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ARIS AUZANS

Development of computational model for nuclear energy systems analysis: natural resources optimisation and radiological impact minimization

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Development of computational model for nuclear energy systems analysis: natural resources optimisation and radiological impact minimization

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Department of Bio and Environmental Physics, Institute of Physics, Faculty of Science and Technology, University of Tartu, Estonia

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CONTENTS

1. LIST OF PUBLICATIONS INCLUDED IN THE THESIS

This thesis is based on the following publications, which are referred to in the text by their Roman numerals.

I **Auzans, Aris**; Teder, Allan; Tkaczyk, Alan H. (2016). Time Delay and Profit Accumulation Effect on a Mine-Based Uranium Market Clearing Model. Nuclear Engineering and Design, 310, 154–162, 10.1016/j.nucengdes.2016.09.031.

II **Auzans, Aris**; Schneider, Erich A.; Flanagan, Robert; Tkaczyk, Alan H. (2014). A Mine-Based Uranium Market Clearing Model. Energies, 7 (11), 7673–7693, 10.3390/en7117673.

III Pelakauskas, Martynas; **Auzans, Aris**; Schneider, Erich A.; Tkaczyk, Alan H. (2013). Autonomous dynamic decision making in a nuclear fuel cycle simulator. Nuclear Engineering and Design, 262, 358–364, 10.1016/j.nucengdes.2013.04.033.

2. AUTHOR'S CONTRIBUTION

The publications included in this thesis are a result of a collective effort by all of the authors. The author of this thesis has contributed as follows:
X – The author of this thesis has contributed at least 50% of the work.

Activity	**Publication I**	**Publication II**	**Publication III**
Hypothesis formation	**X**	**X**	**X**
Data collection	**X**	**X**	**X**
Sample preparation and measurement	**X**	**X**	**X**
Data analysis	**X**	**X**	**X**
Manuscript writing	**X**	**X**	**X**
Publishing	**X**	**X**	**X**

3. LIST OF ABBREVIATIONS

ABM	–	agent based modelling
ACC	–	Amortized capital cost
APWR-UOX	–	Advanced pressurized water reactor burning uranium oxide fuel
ATC	–	Average total cost
AVC	–	Average variable cost
BRW	–	Boiling water reactor
BWR	–	Boiling Water Reactors
CANDU	–	Canada deuterium uranium nuclear rectors
CoE	–	Cost of electricity
CPDF	–	Cumulative probability density function
DD	–	Decommissioning costs
DU	–	Depleted uranium
EMWG	–	Generation-IV Economic Modelling Working Group
EV	–	Economic value
FCC	–	Fuel cycle costs
FP	–	Fission products
GWe	–	Giga watts electric power
HLW	–	High level radioactive waste
ISL	–	In-situ leach
LANL	–	Los Alamos National Laboratory
LEU	–	Low enriched uranium
HEU	–	Highly enriched uranium
LLW	–	Low-level radioactive waste
LCOE	–	Levelized cost of electricity
LWR	–	Light water reactor
MA	–	Minor actinides
MC	–	Marginal costs
MOX	–	Mixed oxide fuel
MWe	–	Megawatts electric power
MWt	–	Megawatts thermal power
NFC	–	Nuclear fuel cycle
NU	–	Natural uranium
OM	–	Operation and maintenance
OP	–	Open pit,
PHWR	–	Pressurized heavy-water reactor

Pu	–	Plutonium
PU	–	Price of uranium
PUREX	–	Plutonium uranium extraction process
PWR	–	Pressurized water reactor
PWR	–	Pressurized Water Reactors
RC	–	Reactor construction costs
SFR	–	Sodium Cooled Fast Burner Reactor
SNF	–	Spent nuclear fuel
SNF	–	Spent nuclear fuel
SWU	–	Separative work unit
TOC	–	Total overnight capital cost
TRL	–	Technological Readiness Level
TRU	–	Transuranium elements
U	–	Uranium
UG	–	Underground
WGPu	–	Weapons grade plutonium

4. INTRODUCTION

Many countries are struggling to limit greenhouse gas emissions and focus on carbon-free energy sources, and therefore nuclear energy is a subject of continuing debate to enhance the worldwide energy production mix and cover the base load requirements. This debate about nuclear energy has spurred the development of a wide range of forecasts and computational models of the uranium (U) requirement to fuel the ongoing growth of nuclear power. Evaluation of uranium supply in a market and resource optimization context is needed to inform decisions impacting the long-term development of nuclear power and warn policy makers about possible uranium market supply-side volatilities and to help choose the technology mix. The aim of this work is to demonstrate and test advanced simulation methods and conceptual ideas to enable realistic fuel cycle simulators and develop a supporting tool for decision makers. Additionally, this work facilitates the selection of the most favorable nuclear fuel cycle, using optimization with respect to multiple criteria to save natural resources, minimize the impact of high level radioactive waste on nature, and decrease nuclear material proliferation risks.

The nuclear fuel cycle (NFC) is a complex system which involves physical and chemical initial metal transmutation and energy production in nuclear reactors. Due to high levels of remaining radioactivity in a spent nuclear fuel (SF), the time delay effect must be taken into account between processing steps. Currently there are about 440 nuclear power plants worldwide, which operate in 31 countries. More than 61 reactors are under construction. Operation period of a nuclear reactor can reach up to 60 years, therefore it is important to ensure nuclear fuel supply in entire operation period. Current yearly natural uranium (NU) demand reaches up to 63 000 tons of uranium from mines, and each newly built reactor will require annually additional 150 tons of uranium. Nuclear reactors are designed to run on a specific nuclear fuel, which cannot be substituted in a short period and any changes requires large investments. Therefore, fuel requirements must be satisfied in a short run (World Nuclear Association, 2017).

Currently mainly all commodities are being traded in an organized commodity exchange market which is opposite to NU market. The uranium trade is based on fixed-long term contracts, negotiated between mines and facilities. Negotiated NU price can be indexed one reference price, but most likely is calculated on basis of various reference prices and corrections indexes. The corrections indexes are based on a spot market price and can have speculative effect. The statistical data shows, that 80% of all NU has been sold on bases of long term contracts and only 20% by spot market price (U.S. Department of Energy, 2014; World Nuclear Association, 2008; OECD Nuclear Energy Agency, 2010).

The first part of this work models uranium market relationships based on a plausible assumption that in nearest future uranium will be sold based on a spot price and each NU producer will compete with other producers. The other part of this work solves optimization paradigm to find the most favorable NFC which help to save natural resources, minimize high level radioactive waste impact on nature and decrees nuclear material proliferation risks.

The aim of this work is to take an advantage of different modelling methods, for example, the agent based modelling (ABM) concept and create more realistic front end NFC model which allows to demonstrate, how the NFC can be modelled in a free market economic condition and measure uranium market price correlation to the different macroeconomic events. The model simulates uranium mines as independent entities – agents, which act based on market conditions and individual economic parameters to maximize profit in a given time period. An agent or autonomous unit concept, where each unit can independently take decisions and learn from overall or individually collected statistical data, allow to simulate large and complex systems with multiple parts supporting actions and interaction between entities based on the case study. However, the model cannot be used to predict uranium market price but rather to measure policy, regional level regulations and natural disasters' effect on a uranium market price and NU utilization factor. Such lightweight model can be used to advice policy makers, can be plugged into another NFC model and can be used to test multiple conceptual methods.

