

## **A Predictive Fuel Cycle Modelling Capability for Safeguards and Non-Proliferation**

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### **Abstract**

A good understanding of the flow of nuclear material through a fuel cycle is a vital aspect of non-proliferation activities. For both the design of new reactors and monitoring of extant fuel cycles, modelling and tracking the flow of material throughout all phases of a fuel cycle may make it possible to highlight possible diversion risks and predict trends in the material volumes and compositions.

ORION is a fuel cycle modelling code developed by the UK's National Nuclear Laboratory for over 20 years. ORION tracks the flow of around 2,500 nuclides throughout the fuel cycle through user-defined enrichment facilities, fabrication processes, reactors, storage facilities and reprocessing techniques.

In modelling reprocessing operations, ORION can model any co-extraction or single-element extraction process. In addition, ORION is capable of calculating the effective fissile mass of fuel required for a reactor to achieve a set cycle length, therefore, enabling prediction of the drawdown rate of stockpiled fissile material utilised in a closed fuel cycle. Minor actinide recycling can be assessed in addition to the total impact for a closed vs open fuel cycle in terms of effective fissile mass, heat generation and radiotoxicity of spent fuel.

The capabilities of ORION are discussed along with examples demonstrating how ORION could be used to model a country or region's fuel cycle providing a predictive tool for modelling and tracking the flow of material in each phase of the cycle - information which can be used to inform safeguards assessments, thereby aiding the peaceful use of nuclear material.

### **Introduction to ORION**

ORION [1] is a fuel cycle simulation code developed by the UK's National Nuclear Laboratory (NNL) over the last 20 years. The code can be used on multiple platforms including Windows, Linux and MacOS. ORION features a graphical user interface (GUI) design where the user places ORION 'objects' representing fuel cycle facilities of various type onto a canvas. A simple pictorial representation of each ORION object type along with visual connections between objects - representing the permitted routes of material flow from one object to another, aids in users' visualization of the fuel cycle. ORION is able to simulate a whole range of nuclear related facilities including storage facilities, fuel fabrication and enrichment plants, reprocessing facilities, waste conditioning plants and reactors.

To correctly represent isotopic composition of material discharged from reactors, ORION relies on either a 1-group point-reactor calculation routine (known as 'MPR') which uses burn-up dependent cross-section data; or fuel inventory calculations specific to the combined reactor design and fuel type being represented in the fuel cycle model. These data are required to be generated beforehand using a neutronics analysis tool or fuel inventory calculation tool. Typically, the MPR method is used with ORION when modelling reactors as this allows the fuel

inventory to be calculated at runtime and allows for more accurate calculations where there is variability in fresh fuel isotopics.

The number of nuclides which ORION tracks is determined by the ORION nuclide library. Typically, a comprehensive library consisting of 2552 nuclides is used although ORION users can implement any size library. Libraries with a reduced number of nuclides may be useful for scoping studies or applications where detailed isotopic inventories are not required. ORION simulates decay of nuclides throughout the duration of a simulated fuel cycle model. ORION calculations work on a discrete timestep basis; timestep length can be selected by the user prior to running a simulation from a range of values between the minimum of 1/8th of a month, up to the maximum of 1 year.

ORION simulates reprocessing by applying transfer coefficients to the masses of individual nuclides and is therefore able to simulate any single-element or multi-element extraction process. Reprocessing facilities in ORION can be set to operate on a limited throughput basis (thereby simulating a facility's limit of reprocessing capacity). Alternatively, unlimited throughput can be set. There is full flexibility in determining the operational start and end dates of such facilities.

For reactor objects, individual unit parameters (related to core-fuel mass, thermal and electrical energy, load factor) are defined by the user; in combination with a total energy production requirement for that reactor type - provided that the quantity of fuel is available – ORION will scale the energy production by a discrete number of reactor units until the total energy requirement is met. Therefore, a single reactor object can represent a single reactor or a multitude of reactors of that design. Multi-batch core loading schemes can be modelled, although the selected simulation timestep must be conducive to the required operational cycle length. There are options available to allow different fuel-enrichment specifications for initial start-up cycles compared with that specified for equilibrium operation. Recent developments implementing the 'user-defined equation' method allows for more complex fuel enrichment and reactor operational energy/fuel demand curves to be modelled.

