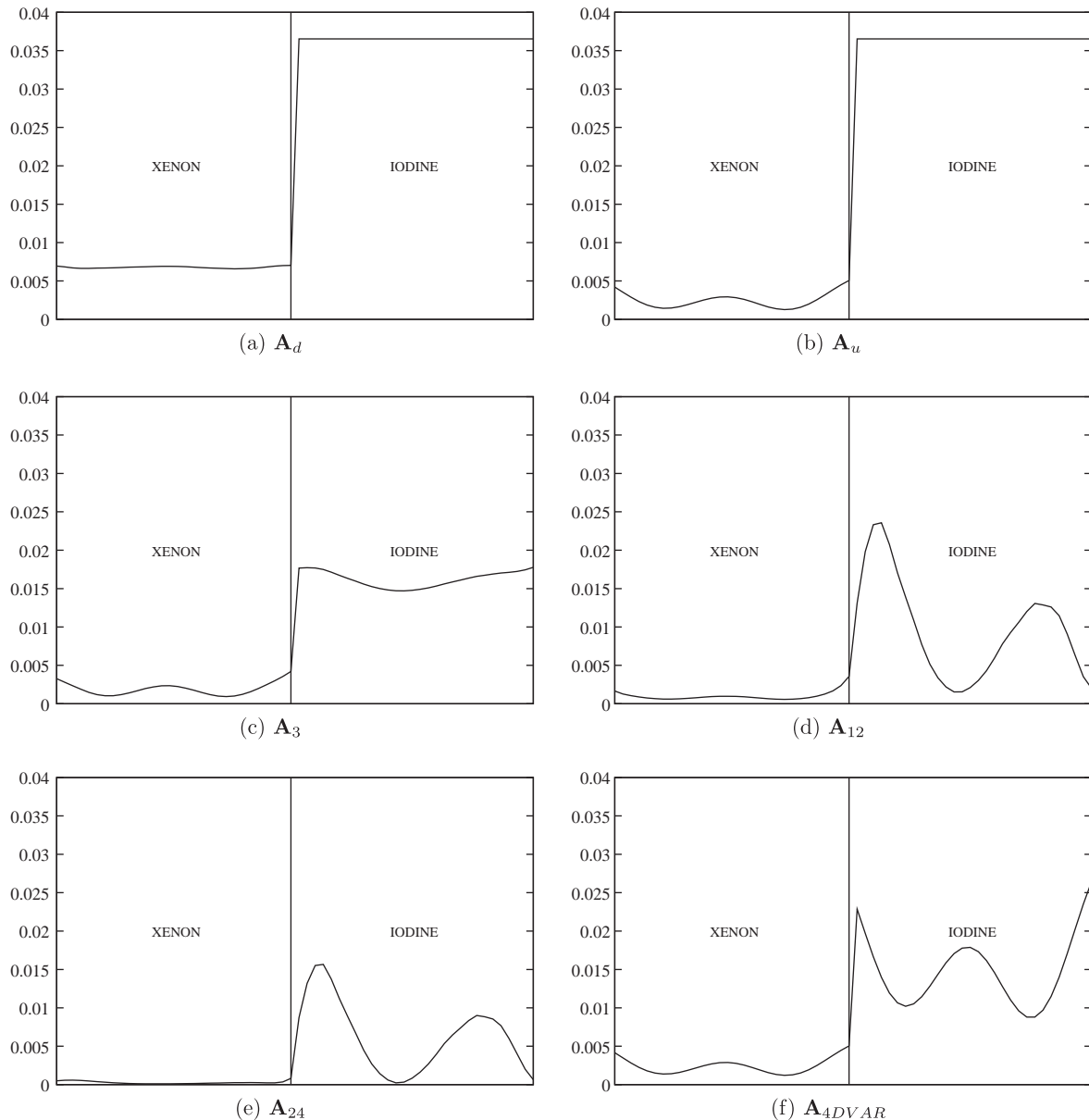
#### 4. Components of the assimilation system

We develop two variational schemes 3DVAR and 4DVAR, in order to improve the xenon and iodine concentration estimation in core, in twin experiments set-up. In this section we describe all the components of the assimilation system except the  $\mathbf{B}$  matrix modelling that will be discussed in detail in Section 5.