The initial work is based on an existing time depending front-end NFC model, which calculates equilibrium conditions in a uranium market taking into account nuclear reactors demand, NU reserves, conversion and enrichment capacity as well as secondary sources – depleted uranium (DU) and weapon graded plutonium (WGPu) (Schneider et al., 2013). The work extends the uranium market-clearing model by adding the ability of individual uranium mines to react on U market price change governed by predefined constraints such as local or regional regulations, natural disasters' or other uncertainties. Such conceptual approach can benefit also other NFC, which depict several fuel cycle actors. These simulators allow realistically model the interaction of different NFC entities to react on market changes.

The initial augmented market model is based on the uranium mines property database, which contains information about 330 uranium resources in a different development stages, unit production costs, total reserves and annual production capacity. The enhanced model version is capable to model competition between uranium mines considering different mines economic characteristics such as total overnight capital cost of construction, operation and maintenance and decommissioning costs. Since the simulator marches forward in time, individual agents (U mines) make decisions not knowing what others are doing, and decisions are based only upon market conditions in the current time step and own historical decisions. Namely, each mine has ability to develop individual strategy and maximize profit. This gives rise to unrealistically myopic behavior for agents, which make decisions based only on current economic conditions or on past data. Therefore, was implemented ability to move back in time and allow the model change agent decision in past. Decision change simulates ability to make long term market predictions for individual agents. In such a way individual agent can modify the strategy which is based on projected evolution of the uranium market. The model tries to find correct strategy for each agent by marching backward and forward in time to ensure that mines operate throughout their lifetime. The model also is capable to simulate unexpected market conditions and the ownership change. To make operation decision which is based on a U market prices, the model must have U mine's economic characteristics such as total overnight capital cost of construction, operation and maintenance and decommissioning costs. But information about individual mines economical characteristics are not available and rather is subjected to market secret, therefore, the methodology presents calculation based on available unit cost data. This lightweight, advanced front-end NFC model is very essential, because it is built on the sandbox principle, where components can be extended, replaced and new concepts and developed multiple scenario can be tested easily.

An optimal backend NFC selection can ensure natural resources optimization and nuclear waste minimization in actinides transmutation process. Based on objective criteria for example resource availability, electricity price, transmutation policy, nuclear materials proliferation constraints and environmental risks it is very important to choose correct nuclear reactor technologies' combination. In fact is possible to define any objective function which contains these criteria and based upon it solve optimization task. Although, in practical applications such decision-making evaluation is very difficult to achieve, because of the highly nonlinear nature of the constraints which are required by the time-dependent material balance model. Therefore in this work is included section about optimal nuclear reactors technology mix finding, based on minimization of cost of electricity. The model calculates entire fuel cycle costs by using traditional present-value and levelized-cost analyses.

To complete the above mentioned tasks current work will include two important sections with different nuclear fuel cycle modelling aims:

1. Front-end nuclear fuel cycle modelling using a mine-based uranium market clearing model, which is based on publications II and II;
2. An optimal fuel cycle scenery evaluation based on a nuclear fuel cycle and economy simulation tool's mass equilibrium model, based on publication III.

5. NUCLEAR FUEL CYCLE OVERVIEW

The nuclear fuel cycle is the series of industrial processes consisting from multiple steps and involves the production of electricity from uranium, plutonium and other fissile materials in nuclear power reactors. These steps accommodate uranium mining, uranium milling, conversion and enrichment, fuel fabrication, power generation and burn-up, used fuel cooling, reprocessing uranium and plutonium recycling, waste treatment. The full fuel cycle scheme with possible materials flow is presented in Figure 1. Although theoretically it is possible to burn transuranic elements and minor actinides only a small fraction of spent nuclear fuel being processed and used again in so called mixed oxide fuel (MOX) in the light water reactors that predominate nuclear power generation. The MOX nuclear reactors fuel is usually consisting of plutonium mixed with natural uranium, reprocessed uranium, or depleted uranium.

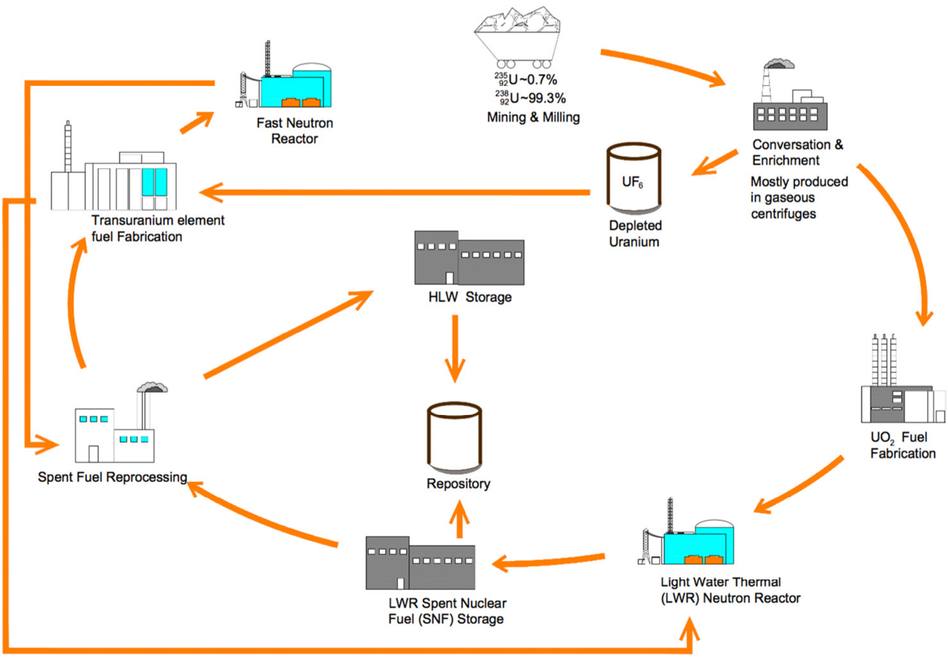


Figure 1. Nuclear fuel cycle overview and possible materials flow

The NFC starts with uranium mining as it is shown in Figure 1. Uranium is a relatively common element that is found throughout the world in earth's crust and oceans, but can only be economically recovered where geological processes have locally increased its concentration. It is mined in a number of countries and must be processed and in most cases enriched before it can be used as fuel for a nuclear reactor. The uranium is mined in an open-pit or underground and then uranium is extracted from the crushed ore in a processing plant (mill) using chemical methods appropriate to the specific mineral form. According to the

World Nuclear Association data current usage of natural uranium is about 63 000 tU/yr. The world's present measured resources of uranium are 5.7 Mt in the cost category to 130 USD/kg U and 7.6 Mt in cost category 260 USD/kg U. Taking into account current natural uranium demand growth rate in conventional reactors, the resources in a cost category until 130 USD/kg U are enough for about 90 years. Further exploration, new technologies and higher prices will certainly, on the basis of present geological knowledge, yield further resources when present ones are used up (World Nuclear Association, 2016). A significant fraction of used fuel may be processed to recover fissile and fertile materials in order to provide fresh fuel for existing and future nuclear power plants. Such options are studied in advanced nuclear fuel cycles with fast neutron reactors usage.