When modelling fuel manufacturing and enrichment facilities, ORION features a multi-isotope enrichment calculation routine in order to accurately calculate uranium isotope composition in enriched uranium fuel. This is particularly relevant to enrichment of reprocessed uranium ('RepU') where 'minor isotope' ( $^{232}\text{U}$ ,  $^{234}\text{U}$ ,  $^{236}\text{U}$ ) concentrations can be significant in regard to the reactivity of the final fuel. ORION can model 'MOX' fuel fabrication facilities – where the term MOX is used to refer to the combination of any fissile and 'carrier' material and does not necessarily refer to mixed oxide fuel.

For reactors utilizing MOX fuel, options are available to the user to allow ORION to automatically vary the relative quantities of fissile and carrier. ORION will take account of the fissile mass requirement needed to produce the required energy in the reactor by adjusting the fissile fraction of the fuel in the upstream MOX fuel manufacturing facility. This is achieved through the calculation of effective fissile mass coefficients which ORION calculates (relative to a reference fissile material vector). This type of calculation requires that cross-section and mean neutron production ( $\bar{\nu}$ ) data is provided as input. A typical use of this feature is in MOX use scenarios where the fraction of Pu in the MOX fuel is varied according to the fissile quality of the available Pu.

ORION's 'preferential processing' function allows consignments of material to be preferentially selected based on a number of available criteria related to age of material, Pu fraction, U enrichment, decay heat (plus numerous others). This feature is available when selecting the

fissile material in MOX manufacture facilities; an equivalent feature, 'preferential treatment', is available when simulating reprocessing plants - the consignment of material reprocessed next is selected according to the criterion selected by the user.

Running on a modern desktop PC, a 100-year long simulation featuring 5 reactor types and utilizing the 2552 nuclide library would take in the order of several hours to complete. ORION features methods to reduce the runtime for spent fuel inventory calculations, most significant of which is the 'MPR memory' option which allows for repeat calculations to be completed in a fraction of the time once an initial run has been completed.

Once a simulation calculation has been completed, the user can obtain mass values from each ORION object and mass-flow values between objects down to the level of individual nuclide mass for each timestep. The program features a plotting routine to draw on-screen results graphs. In addition, the user can export results in the .csv file format for analysis/plotting in external programs such as Excel. A results scripting function facilitates the data extraction process: the user can provide a text file containing specific keywords and parameters which ORION will interpret to produce a named .csv file. As the calculation proceeds on a sequential timestep basis, partial results can be viewed during runtime without pausing the calculation. End-point material masses for periods of time post-scenario can be obtained – this feature is typically used to analyze evolution of spent fuel isotopics in geological disposal facilities. ORION applies nuclear library data to convert mass values to activity, radiotoxicity, toxic potential, spontaneous neutron emission, and decay heat.

In regard to code verification, ORION has been compared against DYMOND, VISION and MARKAL [2] with excellent agreement for test scenario results achieved. ORION features a verification engine whereby a series of test cases are automatically run and results compared against those from previous ORION calculations and/or a number of analytic solutions. Nuclide inventory calculations using the MPR method has been benchmarked with the CMS and ERANOS neutronics packages and the FISPIN inventory code with 'near perfect agreement' between the methods [1].

The purpose of this paper is to describe ORION and to present 'use cases' which are potentially applicable to aiding security and non-proliferation activities. Several past use cases from published literature are discussed along with specific use cases detailing where the features of ORION allow identification of proliferation issues in the context of the whole fuel cycle.

### Past Use Cases of ORION

As presented in the literature, ORION has previously been used to model the UK's power generation enabling nuclear fuel cycle [3] including models to explore future hypothetical scenarios. ORION has been a useful tool to provide high-level conclusions related to constraints on timescales for nuclear expansion and technical specifications for fuel cycle and waste management plants [4]. The models have not been used specifically for proliferation resistance but have focused on highlighting broad practical issues around the management of nuclear material within the context of transitioning to future nuclear energy production scenarios.