#### 4.1. Model

The evolution model corresponds to the xenon dynamics model implemented in CIREP1D. This model is based on the resolution of the xenon and iodine mono-dimensional time equations. Each iteration time step requires a critical boron concentration computation which includes successive stationary neutron/thermal/thermal-hydraulic computations. For such a computation, CIREP1D inputs are:

- initial and final times  $t_0$  and  $t_n$  of transient,
- initial xenon and iodine concentrations at time  $t_0$ ,
- transient data: overall power and control rod position variations over the time interval  $[t_0; t_n]$ .



**Fig. 7.** Diagonal terms of the analysis matrices  $\mathbf{A}$  for 3DVAR and 4DVAR schemes based on univariate and multivariate modelling of  $\mathbf{B}$ .

#### 4.2. State vector

The state vector  $\mathbf{X}$  corresponds to xenon and iodine axial concentrations discretised on the 30 nodes of the 1D axial spatial mesh used in CIREP1D. The dimension of  $\mathbf{X}$  is then 60. The analysis problem is to find a correction  $\delta\mathbf{X}$  such that  $\mathbf{X}^a = \mathbf{X}^b + \delta\mathbf{X}$  is as close as possible to  $\mathbf{X}^f$ . This correction is searched in the same space as the state vector. Thus, the minimisation problem has dimension 60.

#### 4.3. The observation operator $\mathcal{H}$

In the present use of data assimilation the observation operator  $\mathcal{H}$  is given by the model itself. It is nonlinear and roughly corresponds to a critical boron calculation with CIREP1D. Therefore, it depends on xenon but not on iodine as no time evolution are done in such a calculation. Since the 3DVAR scheme does not involve any evolution model, it cannot control iodine concentration. Another important characteristic of this scheme, is the quasi-

equivalence in computational cost of evaluation of the model  $\mathcal{M}$  and observation operator  $\mathcal{H}$ .

