

Technical Workscope Identifier: FC-5.1b

Time Frame: 3 years

Estimated Cost: \$800,000

1 Introduction & Proposed Scope

Nuclear fuel cycle simulation tools can have a large scope of application, from the study of the behavior of a particular type of fuel or reactor inside an existing nuclear fleet to the prospective analysis of a complete nuclear transition. Each use case requires a specific level of confidence, which are up to now very poorly assessed, if assessed at all. Indeed, the only existing way to develop confidence in any fuel cycle calculation/tool, is to compare with other similar tools or historical data. For the former, the conclusion is often a list of why the different software gave different results with no conclusion on the precision of any. The latter only allows validation of existing concepts and has no impact on calculations based on the use of new concepts.

The aim of this project is to add error propagation capability to the CYCLUS fuel cycle simulator [1]. Given the use case of predicting the evolution of a large industrial enterprise in an uncertain future, nuclear fuel cycle simulations are generally based on approximate models and uncertain input data. Since strict validation is largely considered to be impractical, such simulations are seen as indications of trends in future behavior rather than predictions of that behavior. Nevertheless, it would be valuable to be able to place some confidence bounds on those indications, both to assess the robustness of conclusions that derive from those indications and to provide information about the sensitivity of those conclusions to the uncertain data and algorithms. Having a broad distribution for each metric calculated in a fuel cycle simulation instead of unique values will allow a better comparison between different fuel cycle scenarios. Moreover for some critical use cases, it could be extremely valuable to add some degree of confidence on the results of the simulation. This could result in confidence in the use of the tool for such uses, and confidence in the conclusions that follow from those results.

This project will extend the Cyclus concept of resources to include error information and then develop a number of archetypes that can perform operations to propagate that error in a rigorous fashion. **PPHW: Can we guarantee “rigor”?** The ultimate calculation of fuel cycle performance metrics will also need to be updated in order to represent final results as distributions rather than single values.

2 Logical Path to Work Accomplishment

The goal of this project is to add optional extensions to Cyclus that will allow an assessment of the error as it propagates through a fuel cycle.

2.1 Add uncertainty to ressources

The first step of this work, is to update the principal tracked quantity in CYCLUS, the material and associate the isotopic composition, with the concept of uncertainty. **PPHW: I don't know what this next sentence means?** Because for this is the first introduction of uncertainty in CYCLUS (or fuel cycle calculation tool in general), we will consider the uncertainty on the material independent of any previous operation on this materials.

In general, we need to have more to say here.

How will we represent uncertainty in a composition?

We should probably have a specific idea for how to do this

To consider: the composition vector in Cyclus represents a relative composition. Therefore the uncertainty in any single nuclide must be related to the uncertainty in any other nuclide.

Also more on: how this representation will be transparent to archetypes that don't implement error propagation Can we make a representation that will still be correct!?! Perhaps, if we only allow devs to use the available methods to operate on material objects.

2.2 Archetype uncertainty management

When considering a material that is leaving any given facility, there are three different sources of uncertainty or error:

- the uncertainty in the isotopic composition vector of the input material, $\delta\vec{N}_{in}$,
- the uncertainty of parameters that define that facility, τ_p , which correspond to the possible variation, or engineering tolerance, in any physics parameter, i ,
- the modeling error, ϵ_{mod} , introduced by the choice of approximate archetypes models.

The uncertainty of the output material composition is a function of all those uncertainties:

$$\delta\vec{N}_{out} = \mathcal{F}\{ \delta\vec{N}_{in}, \tau_0, \dots, \tau_P, \epsilon_{mod} \}. \quad (1)$$

In this work we propose to introduce archetypes that are able to combine all those sources and compute the resulting uncertainties on the output materials. The following sections indicate which specific archetypes will be considered with some indication of the uncertain paramters that define those archetypes. In some cases, these archetypes are modifications of those that are already part of the Cycamore set of base archetypes. In other cases, entirely new models will be introduced to enable more advanced uncertainty propagation.