Natural uranium contains 0.7% of the ^{235}U isotope and remaining 99.3% is ^{238}U isotope which does not contribute directly to the fission process. Only isotope ^{235}U is fissile and can sustain chain reaction in light water reactors (PWR and BRW) and must be in defined concentration level in a nuclear fuel that is usually 3–5% to guaranty optimal fuel burn-up level (World Nuclear Association, 2017). Uranium isotopes ^{235}U and ^{238}U have identical chemical properties but different physical properties respectively their mass. The difference in mass between two isotopes makes it possible to increase the percentage of ^{235}U in a nuclear fuel. All known enrichment technologies use the mass difference property. There are reactors designed to use natural uranium as a fuel, for example the Canadian-designed CANDU and the British MAGNOX reactors.

The nuclear fission process releases large amounts of energy and for this reason fuel must be assembled to endure high operation temperatures and intense neutron radiation. Fuel structure need to maintain their shape and integrity over a period of several years to prevent the leakage of fission products into the reactor coolant. The standard fuel form comprises a column of ceramic pellets of uranium oxide, clad and sealed into zirconium alloy tubes, which being arranged into fuel assemblies to form regular array of cells. The fission process consumes fuels, therefore old fuel rods must be replaced and rearranged periodically to support optimal fuel burn-up and nominal thermal load in reactor core. For LWRs and PHWRs reactors there are three main stages in fuel fabrication:

1. Producing pure uranium dioxide (UO_2) from incoming uranium hexafluoride (UF_6) or uranium trioxide (UO_3).
2. Producing high-density ceramic UO_2 pellets.
3. Producing the metal framework for the fuel assembly.

A nuclear reactor is complex technological system which produces and controls the release of energy from splitting the atoms of certain elements and the energy released is used as heat to make steam to generate electricity. During nuclear reactor operation, part of the ^{238}U is changed to plutonium in neutron capture reaction, and ^{239}Pu ends up providing about one third of the energy from the fuel. The fuel assemblies, after being in the reactor for 3 to 6 years, are stored underwater for 10 to 20 years. The water serves such purposes:

4. Works as a shield to reduce the radiation levels
5. It cools the fuel assemblies that continue to produce heat (called decay heat) for some time after removal.

After 10 or more years, the radiation from fuel assemblies and decay heat levels are low enough that the fuel may be stored in large casks which can be cooled by air passing on the outside.

Spent fuel management includes storage, transport, processing and recycling or packaging for disposal. According to the Nuclear Energy Institute data the nuclear industry generates a total of about 2000–2300 metric tons of used fuel per year. In past four decades, the entire industry has produced 76 430 metric tons of used nuclear fuel (Nuclear Energy Institute, 2017). Reprocessing of used nuclear fuel to recover uranium and plutonium allow to avoid the wastage of a valuable resource. Yearly reprocessing capacity in several countries is now about 5000 tons per year, which allow recover uranium and plutonium to use it in a nuclear fuel (World Nuclear Association, 2017). Theoretically reprocessing can be done in several courses, separating certain elements from the remainder, which becomes high-level waste. Reprocessing options include:

6. U, Pu recovery (currently is done in several countries). Nowadays all commercial reprocessing plants use the well-proven hydrometallurgical plutonium uranium extraction process (PUREX).
7. Separate U, Pu + U (small amount of U).
8. Separate U, Pu, minor actinides (future objective).
9. Separate U, Pu + Np, Am + Cm (future objective).
10. Separate U + Pu all together (future objective).
11. Separate U, Pu + actinides, certain fission products (future objective).

The separation process has two problems – separated plutonium causes potential proliferation risks and minor actinides remaining in radioactive wastes has longer-lived radioactivity compared with fission products. The minor actinides handling is technically more difficult due to high radioactivity.

The HLW, which classified as highly radioactive and will continue to generate a lot of heat, contains about 3% of the used fuel in the form of fission products and minor actinides (notably Np, Am, Cm). It is conditioned by calcining and incorporation of the dry material into borosilicate glass (process called vitrification), then stored in geologically safe disposal. In principle any compact, stable, insoluble solid is satisfactory for disposal. The LLW are safely stored on site or transported to licensed storage. Waste is stored until it has decayed away and can be disposed of as ordinary trash. The goal of an advanced nuclear fuel cycle which includes actinides transmutation, is to have wastes which become radiologically innocuous in only a few hundred years. The need for a waste repository is not excluded, but it can be smaller, simpler and the hazard posed by the disposed waste materials is greatly reduced.

5.1. The once-through nuclear fuel cycle

The once-through or open nuclear fuel cycle is nowadays the predominant fuel cycle. The open fuel cycle consists of uranium mining and milling, conversion and enrichment, fuel fabrication, power generation in nuclear reactors, used fuel cooling and geological disposal. Historically nuclear reprocessing and plutonium separation was considered to raise nuclear materials proliferation risks and require significant investments in technology. Also, uranium at that time was relatively cheap. Therefore, an open nuclear fuel cycle was considered as a good option. In the open fuel cycle the spent nuclear fuel is considered as a waste and should be encapsulated and disposed of in a deep and safe geological repository after several decades of interim storage for heat decay. The technology for interim storage for at least 50 years is well established. But the technology for encapsulation and disposal is most advanced in Finland and Sweden, where it has been developed to a stage that license applications for construction and operation have been led. The other countries do not have such stable soil, where they could store nuclear waste. Therefore the closed nuclear fuel cycle is very important. It will allow to optimize natural uranium consumption and nuclear reactors will not be so depended from uranium market price and will help to deal with HLW.

5.2. Closed nuclear fuel cycle

In the closed fuel cycle the spent nuclear fuel is reprocessed to separate uranium, plutonium and minor actinides for future use. Full utilization of fissile materials will require multiple reprocessing and recycling of successive generations of fuel. Also, the full nuclear fuel reprocessing cannot be achieved effectively with current nuclear reactors, therefore it will require development and commercial implementation of fast neutron reactors which can enable the extraction of 50 to 100 times more energy from the originally mined uranium than reactors currently in operation (Joint Research Centre et al., 2011). The closed nuclear fuel cycle can include multiple reprocessing targets, these targets are:

12. Plutonium recycling is used in several countries to produce so called MOX fuel, which being burned in LWRs. There are no plans to reuse recycled MOX fuel, because the proportion of the non-fissile even-mass isotopes of plutonium rises with each pass through the cycle.
13. Minor actinides recycling.

With a specific reactor design all the actinides in the fuel can be consumed, leaving only lighter elements with short half-lives. One promising alternative is so called accelerator-driven sub-critical reactor. Here a beam of protons or electrons is directed into a target. In the case of protons beam usage, very fast neutrons will spall off the target, meanwhile in the case of the electrons beam, very high energy photons will be generated. These high-energy neutrons and photons will then cause the fission of the heavy actinides. In Figure 2 plutonium and minor actinides recycling scheme is displayed. In the cycle scheme (Figure 2) multi-recycling plutonium process is displayed, where the only constraint is that the second fuel type must always have the same initial nuclide content as the fresh (first generation) MOX fuel. From FRs spent nuclear fuel can be recovered plutonium which can be reused either as FRs or LWR fuel. The minor actinides cycle is separate cycle which aims into fission element transmutation.