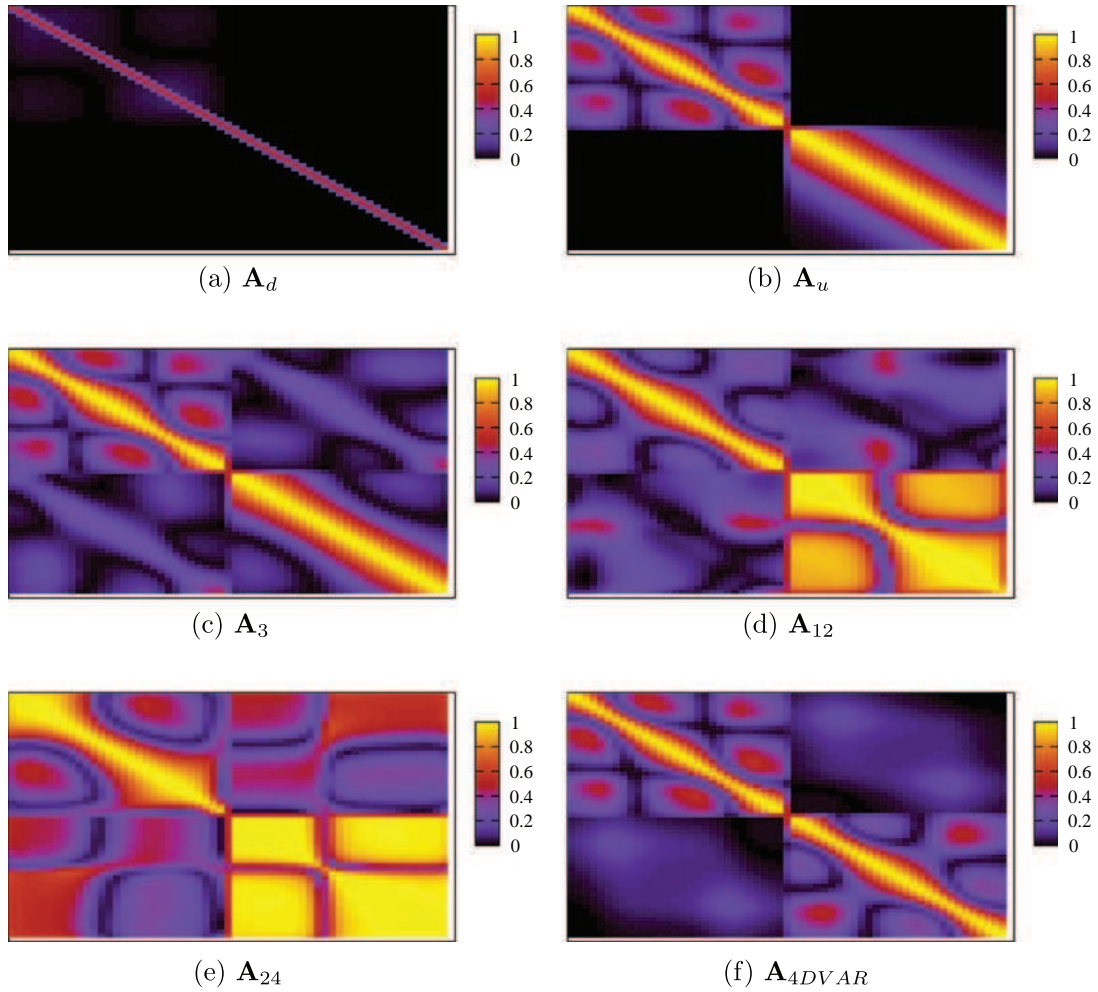
#### 4.4. Observations

In this framework, observations used further in the analysis process are not coming from real core measurements. They come from numerical simulations with CIREP1D, in a twin experiment framework as described in Section 3. The scheme is the following:

1. We compute xenon dynamics initialised by equilibrium concentrations, in a time range of one hour for example. The concentrations obtained after this hour are defined as the real state  $\mathbf{X}^f$  at the initial time  $t_0$  of the future analysis process.
2. We do a reference simulation with CIREP1D to make the real state  $\mathbf{X}^f$  evolve from  $t_0$  to  $t_n$ :

$$\mathbf{X}^f(t_i) = \mathcal{M}_{i,0}(\mathbf{X}(t_0)).$$

3. Observations over time range are obtained by introducing a measurement noise  $\epsilon$  on real data:



**Fig. 8.** Absolute values of the components of the correlations related to the matrices  $\mathbf{A}$  for 3DVAR and 4DVAR schemes based on univariate and multivariate modelling of  $\mathbf{B}$ .

$$\mathbf{Y}_i^o = \mathcal{H}(\mathbf{X}^t(t_i)) + \epsilon.$$

The observation vectors  $\mathbf{Y}_i^{obs}$  at different observation times  $t_i$  are composed of three different measurements: six integrated powers over several cells (index  $P$ ), 1 power axial offset data (index  $AO$ ) and 1 boron concentration data (index  $C_B$ ). The associated error standard deviations are denoted respectively by  $\sigma_{Rp}$ ,  $\sigma_{RAO}$  and  $\sigma_{RCb}$ . The observation vector has dimension 8.

#### 4.5. Error covariance matrices

To build the observation error covariance matrix  $\mathbf{R}$ , we assume that measurement errors are Gaussian, that they are not correlated in space, and that they do not depend on time. In this case  $R_i = R$  and  $\mathbf{R}$  is diagonal and given by:

$$\forall 0 \leq i < n_{obs}, \mathbf{R} = \begin{pmatrix} \sigma_{Rp}^2 & & & 0 \\ & \ddots & & \\ & & \sigma_{Rp}^2 & \\ 0 & & & \sigma_{RAO}^2 \\ & & & & \sigma_{RCb}^2 \end{pmatrix}. \quad (8)$$

Errors introduced in measurements are set to 10%, 5% and 1% of the current value respectively for axial power ( $\sigma_{Rp}$ ), power axial offset ( $\sigma_{RAO}$ ) and boron concentration ( $\sigma_{RCb}$ ) measurements. Those

values correspond to the typical knowledge we got on those measurements considering both their intrinsic error and the representativity error.