2.2.1 Cycamore enrichment facility

The existing Cycamore enrichment facility produces enriched uranium on demand, matching the enrichment of each request, k . Standard models for enrichment flow rates and separative

work requirements are used only to determine the total throughput of the facility in any time step as a function of the:

- inventory, F_{tot} , and composition, x_f , of feed material,
- assay of the tails stream, x_w , and
- total separative work, S_{tot} .

$$F_k = \frac{x_k - x_w}{x_f - x_w} P_k \quad W_k = \frac{x_k - x_f}{x_f - x_w} P_k$$

$$S_k = P_k (2x_k - 1) \ln \frac{x_k}{1 - x_k} + W_k (2x_w - 1) \ln \frac{x_w}{1 - x_w} - F_k (2x_f - 1) \ln \frac{x_f}{1 - x_f}$$

$$\sum_k F_k \leq F_{tot} \quad \sum_k S_k \leq S_{tot}$$

With this model, the uncertainty in the product material is not determined by the inputs or the model itself. Instead, the uncertainty in product enrichment can be introduced with a user-defined tolerance parameter. Conversely, uncertainty in the product enrichment can lead to uncertainty in the amount of feed that is consumed by any request and uncertainty in the amount of separative work capacity that is consumed in order to fulfill each request. A user-specified tolerance on the tails assay can also be introduced to contribute to these uncertainties.

Based on the uncertainty in the product enrichment (and possibly the tails enrichment), it would be possible to determine the uncertainty on the amount of feed material that is consumed by any given request and on the amount of separative work used by any given request.

$$\left(\frac{\delta F_k}{F_k} \right)^2 = \left(\frac{\delta x_k}{x_k} \right)^2 + \left(\frac{\delta x_w}{x_w} \right)^2 \text{????}$$

$$\delta S_k = \dots$$

2.2.2 Other Enrichment Facility??

PPHW: Do we want one of these? Possibly parametrized by something in the way the cascade operates or a single centrifuge?

2.2.3 Cyamore separation facility

The Cycamore separations facility uses a simple separation matrix approach to distribute every nuclide, i , in the input material across K different streams in the output.

$$N_{i,k} = N_{i,in} \cdot e_{i,k} \quad (2)$$

The only parameter which can introduce extra variance is the separation parameter for nuclide i in output stream k , $e_{i,k} \pm \delta e_{i,k}$.

Assuming that the uncertainty of the input material and the tolerance of the separation parameters are independent, the resulting uncertainty on the output material composition can express as :

$$\left(\frac{\delta N_i}{N_j} \right)_k^2 = \left(\frac{\delta N_i}{N_i} \right)_{in}^2 + \left(\frac{\delta e_i}{e_i} \right)_k^2 \quad (3)$$

PPHW: We do need to continue to discuss the interdependence of these uncertainties between different isotopes in the same composition.

2.2.4 Cycamore reactor facility

The reactor archetype included in Cycamore is based on fixed recipes for input and output materials that are provided by the user, in addition of all the classical reactor parameter (batch number, cycle length, power, capacity factor,...). Such a model does not allow any meaningful way to propagate uncertainty from any input quantities into the output composition. Instead, the user will need to provide estimates of the sensitivity of the output recipe to variations in the input recipe. In general, each output isotope will be sensitive to the uncertainty in every input isotope, although in practice some of these can be ignored.

$$\left(\frac{\delta N_j}{N_j} \right)^2 = \sum_i \left(\frac{\delta N_i}{N_i} \right)^2 \sigma_{i,j} \quad (4)$$

Variation consideration on those parameters will affect the discharge time, which should be very difficult to include in the uncertainty calculation. Nevertheless, a brute force study (also sometimes called "Total Monte Carlo method") could allow the determine their impact, running many time the same simulation choosing randomly the parameter value at each cycle of the reactor, the distribution of the results will provides a precise measurement of the sensivity.

We are envisaging two kind of the reactor, which will be both capable to handle uncertainty. The first one will be built as an upgrade of the existing CYCAMORE reactor, making it error aware.

2.2.5 CLASS-based reactor facility

The second version of reactor will be able to calculate the evolution of the fuel provided by the fuel fabrication (see §??). To do so, we propose investigating two ways, both using pre-trained models, allowing the prediction of key physics parameters needed to compute the evolution of a fuel during the irradiation. It has been proven that from pre-trained

neural network models, one can predict the evolution of the one group cross section during the irradiation of the fuel from its initial isotopic composition, and is working for a various range of reactor, from LWR to SFR [?, ?].