Relevant to the UK are plutonium management scenarios, with previous studies having examined issues around MOX use in LWRs and the fuel requirements of a 75 GWe fleet of fast reactors (FRs) [3]. For FRs introduced with the purpose of operating within a closed-fuel cycle, there are unavoidable periods during the initial phases (the initial/first-core fuel requirement, plus the period accounting for irradiation, subsequent discharge, cooling, reprocessing and re-

manufacture of fuel) in which the self-sustaining aspect is lacking, and fissile material must be sourced externally. The study has given consideration to the fleet size of a self-sustaining FR fleet that could be built when the initial tranche of fissile material is sourced from the UK's stockpile of separated plutonium [3]. The impact on the rate of FR fleet deployment due to variations in FR spent fuel cooling time has also been assessed. Plutonium availability and plutonium fissile quality depending on the level of LWR MOX utilization has also been explored.

Other UK specific studies [4] have assessed the impact of the breeding ratio of FR designs during a scenario in which FRs - specifically sodium-cooled fast reactors (SFRs) - become the dominant form of nuclear energy generation in an attempt for the UK to achieve independence from world uranium supply. The conclusions from this study state that there would only be limited benefit in opting for fast reactor designs with high breeding ratio in terms of bringing forward the timescale of independence. As the plutonium source for the fast reactors was sourced from a preceding fleet of LWRs, the study does mention that an increased breeding ratio reduces the number of LWRs needed to meet the fuel demands of the FR fleet.

These studies therefore have specifically looked at fissile quality of plutonium used for FR fuel and also issues around the breeding of fissile material and the effects on timescales of FR fleet deployment.