#### 4.6. Minimisation

Finally, to solve the nonlinear minimisation problem, we use the quasi-Newton method LBFGS (Liu and Nocedal, 1989). This method requires the computation of the gradient of  $\mathcal{J}$  which is done using the adjoint of the xenon dynamics model. In our case, the adjoint is obtained by automatic differentiation of CIREP1D using TAPENADE software (INRIA, 2004). Both  $\mathcal{J}$  and  $\nabla \mathcal{J}$  are computed in the framework of the PALM assimilation coupler (CERFACS and O-PALM, xxxx; Lagarde et al., 2001).

### 5. Background error covariance matrix modelling

The  $\mathbf{B}$  matrix is one of the most important point of the data assimilation, in particular for the 3DVAR method. For the 4DVAR method, the matrix is less crucial since the model itself contributes to spread the information. Thus in order to have a reliable comparison between both methods a careful study of  $\mathbf{B}$  is presented here.

We recall that the state vector of size 60 is composed by the values of the physical fields xenon and iodine at the 30 mesh nodes (finite differences discretisation), the mesh node numbering starting from the bottom of the core. The vector  $\epsilon^b$  of size 60 represent

the background error made on each of the 30 mesh nodes, which is assumed Gaussian. The error covariance matrix  $\mathbf{B}$  is defined by:

$$\mathbf{B} = E[(\boldsymbol{\epsilon}^b - E[\boldsymbol{\epsilon}^b])(\boldsymbol{\epsilon}^b - E[\boldsymbol{\epsilon}^b])^T].$$

We study three different types of modelling for the background covariance matrix  $\mathbf{B}$ : an elementary modelling where  $\mathbf{B}$  is diagonal, a univariate modelling where  $\mathbf{B}$  is block diagonal and at last a multivariate modelling.

### 5.1. Settings used for the modelling

In what follows, we need to set up a simulated case to use the evolution model  $\mathcal{M}$ . We are working in the twin experiment framework. The simulated case is a regular transient where the produced power is close to the nominal power and control rods are partially inserted in core. The state of the core corresponds to the end of a fuel cycle. The true and background trajectories  $\mathbf{X}^t(t)$  and  $\mathbf{X}^b(t)$  are computed with non equilibrium initial states issued from close but not identical previous calculations.

We use standard deviations  $\sigma_{Xe}$  and  $\sigma_I$  close to 3% for the initial  $\mathbf{B}$  matrix. Those values can evolve with respect to the treatment we do on this initial matrix. Those values come from comparison between CIREP1D and other models. Moreover they are in the typical range of values used in Argaud et al. (2009), Bouriquet et al. (2011) and Bouriquet et al. (2011).

### 5.2. Elementary modelling

As a first step to build the  $\mathbf{B}$  matrix, we omit correlation in space and between species consider the diagonal matrix given by:

$$\mathbf{B}_d = \begin{pmatrix} \sigma_{Xe}^2 & 0 & 0 & 0 \\ 0 & \ddots & 0 & 0 \\ 0 & 0 & \sigma_I^2 & 0 \\ 0 & 0 & 0 & \ddots \end{pmatrix}.$$

### 5.3. Univariate modelling

Before developing a multivariate modelling, we propose to take into account spatial correlations for xenon and iodine. We are looking for a block diagonal matrix:

$$\mathbf{B}_u = \begin{pmatrix} \mathbf{B}_{Xe} & 0 \\ 0 & \mathbf{B}_I \end{pmatrix},$$

where the block diagonals are given by:

$$\mathbf{B}_{Xe} = \mathbf{B}_{d,Xe} \boldsymbol{\Gamma} \mathbf{B}_{d,Xe},$$

$$\mathbf{B}_I = \mathbf{B}_{d,I} \boldsymbol{\Gamma} \mathbf{B}_{d,I}.$$

The matrices  $\mathbf{B}_{d,Xe}$  and  $\mathbf{B}_{d,I}$  correspond to the sub-matrices extracted from  $\mathbf{B}_d$ . The matrix  $\boldsymbol{\Gamma}$  is built thanks to the Balgovind correlation (Gaspari and Cohn, 1999) between two nodes of the spatial mesh  $z_i$  and  $z_j$  numbered from 1 to 30, which reads:

$$\boldsymbol{\Gamma}(z_i, z_j) = (1 + |z_i - z_j|/L) \exp(-|z_i - z_j|/L),$$

where the parameter  $L$  corresponds to the correlation scale to set up.