The first application using the neural network predictive models, is to train a model to directly predict the composition evolution as the function of the burnup. This application might not work, since the usage of neural network has been proven to predict one group macroscopic cross section.

If the neural network model fail to directly predict precisely the isotopic composition evolution, one have to consider the second option, which imply to predict the 1 group cross section, then integrate the Bateman equation.

The main reason leading the try of direct prediction of the isotopic evolution, is the error/uncertainty propagation. As express previously :

$$\delta \vec{N}_{out} = \mathcal{F}\{ \delta \vec{N}_{in}, \tau_0, \dots, \tau_n, \epsilon_{mod} \} \quad (5)$$

The determination and the propagation of all uncertainty source is, for this kind of reactor, a complicated matter. The error due to the computation of the depletion calculation are wild:

- the error of the neural network predictor, ϵ_i^{nn} , with $i \in [0..N]$, N the number of predicted parameter,
- the convolution of the uncertainty on the material composition with the neural network prediction.
- the calculation error on the data sets used to train the neural network, $\epsilon_{T.D.}$.

And then can be expressed as :

$$\epsilon_{mod} = \mathcal{G}\{ \delta \vec{N}_{in}, \epsilon_0^{nn}, \dots, \epsilon_n^{nn}, \epsilon_{T.D.} \} \quad (6)$$

Because, the predictive model are trained on sample populated using few thousand of depletion calculation, which are subject to computation error, $\epsilon_{T.D.}$. On one side, a depletion calculation take as input, the nuclear data. Those nuclear data are interpolated/extrapolated from many different experimental measurement using many different models. Therefore the nuclear data contain uncertainty... Those uncertainty are extremely difficult to propagate properly through a full depletion calculation because of the coupling between neutron transport and depletion calculation: the composition of the fuel impact the shape of the neutron spectrum, which impact the reaction rate on the nuclei... On the other side, the depletion calculation require different approximation to be completed. There is nearly impossible using Monte Carlo technique on a PWR full core calculation due to source convergence issue. It is also extremely complicate to follow precisely the different reactor parameter, such as boron concentration, rod control management, charge factor evolution, neutron leakage...

The study and the propagation of the modeling uncertainty, such as the modeling simplification and the nuclear data uncertainty is way beyond the scope of this project...

This require a full dedicated research project (and probably more). Therefore, those error, $\epsilon_{T.D.}$, will not be considered on the first version of this work. This might need to be reconsidered when the depletion calculation error propagation capacity will have done important progress.

The direct error induced by the use of predictive model, ϵ_i^{nn} on each parameter, i , need to be assessed. This could be performed with a mapping the error on the isotopic space populated with the training sample. This will allow to determine the error of the model on each point on the isotopic space populated. We might use then a other neural network, or other interpolation method to predict the error of the prediction as the function of the isotopic composition.

Once we have a working predictive model and a map of the error on the prediction, one need to build the covariance matrix which will allow to convolute the uncertainty on the input material, δN_{in} , with the prediction of the model.

If the direct prediction of the composition is not precise enough, one have to use solve Bateman equation using predicted one group cross section and then compute the error coming from a numerical resolution of the Bateman equation and propagate the error of the one group cross section. The Bateman equation resolution will be a step by step process. After having discretize the irradiation time (or burnup), one will use the model to predict the cross section at each time step (closer the time step are preciser the calculation will be) and then solve numerically the Bateman equation step after step, ending with the final isotopic composition of the fuel. Because the predictive model will be able to predict the one cross section as the function of time (or burnup), one should be able to propagate those error using sensitivity analysis. The time discretization as well as the other approximation require to solve the Bateman equation will also introduce computation error that need to be determined and added to the final uncertainty. This could be made with the comparison of depletion calculation made with those extra approximation with the reference one performed using the same modeling approximation as the training depletion all along the isotopic space.