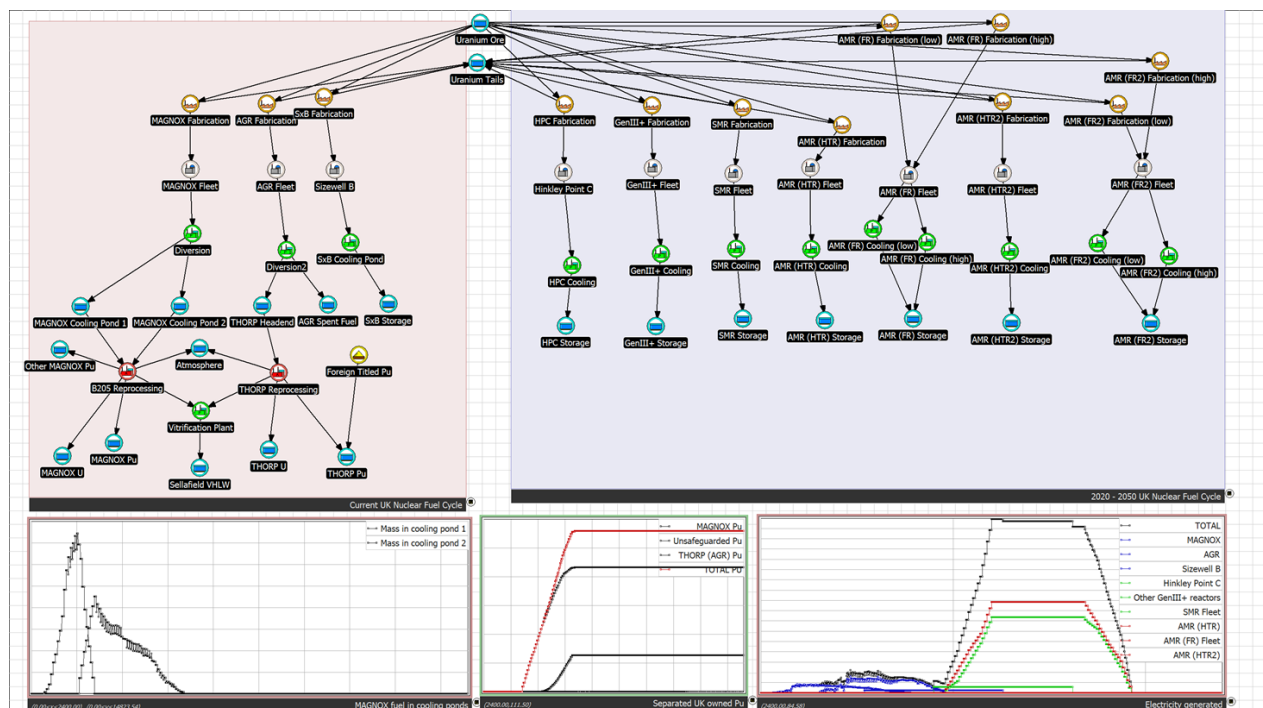


Figure 1: ORION Canvas view of a UK-wide fuel cycle scenario

### Applicability of ORION to Proliferation Resistance and Safeguarding

Whilst numerous proliferation resistance assessment methodologies are known to exist, in this instance, work in references [5] and [6] have been examined and relevant proliferation resistance assessment criteria have been identified that have relevance to ORION. ORION's strengths are its ability to provide accurate isotopic representation of material at any point in the fuel cycle and at any time (including post-scenario). From isotopic mass, a number of material

properties (activity, radiotoxicity, toxic potential, spontaneous neutron emission, and decay heat) can be calculated. This makes ORION a useful tool for identification of proliferation resistance metrics such as; isotopic barrier, radiological barrier, detectability (uniqueness of a material's signature), available mass and available time. In addition, results from ORION can be used to determine the classification of fissile material type (for example, as per categories stated in [7] where proliferation resistance qualitative descriptions range from 'very low' to 'very high'), making ORION a tool for identifying material which is of most concern (has 'attractiveness') in terms of proliferation potential.

In future fuel cycle scenario planning, ORION can be used to identify where attractive material may exist in the fuel cycle, how long it will exist for (within a given scenario), through what fuel cycle facilities it will pass (excluding covert diversion scenarios) and the evolution of that material with time – including the legacy evolution over millennia.

ORION has some limitations and is not able to model explicit chemical processes, so the form of material (for example, sludge, liquid, oxide, metal) arising from a process is not known. Any extrinsic barriers such as IAEA applied Safeguards, access control, security etc cannot be modelled in ORION. Likewise, ORION models do not provide detail on facility attractiveness, facility accessibility or diversion detectability. Accurate modelling of fuel cycle facilities, including reactors, requires technical data on facility operation and specification.

The ORION tool allows a modeller to relatively easily alter multiple variables that can impact material attractiveness, including reprocessing extraction options (UREX, PUREX, COEX etc.), length of spent fuel cooling time, mixing/dilution of material, fuel burnup, reprocessing extraction efficiency. Reference [7] examined the relative attractiveness of material obtained from different fuel cycle options and concluded that there is no 'silver bullet fuel cycle' indicating that there is no ideal fuel cycle and so the exploration of options to minimize proliferation potential while enabling electrical generation is important.

The use of the term 'attractiveness' in this paper is taken to refer to material with high fissile content and low radiological barriers. No formal classification of material is intended and distinction between material of high and low attractiveness is based on the perceived relative difference in fissile content. Requirements for safeguarding of material is beyond the scope of this paper.

#### ORION Use Cases: National-level Fuel Cycle Modelling

Although the focus on ORION development has been geared toward fuel cycle facilities concerned with commercial electrical generation, the code has sufficient flexibility to include military and small-scale research facilities. Almost any reactor type can be modelled provided that a suitable neutronics model to generate cross-section data can be procured. Therefore, the entire nuclear operations of a country could be included in an ORION model.