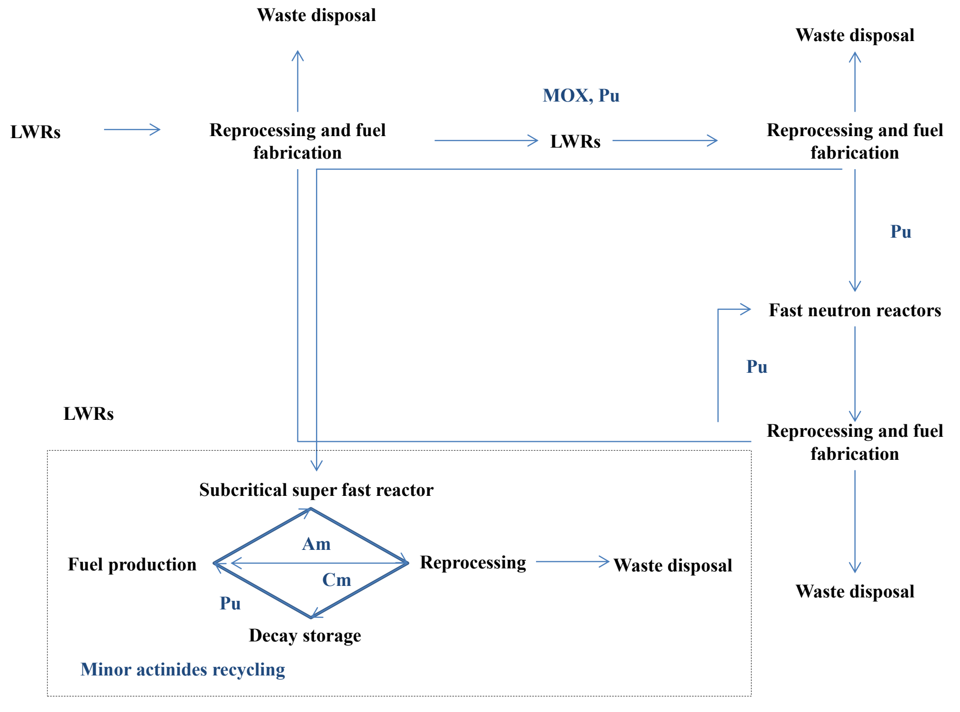


Figure 2. Plutonium and minor actinides recycling

5.3. Nuclear fuel cycle costs calculation

Nuclear fuel cycle costs can be divided into two parts. i.e., front-end components which include uranium purchase, conversion to uranium hexafluoride, enrichment and fuel fabrication, and back-end components. The back-end components depends from chosen strategy of fuel cycle, either it is open fuel cycle or partially/fully closed nuclear fuel cycle. In an open fuel cycle cost components include permanent waste disposal and waste processing costs (vitrification), meanwhile in a closed fuel cycle the plutonium separation and leftover waste disposal must be accounted. Different studies show, than partially or closed nuclear fuel cycle total costs are higher that open fuel cycle costs due to required infrastructure costs and additional technical processes (Technical Subcommittee on Nuclear Power, Nuclear Fuel Cycle, 2011; Nuclear Energy Agency, 1994). However open fuel cycle costs analysis does not take into account future social costs for HLW. The techniques to estimate total NFC costs include separate component analysis and cost evaluation for each element. There is no many reprocessing facilities or enrichment facilities in countries with advanced nuclear power generation technology, the nuclear fuel cycle cost data are rather estimated costs instead of real costs. It is very difficult to obtain relevant costs for each facility. Thus, the nuclear fuel cycle cost as an estimated cost is inevitably subject to uncertainty and calculation required probability distribution or also can be applied deterministic method where an input variable as a representative value. The total cost of the nuclear fuel cycle is generally calculated by multiplying the process quantity in each phase of the nuclear fuel cycle process with the unit cost. These costs will be completely different for each country due to labor cost, tax etc. difference. Figures 3, 4 are show time scale model for each fuel cycle. It will take many years to start SF reprocessing and economic reason for closed nuclear fuel cycle would be NU price and HLW social costs.

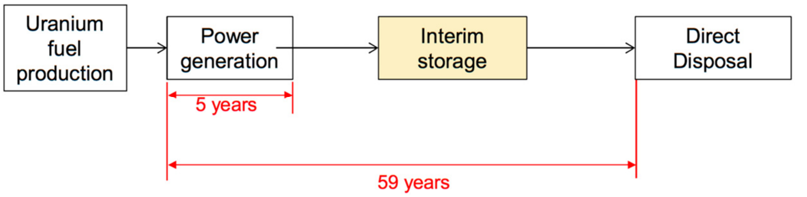


Figure 3. Direct disposal model time frame

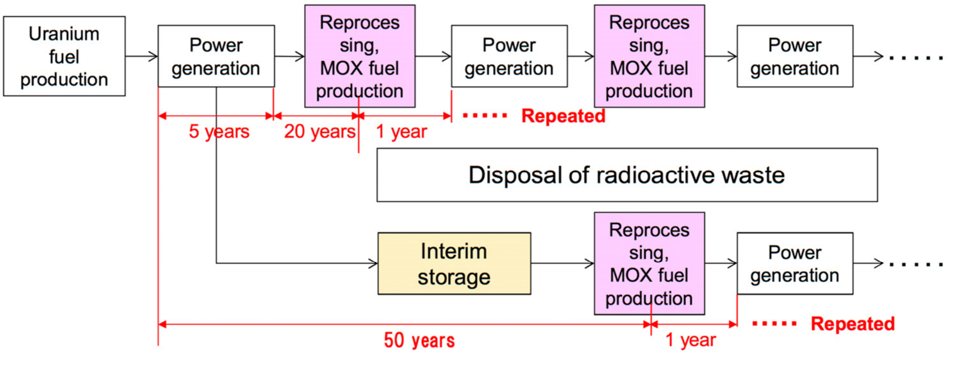


Figure 4. Plutonium recycling model time frame

6. NUCLEAR FUEL CYCLE NUMERICAL MODELLING (BASED ON PUBLICATIONS I AND II)

Nuclear fuel cycle is a complex system with multiple components where each step can add unit costs. The nuclear fuel cycle numerical models are intended to simulate the evolution of cycles over a period of time and then to provide output data relevant to the input parameters. A numerical nuclear fuel cycle modelling can have multiple targets (JUCHAU et. al, 2010):

14. Analyze nuclear fuel cycle different strategies and options to help decision makers and calculate levelized cost of electricity for a simulation. Evaluate reprocessing-recycling strategies as well analyze new reactor deployment and existing fleet replacement.
15. Perform an uncertainty analysis for each fuel cycle element.
16. Uranium resource evaluation for different nuclear fuel cycle strategies and optimization task solving across multiple objective functions.
17. A transport modelling to track material balance and its isotopic composition evaluation in every fuel cycle stage. Isotopic composition in spent nuclear fuel is calculated by the fuel depletion code. Detailed isotopic tracking, particular plutonium and minor actinides are required to address advanced fuel cycle viability questions, optimal resource usage and HLW issue analyze.
18. Open access to simulation code and documentation.

Currently there are many different nuclear fuel cycle simulation codes which fulfil one or several above mentioned technical targets but only few codes are reviewed in this study. In the Table 1 there are compared several NFC simulation codes according to the above mentioned technical targets. Although many of NFC codes only partially supported one or several technical targets they are included in the results table.