2.2.6 Fabrication

The aim of the fuel fabrication is to mix different incoming material streams in order to build a fuel which validate the neutronics/physics requirement of the reactor. Depending of the reactor, the criterium could be various. We are considering in the first time including fabrication model for MOX fuel only, in LWR and SFR, used as burner and breeder for SFR. One will use algorithm building fuel allowing to build fuel reaching the targeted burnup according to either criticality criterium either conversion ratio criterium. Those algorithm will relies on the capabilities of some predictive model to predict the maximal achievable burnup depending on the the criticality or conversion ratio evolution according to burnup. The predictive model as the reactor model, will be based on the use of neural network formerly

trained on the same set of training depletion calculation used for the reactor models. The capability of the neural network have been proven to predict the evolution of the criticality in PWR reactor using MOX fuel [?, ?], as well as the the initial criticality of MOX fuel in SFR [?] and should be possible to extend it to conversion ratio evolution.

The error/uncertainty propagation for fuel fabrication should be pretty similar than for reactor. Indeed the uncertainty can be expressed as :

$$\delta \vec{N}_{out} = \mathcal{H}\{ \delta \vec{N}_{in}, \epsilon_{mod} \}. \quad (7)$$

In this case there is no tolerance, since the parameter are goal to achieve, not physicals characteristics. As well as previously the error of the model can be expressed as :

$$\epsilon_{mod} = \mathcal{K}\{ \delta \vec{N}_{in}, \epsilon_0^{nn}, \dots, \epsilon_n^{nn}, \epsilon_{T.D.} \}, \quad (8)$$

where ϵ_i^{nn} represent the error on the prediction of the parameter i by the neural network predictive model and $\epsilon_{T.D.}$ the error due to the error on the depletion calculation composing the training set, which will not be considered since we dont have any way to correctly estimate it.

As for the reactor model, the ϵ_i^{nn} component of the error can be determined through a mapping of the error along the isotopic space, and the impact of the material input uncertainty needed the be assessed by the calculation of the covariance matrix which need to be build.

2.3 Problems/Applications/Validations

During the realization of this work we would like to validate each step of the uncertainty propagation process. First, with a mid/early-term validation, after the enrichment facilities, the separation and the recipes reactor will be implemented, it will be possible to confirm the uncertainty is correctly propagated, using a brute force validation (with the "Total Monte Carlo" method). This validation will be continued with new archetypes will be implemented in CYCLUS...

An other gaol we want to achieve, is an sensitivity analysis, allowing to determine the impact of the different uncertainty/error/tolerance on the final calculation uncertainty. This should allow to define precisely where the future effort should be focus to reduce those uncertainty sources accordingly to the object of the calculation and also to validate (or un-validate) the use of fuel cycle simulation tool for some specialized study (such as non-proliferation study...) With all the necessary components in place, a series of demonstration simulations will be conducted using fuel cycles of increasing complexity: once through, MOX LWR recycle, and fast reactor recycle. These scenarios will be constructed to highlight the role of error and uncertainty and identify metrics in which the presence uncertainty may impact fuel cycle analysis conclusions.

3 Relevance of Proposed Research

This proposal aims to provide an important feature needed in the fuel cycle simulator. Given the appropriate estimation of the error relative to any fuel cycle simulation, the simulator would be able to make decisions about fuel cycle transition like fuel reprocessing, or the launching of new technologies or types of reactors. Furthermore, the project will be one of the first of its kind to introducing error propagation in fuel cycle calculation, increasing the utility of the Cyclus kernel. Since the precision of fuel cycle tool have never been assessed, this work might the first step providing more confidence in the fuel cycle calculation. And even if this wok will be applied to the fuel cycle simulation tool CYCLUS, the concept should be a theoretically applicable on any agent based fuel cycle simulation tool.

Additionally, new archetypes will be contributed to the Cyclus ecosystem, including not only error propagation but also different fuel fabrication methods, cross-section prediction models and a Bateman equation solver. These features will permit future comparison between the different fuel fabrication models and improve the user experience and confidence in the interpretations of Cyclus simulations.