Many countries have indicated ambition to increase nuclear generation capacity or are in the process of doing so. Creating an ORION model for such countries could be a way to inform through providing a visual indication of nuclear facilities and associated material paths between them. The model could allow a tool for modelling probable pathways toward that country's stated nuclear ambitions: scoping studies to show the future facilities and operations that nation may engage require. Previous studies completed for the UK fuel cycle have modelled historic operations [3]. This has facilitated studies on future options to manage/utilize legacy material.

When modelling future scenarios, ORION can be used to identify bottlenecks in supply, or used in conjunction with forecasts around uranium ore availability to predict difficulty in supply which may result in nuclear nations seeking alternative fuel types.

To extend beyond an individual nation's nuclear activities, concepts such as 'GNEP' [8] or the International Fuel Cycle Center Concept (IFNEC) could be modelled through a collation of data from national ORION models. This could inform the scale of operations required and magnitude of nuclear materials passing between 'supply' and 'recipient' nations.

#### ORION Use Cases: Transition to a Gen IV Closed-fuel Cycle Scenario

A common use for fuel cycle codes is as a tool to examine issues around transition between Gen III/III+ to Gen IV reactor technology. The transition studies, such as those in reference [1] and [4], examine the high-level conclusions related to issues such as possible timescales for deployment, scale of expansion of nuclear capacity and the required technical specifications for associated fuel cycle and waste management facilities.

A key issue for such transitional scenarios involving replacement of existing Gen III technology with Fast Reactor Technology is the ability to procure suitable fissile material for the initial phase of FR operations – in the interim period before FRs can become fully self-sustaining. As common FR designs, such as the SFR, require high fissile content fuel, there are issues around proliferation potential of this material and its management.

Options for procuring such material may involve stockpiling of fissile material (such as separated plutonium) sourced from legacy operations and/or reprocessing of spent fuel from current generation reactors. As in the study presented in [4], ORION has been used to examine the merits of pursuing fast reactor designs with high breeding gains to expedite transition to a closed-fuel cycle. Such studies can therefore inform the reactor design: in this instance it was concluded that the pursuit of designs with high breeding gains did not provide significant benefit in expediting the transition.