Table 1. Summary of different nuclear fuel cycles code comparison results

T*	CAFCA	COSI	CEPMNFC	DANESS	NFCSim	VEGAS	VISION	NFCSS	GENIUS 1	U-Clearing model**
1		X	X		X				X	
2										
3						X				
4		X								
5	X			X	X	X	X	X	X	X

* Technical targets to fuel cycle model

**A Mine-Based Uranium Market Clearing Model

As we can see, all nuclear fuel cycle simulation codes (included in the Table 1) can be divided into two groups, those who track material movement in discrete fuel batches and those who do not. For example, the VEGAS was originally created at Los Alamos National Laboratory (LANL) with the aim to minimize TRU materials and complement other simulator. A mine-based uranium market clearing model is created to evaluate uranium supply effect on natural uranium price and demonstrate agent-based simulation concept. CAFCA performs economic analyses for a simulation calculating the average total cost of electricity for a scenario and the final goal is to minimize TRU inventory of a given scenario. DANESS can simulate ten different reactor fuel combinations. Reactors and facilities are characterized by types, not individually. Material flows are tracked isotopically and radioactive decay is incorporated. It calculates a levelized cost of electricity for a scenario. VISION code is capable of modelling nuclear fuel cycle scenarios using multiple reactor and fuel combinations to calculate the levelized cost of electricity for a simulation. The code also calculates radioactive decay and tracks material flows isotopically. In the NFCSS reactors and fuel cycle facilities are characterized by types and cannot be added with individual parameters to simulation. Materials are tracked by isotopes, and radioactive decay is included in a simulation. The NFCSS can simulate four different reprocessing scenarios.

The second group of nuclear fuel cycle modelling codes tracks material movement in discrete fuel batches or fuel assemblies. COSI works as engine which is composed of several interconnected codes, including a cycle-by-cycle burn-up and depletion engine. The code can be used to provide an economic analysis of a nuclear fuel cycle including calculations for levelized cost of electricity. CEPMNFC code also incorporates a cycle-by-cycle burn-up and depletion engine. In the code actinides are tracked at the isotopic level, while fission products are tracked as a group. Radioactive decay is incorporated. The code calculates the levelized cost of electricity for predefined scenarios. The GENIUS 1 code is a multi-regional simulator in which individually characterized reactors and fuel cycle facilities may be included in a simulation. Also, materials are tracked isotopically. GENIUS 1 can be used to simulate three basic fuel cycle arrangements. NFCSim code was developed primarily to explore different fuel cycle options for the United States. There can be individually characterized deployment of reactors, fuel cycle facilities, and accelerator driven systems. Materials are tracked in isotopic level and radioactive decay is calculated. The code calculates a levelized cost of electricity for a modelled scenario.

Simulation tool developers must find a balance between usefulness and credibility, because models can very easily become complex and any new simulation can require significant effort as well data analysis and validation can become almost impossible. A lot of simulation tools work with arbitrary chosen data due to lack of information.

7. URANIUM MINING MARKET CLEARING MODEL

This chapter will be discuss technical information about a mine-based uranium market clearing model, its technical characteristics and individual U mines decision making strategy economic background. Subchapters will provide depiction of individual U mine's mining cost calculation, NU market supply curve creation, U demand curve creation and U market price calculation.

7.1. Uranium mines economic characteristic calculation

The advanced model builds upon the market clearing model of the uranium and enrichment industries described in (Schneider et al., 2013). That model is built upon databases of primary and secondary uranium resources as well as enrichment facilities, with each enrichment facility having a unique cost structure. The model derives market-clearing conditions by locating the intersections between the annual supply and demand curves for uranium and enrichment services while also considering the effects of secondary supplies including highly enriched uranium down blending and sale of natural uranium inventories, which come for zero price. Therefore, the model incorporates the coupling between the uranium and enrichment markets. For instance, an increase in uranium price will lead to decreased tails assays, more demand for enrichment, higher enrichment prices and ultimately reduced demand for natural uranium. In special conditions when enrichment industry experiences NU supply shortages, enrichment services can guaranty short-term U market price elasticity and continuous low enriched uranium (LEU) supply by using DU tails assay. The short-term U market price elasticity can also be regulated by secondary uranium management policies.

Each mine in the core database has unique characteristics including total uranium reserves, earliest feasible opening date, capital and operating costs and others detailed below and in (Schneider et al., 2013). Since these characteristics are fixed, the supply curve for each individual mine is also the same in every time period as long as the mine still possesses uranium reserves it can produce. Therefore, the production decisions of each mine can be determined based on the short-run market price, which is in turn set by the industry short run supply curve aggregated over all mines that are able to produce in that time period. The aggregated short run industry supply curve displays all uranium mines which can potentially produce in a given time period if the price is high enough.

Figure 5 distinction between an individual mine "shutting down" in the short run and "exiting" price in the long run. Figure 5 follows the economic rules, which are described in (Nechyba et al., 2011). The marginal cost (MC) is the variable cost incurred by producing one additional unit of output. The average variable cost (AVC) is the average value of the MC for all units of output produced. The average total cost (ATC) is the AVC plus the amortized capital cost

(ACC) divided by the number of units of output. For a mine to operate, its economic costs must be covered either from direct NU sell in a current time period or from accumulated profit gained in previous periods. The MC curve crosses ATC at its lowest point (E1) because the MC is of producing an additional unit of output is averaged into the ATC. When the MC is less than the ATC, each new unit of output lowers the ATC. A new mine will not begin to operate unless its average total cost of producing uranium is less than or equal to the mine's MC. This point is known as the short-run breakeven point (E1 in Figure 5). If a mine is currently operating it will continue to operate until the market price drops below the minimum value of its AVC and all accumulated profit will be spent to cover U mine's operation and annual maintenance costs. This is known as the long-run industry exiting point (E2).

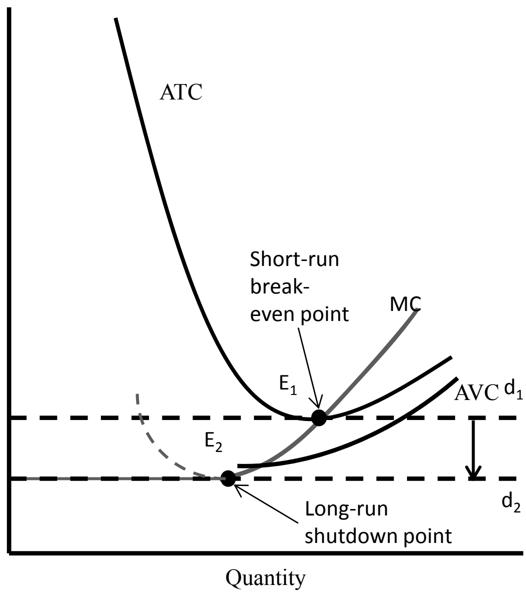


Figure 5. Cost curves for a single uranium mine

The original model's database does not include information about capital, operation and maintenance or decommissioning costs for individual uranium mines, only their unit cost of uranium production at a reference output level. Operating cost information is required to allow the simulator to make short run operation decisions, while capital costs become relevant when determining whether to open or decommission a mine. Disaggregated capital, operating and decommissioning cost data is available from WISE Uranium Project for a limited number of mines (Diehl, 2011).