This modelling assures the definite positivity of  $\mathbf{B}_u$ . The choice of  $L$  has consequences in:

- the structure of  $\mathbf{B}_u$  (decay property of the matrix elements away from the main diagonal),
- the conditioning of  $\mathbf{B}_u$  (the larger  $L$  is, the worse the conditioning is),

- and the quality of the analysis.

In practice, the choice of  $L = 4$  for both species gives satisfactory results (Ponçot, 2008).

### 5.4. Multivariate modelling

We propose to build correlations thanks to the evolution model  $\mathcal{M}_{i,0}$  between times  $t_0$  and  $t_i$ . This method is very close to what is done in Kalman filter. However we do not consider each step of evolution.

If we consider a small initial perturbation  $\boldsymbol{\epsilon}$  on the state  $\mathbf{X}$  at time  $t_0$ , one can write:

$$\mathcal{M}_{i,0}(\mathbf{X}(t_0) + \boldsymbol{\epsilon}(t_0)) \approx \mathcal{M}_{i,0}(\mathbf{X}(t_0)) + \mathbf{M}_{i,0|\mathbf{X}} \cdot \boldsymbol{\epsilon}(t_0),$$

where  $\mathbf{M}_{i,0|\mathbf{X}}$  represents the tangent linear of  $\mathcal{M}_{i,0}$  with respect to the vector  $\mathbf{X}$ . Then, if we set  $\boldsymbol{\epsilon}(t_i) = \mathcal{M}_{i,0}(\mathbf{X}(t_0) + \boldsymbol{\epsilon}(t_0)) - \mathcal{M}_{i,0}(\mathbf{X}(t_0))$ , the last relation can be expressed in terms of the error as follows:

$$\boldsymbol{\epsilon}(t_i) \approx \mathbf{M}_{i,0|\mathbf{X}} \cdot \boldsymbol{\epsilon}(t_0).$$

Then we get an approximation of the covariance matrix at  $t_i$  as a function of the covariance matrix at  $t_0$ :

$$\text{cov}(\boldsymbol{\epsilon}(t_i), \boldsymbol{\epsilon}(t_i)) \approx \mathbf{M}_{i,0|\mathbf{X}} \text{cov}(\boldsymbol{\epsilon}(t_0), \boldsymbol{\epsilon}(t_0)) \mathbf{M}_{i,0|\mathbf{X}}^T. \quad (9)$$

It is noted that it can be difficult to get the tangent linear operator  $\mathbf{M}$  for an industrial code, since it usually requires to be written at the same time as the direct code. Thanks to Eq. (9) we can model correlations between xenon and iodine by multiplying an univariate matrix  $\mathbf{B}_u$  by  $\mathbf{M}_{i,0|\mathbf{X}}$  and  $\mathbf{M}_{i,0|\mathbf{X}}^T$ :

$$\mathbf{B}_i = \mathbf{M}_{i,0|\mathbf{X}} \mathbf{B}_u \mathbf{M}_{i,0|\mathbf{X}}^T.$$

In what follows, we compare the univariate matrices  $\mathbf{B}_d$ ,  $\mathbf{B}_u$  to the multivariate matrices  $\mathbf{B}_3$ ,  $\mathbf{B}_{12}$  and  $\mathbf{B}_{24}$ .