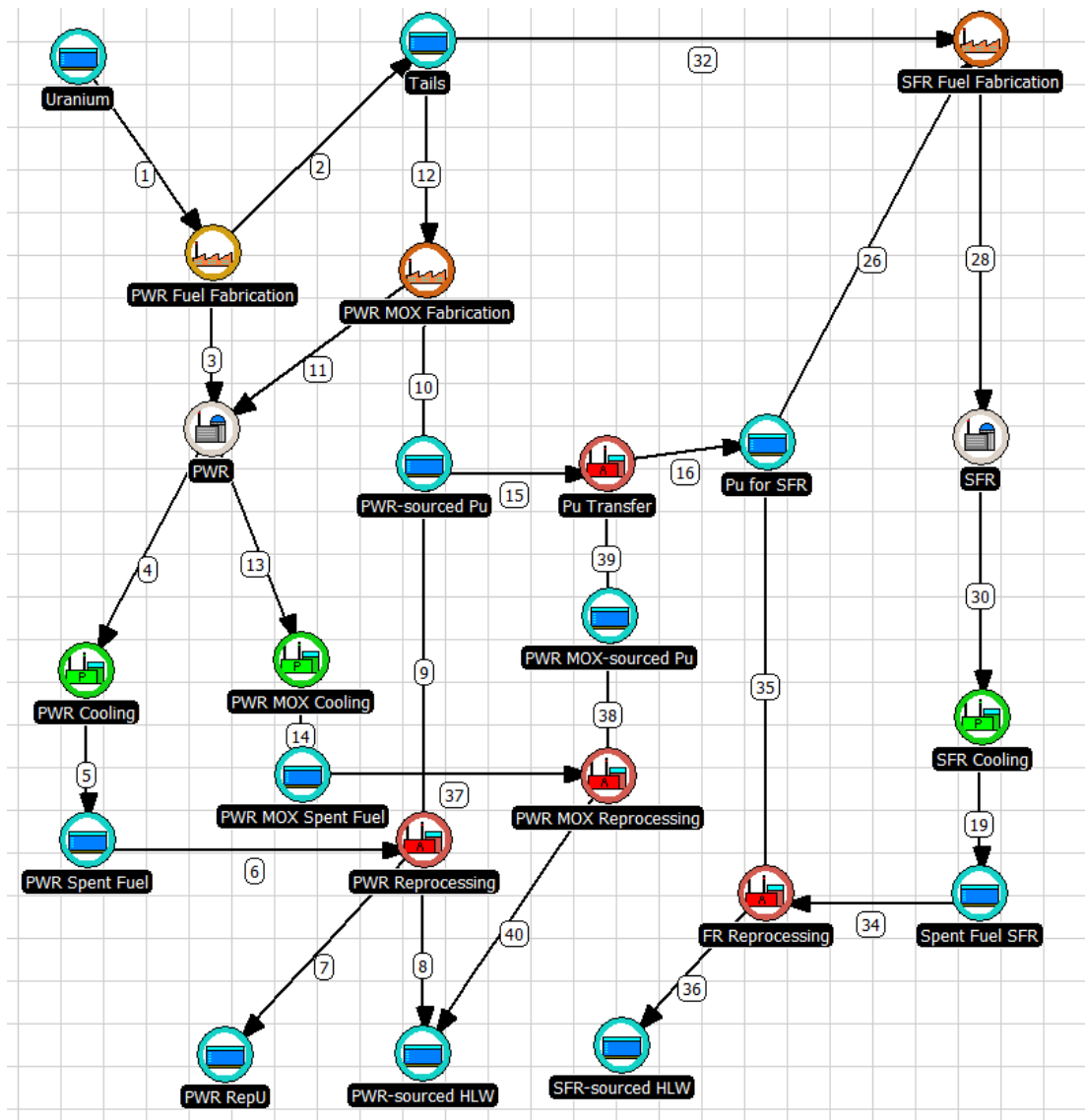


Figure 2: ORION canvas view showing a simple PWR to SFR transition scenario.

### ORION Use Cases: Evaluation of Strategies for the Seeding of Fast Reactor Breeder Material

In the production of fissile material through breeder regions in fast reactors, the material bred in this manner can have high level of attractiveness. To mitigate this, a ‘seed material’ can be added to the breeder material at the manufacturing stage: the nuclides in the seed material have consequences on the subsequent attractiveness of fissile material generated (changing the overall isotopic composition). An example of this strategy is the addition of Np to SFR breeder blankets.

A study presented in [9] indicates that obtaining sufficient quantities of Np to seed the SFR blanket material is challenging when sourcing the Np from fast reactor operations alone - stating that Np is only available in sufficient quantities to provide a seeding concentration of approximately 0.1 w/o. However, the quantity of Np available in PWR spent fuel is around an order-of-magnitude higher. It is therefore important to consider the available supply of seed material within the context of the overall fuel cycle if such strategies are to be successful. ORION can facilitate such considerations for MA separation and seeding strategies by providing

a coherent fuel cycle model which includes the supporting facilities required (along with their capacities and timescales of operation).

## Summary and Conclusions

The key features and capabilities of the ORION fuel cycle modelling tool have been discussed. ORION is capable of modelling a wide range of fuel cycle facilities and, due to the large number of nuclides the code can track, the flexibility of reactor designs that can be modelled, it is a useful tool for isotopic characterization of material at all points in the fuel cycle. Orion facilitates quick exploration of fuel cycle options to allow assessment of the proliferation potential of material in the context of the whole fuel cycle

A number of use cases have been discussed where the features of ORION aid the modeller in identifying and exploring non-proliferation issues – particularly with regard to creation and destruction of material within the context of a whole fuel cycle where the need to deploy generation capacity and transition to new reactor technology needs to be balanced against a range of criteria. Such assessments are useful for planning and identifying points of vulnerability: identifying where there is material with weak radiological barriers and of high attractiveness to proliferators, when this material might come into creation, its quantity and assessing fuel cycle technologies to aid in reducing the risk of proliferation.

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