4 Milestone Task Listing

This research project consist in four major tasks that could be conducted in parallel. The first one will be very short (< 6 month), dedicated to update CYCLUS and allow it to handle uncertainty. The second one should be the longer task (12 - 24 months) where the models will be developed. The predictive model development can/should/will be started at the start of the project. The third will be started after the end of the TASK 1 and corresponds to CYCLUS archetypes update and included in a separated package. The development of some archetypes will depends on the progress on the TASK2. The last task is the validation and application one and will be started with the completion of the different TASK3-subtasks. The ideal progression is represented on the figure ??.

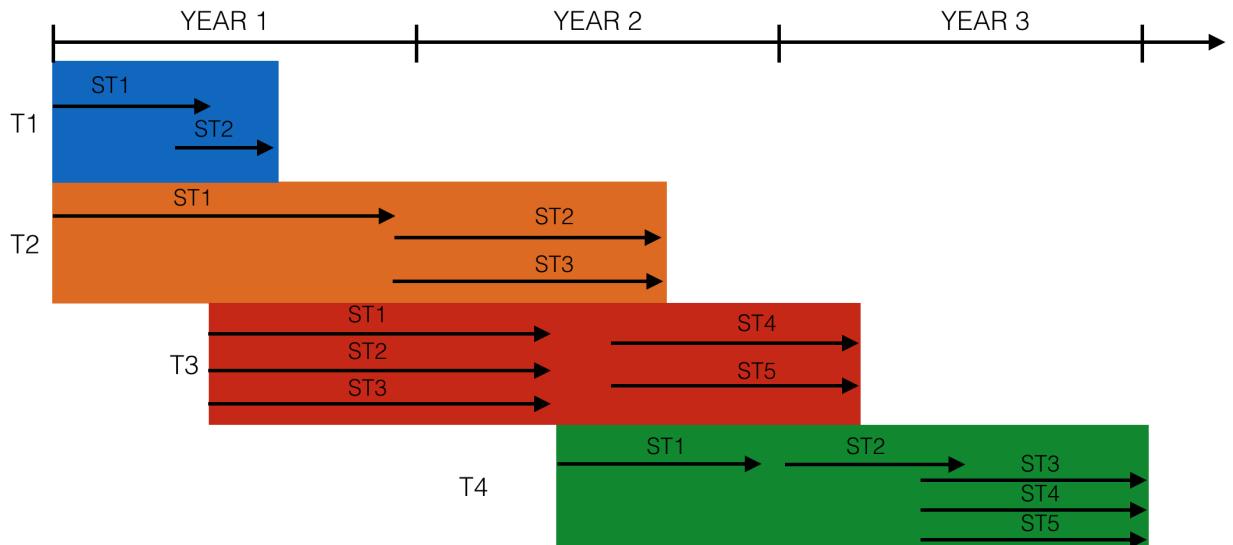


Figure 1: Preliminary schedule of the project, with the different Task (T#) (1 in blue, 2 orange, 3 red, 4 green) and the corresponding subtask (SB#).

TASK 1: CYCLUS update for uncertainty awareness

- subtask 1: update material to uncertainty,
- subtask 2: validate the backward compatibility,
- subtask 3: Add a default uncertainty behavior when using both uncertainty aware archetypes and standard one in the same time ?

TASK 2: Updating the CYCLUS Archetypes to uncertainty management

- subtask 1: enrichment facility,
- subtask 2: separation facility,

- subtask 3: recipe reactor,
- subtask 4: reactor archetypes, depletion calculation/prediction, uncertainty propagation,
- subtask 5: fuel fab archetypes, mixing calculation/prediction, uncertainty propagation.

TASK 3: Modeling development

- subtask 1: isotopic space definition, training sample realization
- subtask 2: reactor models development: parameter prediction, error analysis
- subtask 3: fuel fabrication model development: parameter prediction, error analysis

TASK 4: Validation & application

- subtask 1: validation of the overall process with simple calculation : enrichment + separation + recipe reactor
- subtask 2: validation of modeling capabilities (Fab + reactor)
- subtask 3: exemple calculation: PWR, transition from PWR to FBR
- subtask 4: full sensitivity analysis
- subtask 5: time dependent parameters sensitivity analysis (discharge burnup, capacity factor...)
- subtask X: comparison with other physic modeling capabilities such as Bright-Lite ?