### 5.5. Overview of the estimated covariance matrices

Fig. 2 shows the diagonals of the various  $\mathbf{B}$  matrices. These diagonals correspond to the error variance of the background state vector for each node of the spatial mesh ( $x$ -axis in the Fig. 2). We may notice:

- In the diagonal and univariate modellings (Fig. 2a and b), the variance is the same for all the spatial discretisation points, though it is known that the lower and upper regions of the core are quite inaccurately modelled. The iodine error variance is larger than the xenon one but it is due to the fact that iodine concentration in core is bigger than the xenon concentration. In terms of relative errors, they are similar.
- For multivariate modellings (Fig. 2c–e), 3 regions can be seen (easier to see for the iodine part than for the xenon part): two large regions for half lower and upper parts of the core and a small one for the central part of the core. The variances are lower for the median part than for the two others (also easier to see for the iodine than for the xenon)
- The variances are lower in the multivariate modelling than in the univariate modelling, that is to say  $\text{tr}(\mathbf{B}_{\text{multi}}) < \text{tr}(\mathbf{B}_u)$ . But the multivariate modelling takes into account correlations between species: thus error statistics are spread all around the elements of the covariance matrix.

To get an idea of the diffusion of the xenon error to the iodine error in the multivariate modelling, Fig. 3 gives the absolute values (for the clarity of the figure) of the correlations with respect to the nodes of the spatial mesh, where the correlations are defined as

$$\text{corr}(i,j) = \mathbf{B}(i,j) / \sqrt{\mathbf{B}(i,i)\mathbf{B}(j,j)},$$

where the element  $(i, i)$  of the matrix  $\mathbf{B}$  corresponds to the variance of the background error on xenon at the node number  $i$  (resp. iodine at the node number  $i - 30$ ) if  $i < 30$  (resp.  $i > 31$ ) and the element  $(i, j)$  (or  $(j, i)$  since  $\mathbf{B}$  is symmetric) corresponds to the covariance of the background error between xenon and iodine at the node  $i$ . Then the range of the scale varies from 0 to 1.

We may notice:

- Compared to the univariate modellings for which extra block diagonal terms are obviously null, introduction of spatial correlations fills in the two diagonal blocks in Fig. 3b. The choice of the correlation scale will be discussed later.
- In the multivariate modellings (Fig. 3c–e), the correlation matrices present an internal structure more or less pronounced with respect to the use of an evolution model on a more or less long time range. As for the variances, one can see two large regions for the half upper and lower parts of the core and a narrower region for the central part of the core.
  - Diagonal blocks: they correspond to the spatial correlations for a given species. Spatial correlations increase with the length of the time range used in the evolution model, first for the iodine correlations (e.g.  $\mathcal{M}_{12}$ ) and then for the xenon ones. This can be explained by the way of production of xenon which is produced by radioactive decay of the iodine. For the matrix  $\mathbf{B}_{24}$ , correlations between upper and lower regions of the core are almost as strong as the spatial correlations inside these regions.
  - Extra-diagonal blocks: they correspond to the correlations between the xenon and the iodine. The same correlation increase is noticed with the length of the time range used in the evolution model. But these correlations stay below the spatial correlation level inside the same species.
  - Central blocks: a region including very few nodes of the middle of the core seems to be insensitive to the time range used in the evolution model: the background error for these nodes is slightly correlated to the background error of the other nodes. At last, one can notice that the correlation scale for these nodes seems to be shorter to the scale  $L = 4$  set up in the correlation scale modelling described in Section 5.3.

## 6. Comparison between 4DVAR and 3DVAR schemes

We are in the twin experiment framework: the true state  $\mathbf{X}^t$  is a simulated state. The simulated case was briefly described in the previous section. We always assume that background and measurement errors are Gaussian. Errors introduced in measurements are set to 10%, 5% and 1% respectively for axial power, power axial offset and boron concentration measurements.

The purpose is to compare the result of the 3DVAR and 4DVAR schemes at the assimilation time but also after at a forecast of 10 h (typical time for xenon oscillation). In the case of the 3DVAR assimilation, various modelling of the  $\mathbf{B}$  matrix will be under consideration. The 3DVAR results are compared to a 4DVAR result whose characteristics are set up according to Ponçot et al. (2009): the window size is set to 6 h and the observation frequency is set to 2 h (then 3 observation sets are used).