One representative mine of each type – underground (UG), open pit (OP) and in-situ leach (ISL), is chosen from this data set. The Generation-IV Economic Modelling Working Group (EMWG) unit cost calculation procedure is applied to compute unit production costs — UC ($/kg U), for these mines

(EMWG, 2007). All other mines of that type are assumed to adhere to the same relative distribution of capital, operating and decommissioning costs. Hence these costs are obtained by scaling the costs for the reference mine by the ratio of unit costs, as detailed below. This simplification was made in response to the unavailability of detailed cost structure breakdowns for individual mines. The representative disaggregated costs available in (Diehl, 2011) are used in this in order to demonstrate the implementation of the model.

Table 2 provides the reference data set for each mine type. The methodology for relating TOC, OM, and DD to UC is described next. The unit cost, UC, is calculated as a sum of all costs components divided by total annual production output. In equation it can be written as:

$$\mathrm{UC} = (\mathrm{ACC} + \mathrm{ADD} + \mathrm{OM})/\mathrm{M} \tag{1}$$

Where M: Annual production (throughput) of product in kg of basis unit/yr: technology-specific basis unit may be U, separative work unit (SWU), etc. ADD: Amortized annual decommissioning costs.

The unit cost components are calculated as above. The amortization factor (AF) is given by:

$$\mathrm{AF} = \frac{r}{1-(1+r)^{-T_0}}, \tag{2}$$

where r: Real discount rate, T_0: Duration (years) of operation. An amortization factor used to determine the periodic payment amount due on a loan, based on the amortization process.

A sinking fund amortization factor (SFF) with a lower rate of return applies to decommissioning costs. It is calculated from:

$$\mathrm{SFF} = \frac{r_{\mathrm{SF}}}{(1+r_{\mathrm{SF}})^{T_0-1}} \tag{3}$$

where r_{SF}: Real sinking fund rate, T_0: Duration (years) of operation. In finance, a sinking fund is a method by which firm's sets aside money over time to retire its indebtedness. Namely, it is a fund into which money can be deposited, so that over time preferred stock, debentures or stocks can be retired. Then TOC, interest during construction (IDC) and decommission costs (DD) are calculated from the reference data:

$$\mathrm{TOC} = \frac{\mathrm{ACC} \times \mathrm{M}}{\mathrm{AF}} \text{-IDC} \tag{4}$$

$$\mathrm{IDC} = \sum_{i=1}^{Tc} \mathrm{TOC} \times f_i \times ((1+r)^{Tc-j} - 1) \tag{5}$$

$$\mathrm{DD} = \frac{\mathrm{ADD}}{\mathrm{SFF}}, \tag{6}$$

where T_c: Duration (years) of construction. Total operating costs are expenses associated with U mine maintenance and administration on a time basis. Interest costs during construction refers to the financing charges incurred during the U mine construction. Decommissioning cost or asset retirement obligation is the cost incurred by firms in reversing the modifications made to landscape when U mining operation is ended.

The next step is to calculate the scaled costs for other mines of the same type by using economic decomposition method incorporating throughout mass scale approach. In the discussion that follows, variables subscripted "*r*" apply to the reference mine of a given type (OP, UG, ISL). Unsubscripted quantities apply to another mine of the same type. The amortized annual capital, OM and DD costs and interest during construction are scaled from reference values as follows:

$$\mathrm{ACC} = \frac{\mathrm{UC}}{\mathrm{UC_r}} \cdot \frac{\mathrm{ACC_r}}{\frac{\mathrm{M}}{\mathrm{M_r}}} \tag{7}$$

$$\mathrm{OM} = \mathrm{OM_r} \cdot \frac{\mathrm{UC}}{\mathrm{UC_r} \cdot \frac{\mathrm{M}}{\mathrm{M_r}}} \tag{8}$$

$$\mathrm{DD} = \mathrm{ADD_r} \cdot \frac{\mathrm{UC}}{\mathrm{UC_r} \cdot \frac{\mathrm{M}}{\mathrm{M_r}}} \tag{9}$$

$$\mathrm{IDC} = \mathrm{IDC_r} \cdot \frac{\mathrm{UC}}{\mathrm{UC_r} \cdot \frac{\mathrm{M}}{\mathrm{M_r}}} \tag{10}$$

The OM, is interpreted as the AVC at the reference annual production level, M. In reality, individual mines would increase or curb production as conditions warranted; however, the reference existing model (Schneider et al., 2013) permits mines to function at their reference capacity or not at all. By formulating a mine-specific supply curve, the modification described next enables each mine to select its own production level at every time step.

A bottom-up engineering cost analysis would be needed to construct such a supply curve. Since the objective of this work is to demonstrate a method for making use of such data in a simulation, a plausible functional form was chosen to represent a generic short run supply curve, which shows the quantity supplied by individual U mine at certain price level. The form chosen is second order polynomial equation, as was proposed in (Harshbarger et al., 2009). It is and given by:

$$P = \mathrm{a}Q^2 + \mathrm{b}Q + \mathrm{c}, \tag{11}$$

where Q: supply quantity in given period (usually one year), P: marginal cost of supplying an additional unit at quantity Q; a, b, c: coefficients to be determined.

For each uranium mine, the existing database from (World Nuclear Association, 2008) provides a reference capacity (tons of uranium produced per year) and a reference production cost ($ per kilogram of uranium produced), from which is calculated marginal cost of supplying. Therefore, to determine the coefficients a, b, and c the following criteria are imposed:

$$\begin{cases} P_1 = \mathrm{a}Q_1^2 + \mathrm{b}Q_1 + \mathrm{c} \\ P_2 = \mathrm{a}Q_2^2 + \mathrm{b}Q_2 + \mathrm{c} \\ \quad 0 = 2\mathrm{a}Q_2 + \mathrm{b} \end{cases} \tag{12}$$

Here Q_1 and P_1 are the reference capacity and cost from the database. Economic theory provides that a firm's short run marginal cost curve exhibits a U shape, as predicted by Equations (12). The shape arises because costs per unit of production first decrease as production rises from very low levels and scale benefits are realised. As additional capital and labor inputs are applied to increase production, though, the marginal benefit of these inputs begin to decline as they outstrip the ability of a firm's infrastructure to effectively use them. Although there exists insufficient historical mine data to calibrate the marginal cost curve, the U shape of Equations (12) provides the correct type of feedback to the cost model. The point P_2 = 0.5P_1 and Q_2 = 0.7 Q_1 the marginal cost of mining an additional unit of uranium is assumed to reach its lowest value, 70% of the reference cost P_1, when the mine's production stands at half of the reference level Q_1.

The individual mine supply curve is the upward sloping part of the marginal cost curve (the part above the average cost curve). The portion of the marginal cost curve above ATC (Figure 6) is a profit maximizing individual mine supply curve. Portions of the marginal cost curve to the left of the shut-down point (E_2) are not part of the short run supply curve, because to produce on the left side of the E_2 MC costs increase (dashed line in Figure 6) and ATC costs significantly increase. Operation in this part of the MC curve is uneconomical.

Table 2. Reference data for costs calculation from the WISE Uranium Project Calculators.