The various  $\mathbf{B}$  matrices used for the 3DVAR schemes are the following:

- $\mathbf{B}_d$  corresponds to the univariate modelling of  $\mathbf{B}$  without any spatial correlation;
- $\mathbf{B}_u$  corresponds to the univariate modelling with spatial correlation;

- $\mathbf{B}_i$  corresponds to the multivariate modelling where the time range used in the evolution model equals to  $i$  hours (here 3, 12 or 24 h).

Results are organised as follows: firstly we are analysing the 4DVAR results. Secondly we are comparing 1D errors on axial shape of xenon, iodine and power. Then we show the time evolution of the mean error. At last we discuss the statistics of the analysis given by the analysis matrices.

### 6.1. 4DVAR results

First we will look at the results of the 4DVAR scheme that is known to be the most efficient for forecasting. With this scheme, the modelling of xenon/iodine correlation for  $\mathbf{B}$  has a weaker influence on the quality of the analysis and then we use the  $\mathbf{B}_u$  matrix. Fig. 4 shows relative errors<sup>1</sup> on xenon, iodine at the assimilation time  $t_0$  and on power at  $t_0$  and  $t_0 + 10h$  for two computations: the background computation which gives the background state and a 4DVAR computation with the assimilation characteristics given before.

On this Fig. 4, one can see that the 4DVAR computation allows to reduce errors on xenon and iodine axial shape at least by a factor of 2. For the axial power shape the decrease is even more important since the errors are reduced by a factor of 4. What follows aims at showing that it is possible to approach the 4DVAR results quality with 3DVAR schemes using multivariate  $\mathbf{B}$  matrices.

### 6.2. Comparison between 4DVAR and 3DVAR

Fig. 5 gives the 1D relative errors respect to the true state on axial shape of xenon, iodine and power for the different assimilation schemes. We see that the 4DVAR results are better than the 3DVAR ones independently of the choice of  $\mathbf{B}$ . However, looking at 3DVAR results at analysis time, we notice that xenon is rather well estimated in all variational schemes except for the scheme which uses the elementary modelling of  $\mathbf{B}$ . The xenon estimation is not as good for the bottom half as for the top half, but it is everywhere better than the state given by the background computation. This good result can be explained by the fact that the xenon level at the assimilation time is directly related to the assimilated observations, that is to say to the integrated powers.

On the opposite, iodine is not directly related to the power level but through the production of xenon since xenon is essentially produced by the radioactive decay of the iodine. Thus the observation operator  $\mathcal{H}$  does not depend on iodine. Therefore it is not possible to correct iodine state with a 3DVAR scheme unless correlations between xenon and iodine are introduced in  $\mathbf{B}$ . As a consequence the 3DVAR analysis error is equal to the background one for the computation with the matrices  $\mathbf{B}_d$  and  $\mathbf{B}_i$ . With a multivariate modelling of  $\mathbf{B}$  it can be seen that the time range used to build the extra-species correlations influences the quality of the iodine analysis. It seems that the longer the time range is, the better the analysis is. In fact there is no convergence towards the 4DVAR analysis quality, and taking a 48 h time range does not allow to improve 3DVAR results. One can assume that the optimal time range is related to the time constants of radioactivity decay of the xenon and iodine.

The knowledge of the iodine level is not important for the monitoring operator system. We are expecting to improve axial power forecasts with the assimilation techniques. If we take a look at the power estimation after 10 h, we notice that background and diag-

<sup>1</sup> The “true” value of the fields xenon, iodine and power is known since we are working in the framework of twin experiments.

onal and univariate 3DVAR analysis axial power shapes are very close. Since xenon is essentially produced by radioactive decay of iodine, a bad estimation of the initial iodine concentration will affect the xenon concentration estimation later. As expected the multivariate modelling leads to a significant improvement in the 3DVAR forecast (up to a factor of 2 to 3 on the errors for the use of the matrices  $\mathbf{B}_{12}$  and  $\mathbf{B}_{24}$ ). The multivariate modelling resulting from the use of a time range of 3 h in the evolution model does not seem to be sufficient to really improve power forecasts. As a first conclusion, the optimal time range seems to be around 12 h: the 24 h time range does not improve much the forecasts compared to the 12 h time range but it increases the amount of computation for  $\mathbf{B}$ .

### 6.3. Time evolution of the $L^2$ -norm error

We would like to confirm what has been shown at the assimilation time  $t_0$  and  $t_0 + 10h$ . Fig. 6 presents the time evolution of the  $L^2$ -norm error of the three studied fields for the different matrices  $\mathbf{B}$  used. An oscillation which tends to damp can be seen. But it does not change the previous conclusion. Two groups can be seen: the first one composed by the analysis computed by the 3DVAR schemes using the matrices  $\mathbf{B}_d$ ,  $\mathbf{B}_u$ ,  $\mathbf{B}_3$ ; the second one composed by the analysis computed by the 3DVAR schemes using the multivariate matrices  $\mathbf{B}_{12}$ ,  $\mathbf{B}_{24}$  plus the analysis computed by the 4DVAR scheme based on the matrix  $\mathbf{B}_u$ . As one can see on the Fig. 6, the latter still represents a "reference" towards one can expect to tend with a 3DVAR scheme based on a multivariate modelling. And the 3DVAR schemes where no or very few correlation between xenon and iodine is modelled are unable to give good forecasts. We can deduce that the 3DVAR assimilation results depending a lot on the  $\mathbf{B}$  involved.

### 6.4. Analysis matrices

Assimilation techniques offer a *a posteriori* diagnostic on the computed analysis by the mean of the analysis matrix. We use this opportunity to go more deeply into the study of the respective quality of the various approaches.

Figs. 7 and 8 are to be compared to Figs. 2 and 3 that show the structure and amplitude of the elements of the background matrix  $\mathbf{B}$ . Fig. 7a and b show that the 3DVAR schemes based on univariate process is not able to reduce the variance (represented by the diagonal of  $\mathbf{A}$ ) of the iodine error. Though the scheme based on the multivariate matrix  $\mathbf{A}_3$  has been proved not being good for forecast, Fig. 7c shows that it is much better than the previous ones since it allows to reduce by a factor of 2 the error on iodine.

Fig. 8 gives absolute values of the correlations with respect to the nodes of the spatial meshes. It is to be noted that if the matrix  $\mathbf{B}$  does not contain correlations between the xenon and iodine errors (extra diagonal blocks), the analysis matrix  $\mathbf{A}$  issued from a 3DVAR scheme does not contain any correlation between them neither. The 4DVAR scheme is based on the univariate  $\mathbf{B}_u$  but the corresponding analysis matrix  $\mathbf{A}_{4DVAR}$  shows correlations between xenon and iodine. These latter are brought by the 4DVAR scheme through the use of the evolution model on a 6 h time range but they are shorter than the ones in the matrices  $\mathbf{A}_3$ ,  $\mathbf{A}_{12}$  and  $\mathbf{A}_{24}$ .

Fig. 8 also presents the spatial correlations intra species (diagonal blocks). It can be compared to the spatial correlations shown in Fig. 3. It can be seen that spatial correlations after the assimilation process are a little bit shorter than they were in the matrix  $\mathbf{B}$ .

## 7. Conclusions

In this paper, we have shown how variational data assimilation methods can be used to improve the accuracy of the prediction of

the xenon concentration in PWRs. A monodimensional xenon dynamics code CIREPID was developed for this purpose.

The investigation done here in twin experiments proves that the 4DVAR scheme is a very efficient method to improve the accuracy of the prediction of the xenon concentration as well as the axial power shape in PWRs. However this method is computationally costly and the development of the adjoint of the model is mandatory.

A computationally cheaper solution is the 3DVAR that can lead to rather good result. Nevertheless these latter can only be obtained through a careful modelling on the associated background error covariance matrix  $\mathbf{B}$ . Among the various modellings of  $\mathbf{B}$  studied here the one based on the multivariate modelling is the most satisfactory.

The next stage for the 3DVAR approach could consist in setting up an assimilation chain where the  $\mathbf{B}$  matrix is updated at each analysis step as it is successfully done for meteorological operational forecasts.

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