Reference U mines	**Type**	**UG**	**OP**	**ISL**
Data from (Nuclear Energy Data, 2010):	TOC, $	2.81×10^8	3.47×10^8	1.11×10^8
	OM, $/yr	1.04×10^8	1.62×10^8	1.73×10^7
	DD, $	3.39×10^7	5.92×10^7	2.86×10^7
	M, kg/yr	7.72×10^5	3.16×10^6	4.12×10^5
Calculated from data following procedure in text	ACC, $/yr	4.25×10^7	7.93×10^7	2.67×10^7
	ADD, $/yr	1.07×10^6	5.78×10^6	3.07×10^6
	IDC, $	4.36×10^7	5.37×10^7	1.72×10^7
	UC, $/kg U	192	77.9	114

7.2. Short Run Market Supply and Demand Curves

The short run market supply curve is defined as the horizontal sum of the individual mines' supply curves, so that the amount that would be supplied Q by all agents at a price level p is:

$$Q = \sum_{i=1}^{n} Q_i(p), \tag{13}$$

where n: number of U mines, $Q_i(p)$: supply curve of firm i from Equation (11).

The graphical representation of the market supply curve construction is shown in Figure 6.

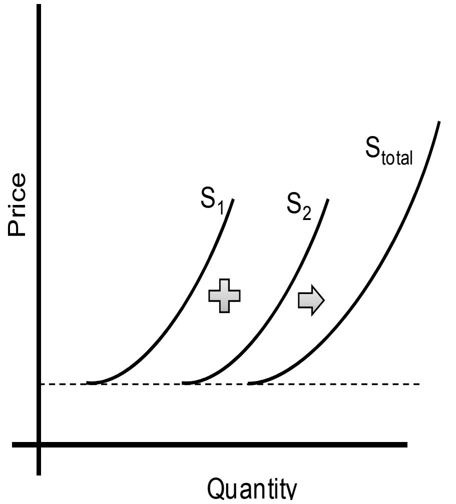


Figure 6. Uranium market supply curve creation.

The quantity of uranium supplied, the sources of that supply, and the U market price are all affected by the demand curve. Although in the short term the demand for LEU, i.e., nuclear reactor fuel may be treated as constant, the NU required to meet this need can be varied by secondary uranium management policies. It can also be modified by trading NU for SWU through adjustment of the tails assay from the enrichment process. This trade-off causes the demand curve for Figure 7 to be non-vertical; if it were not present, in the short run utilities would always require the same amount of NU (or its equivalent) to fuel reactors regardless of uranium price. The supply curve has horizontal parts, it means that multiple producers (U mines) offer uranium for the same price in given time period.

The demand curve creation mechanism was developed and described in the reference model (Schneider et al., 2013), in short the algorithm involves finding the NU price P_U [$/tonne U] for which each tails weight fraction would be cost-minimizing when NU, SWU and conversion costs (for conversion services purchased at user-specified price PC [$/tonne U], Table 3.) are all incorporated. The cost C [$/yr] of making LEU hexafluoride is given by summing the costs of purchasing uranium, conversion services and SWUs:

$$C = (P_U + P_C) \cdot U_d + P_{SWU} \cdot SWU_d + P_U \cdot NU_d \qquad (14)$$

Here NU_d is the (fixed for the time interval) NU demanded by reactors consuming unenriched uranium as fuel (i.e. CANDU rectors), while U_d is the demand for NU to be enriched to LEU. To find the NU price for which a DU ^{235}U weight (fissile uranium isotope with atomic mass number 235) fraction x_w minimizes C, Equation 14 is differentiated with respect to x_w, holding the other parameters constant, set equal to zero, and solved for P_U. The process is laborious because U_d and SWU_d depend from LEU tails weight fraction. It results in quite complex series of equations:

$$0 = (P_U + P_C)\frac{\partial}{\partial x_w}\left[\frac{x_p - x_w}{x_f - x_w}\right] + P_{SWU}\left[\frac{\partial}{\partial x_w}\left[\frac{x_p - x_w}{x_f - x_w}\right]\left(V(x_w) - V(x_f)\right) + \left[\frac{x_p - x_w}{x_f - x_w} - 1\right]\frac{\partial V(x_w)}{\partial x_w}\right], \qquad (15)$$

where

$$\frac{\partial}{\partial x_w}\left[\frac{x_p - x_w}{x_f - x_w}\right] = \frac{1}{x_f - x_w}\left(\frac{x_p - x_w}{x_f - x_w} - 1\right) \qquad (16)$$

and

$$\frac{\partial V(x_w)}{\partial x_w} = -2ln\left(\frac{1 - x_w}{x_w}\right) - \left(\frac{1 - 2x_w}{1 - x_w}\right)\left(1 + \frac{1 - x_w}{x_w}\right), \qquad (17)$$

where x_f : NU feed ^{235}U weight fraction is known $x_f = 0.00711$; x_p: ^{235}U product fraction.

This expression can be rearranged to solve for P_U. The process is repeated for each tails 235U weight fractions on 0.1% to 0.4% ^{235}U, resulting in a set of (U_d, P_U) points. Each point defines 'the best' the industry can do if it is able to purchase uranium at P_U: purchase U_d kg of NU, tell enrichment plant operators to take tails to DU ^{235}U fraction x_w, and purchase SWU_d separative work units at the market price P_{SWU}. The set of points then traces out the demand curve, see in Figure 7.

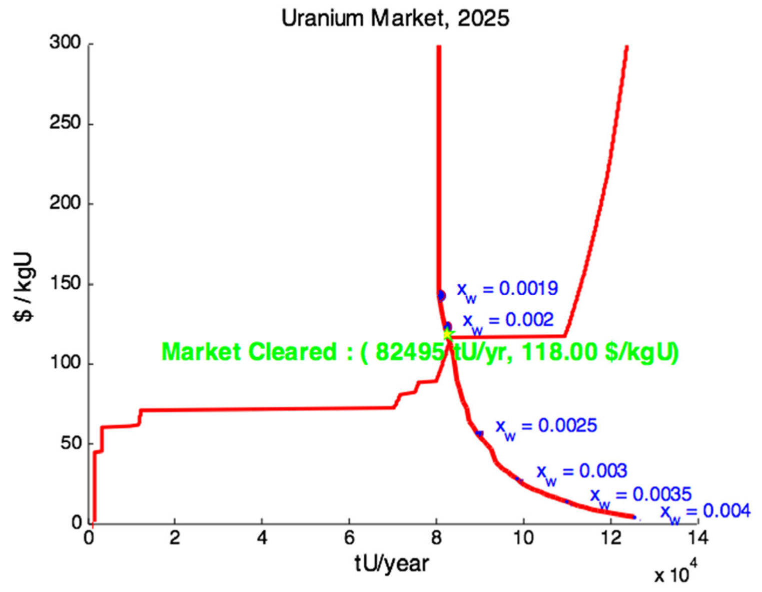


Figure 7. Uranium market supply and demand curves in 2025.

Table 3. Global input parameters

Description	**Mean Value**
World LEU fuel demand in 2010	6790 tonnes/yr
World NU fuel demand in 2010 *	3390 tonnes/yr
Average ^{235}U content of LEU fuel	4.3 wt%
World LEU & NU fuel demand growth rate	2.6%/yr
Year continuous enrichment facility capacity growth commences	2018
Enrichment facility capacity growth rate	2.6%/yr
Cost of yellowcake-to-fluoride conversion	$10/kg U
WGPu fraction in MOX**	5 wt% of IHM
^{235}U content of HEU downblend stock	0.25 wt%
Uranium Production Cost Multiplier	1.0
SWU Production Cost Multiplier	1.0
Mine Capacity Factor Multiplier	1.0

* Certain reactors, e.g. CANDU, consume fuel fabricated from unenriched natural uranium.
** Mixed oxide fuel

7.3. A uranium market clearing model general sandbox scheme

A uranium market clearing model is written in the MATLAB programming language, which is quite commonly used in academia and allows generate graphs without additional packages. The main NFC module structure is built from several components and graphically can be seen in Figure 8:

1. Database and input parameter block – contains information about U mines, secondary supply sources, enrichment services and other parameters.
2. The model core – marching through simulation time period and executes subcomponents logic.
3. Supply block – contains from several logical structures, i.e., individual U mine's decision – making algorithm, mine's supply curve construction logic, market supply curve construction, demand curve construction and market price calculation logic.
4. Economic characteristic calculation block – contains logic which calculates actual selling and individual U mines profit or loses in given time period. As well this block contains logic, which decrement U mines reserves.
5. Output data collection – store information about every simulation time period and construct graphs.

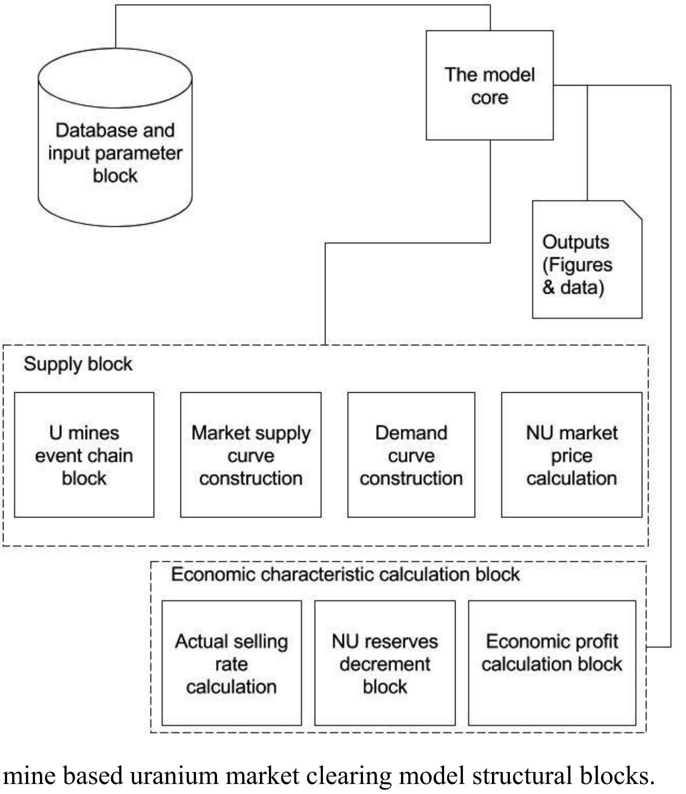


Figure 8. A mine based uranium market clearing model structural blocks.

8. AN AGENT-BASED MODELLING APPROACH

The agent-based modelling concept is widely used in energy systems modelling (Lakić et al., 2015; Gonzalez de Durana et al., 2014) and other fields to model individual agent's behavior in ecosystem where each agent solves optimization task and makes individual decisions. In such a way it allows to model the behavior of a system by simulating the behavior of each individual agent. In the nuclear fuel cycle simulators this concept is used in the Cyclus project, which is the next-generation agent-based nuclear fuel cycle simulator where each components act like an agent plugged to the main engine (Matthew et al., 2014).

The current model uses a cycle type ABM approach that can be broken down into three steps:

1. Initialize the model and uranium mines as agents with input parameters, global constraints and initial market conditions.
2. Each agent observes outside information, i.e., uranium market price.
3. Each agent takes an action based on the current observations, and the model repeats by going back to 2.

This cycle becomes an adaptive ABM if we incorporate a fourth step between 1 and 3 where each agent updates their internal parameters, and decides what action to take based on that internal model. The structural scheme of such approach can be seen in Figure 9 (Wolpert et al., 1999).

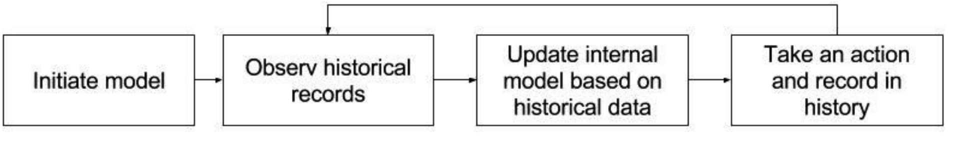


Figure 9. An adaptive ABM concept.

In majority of cases agents are small units in large ecosystem, where single unit decisions cannot affect whole ecosystem. In a uranium mine based market clearing model an individual agent can represent large U mine, which has significant effect on a uranium market share. Therefore, such agents have weight fraction on NU market and individual decisions can affect market price. An ABM decision making capability can be built with multiple techniques depending on needs. In case, if is requires agents which can learn and develop new decision dynamically a machine learning concept must be used. Neural networks for instance, are good at classifying large amounts of data very quickly, but in the end, they do not yield how decisions are actually taken. Therefore, complexes reverse engineering procedure need to be applied and in many cases decision has no rational explanation. Alternative options is to use decision trees to create very white box results, but are not very good at classifying continuous data. There are variety information in literature that discuss machine learning algorithms, their implementations and their pros and cons (Mitchell 1997; Hastie, Tibshirani et al. 2001).

8.1. Uranium mine agent decision tree

During each year of the simulation the market clearing model uses the decision tree criteria summarized at the beginning of this section to determine whether each mine will operate. It then must decide how much uranium the mine will contribute to the total amount supplied across the industry. The model simulates the uranium market for each year of the simulation using the following scheme, starting with the first year of the simulation ($t = 1$) and running through the last year, $t = T$ and is built around the database that contains information about mines availability for production, annual production capacity and total reserves (Eggert et al., 2011). This loop is visualized in Figure 10:

1. The supply curve is drawn by finding the amount supplied as a function of price. To begin, the market price is set to 0.
2. The secondary supplies are added to the supply curve.
3. The offer loop is performed for the set price. In this step the model determines which mines are operating and how much material they are producing. The offer logic is described below.
4. The total suppliable amount from the available mines in current time period at the set price level is summed to determine the cumulative supply.
5. A check is performed to see if the current model price is equal to a user-specified maximum modelled price.
    a. If the market price equals the maximum, proceed to step 6.
    b. If the market price is not yet equal to the maximum price, the market price is increased by a small user-specified increment and returned to step 2 above.
6. The supply curve is now drawn. The uranium demand curve for the time step is next drawn using methods that were described in (World Nuclear Association, 2008).
7. The intersection of the supply and demand curves is found and determines the market price for the time step.
8. The mine reserves are updated by deducting the offered amount (quantity supplied at the market price) from each mine currently operating. This block simulates actual market where U supplier meets its buyer. Here are few predefined conditions about priorities for new market participants and a long-term player. Predefined rules are important in case when multiple U mines try to sell uranium by the same price. In this case can be said, that U mines has equal chance to sell uranium. The predefined selling chance conditions for U mines are:
    a. The model checks whether mine sold uranium in a previous simulation time period. If U mine was selling uranium in a previous simulation period, that such mines has advantage over newly market players. Such condition simulates long term relationship between supplier and buyer.
    b. Cheaper producers, has bigger probability to sell more uranium in a market and make bigger profit.

9. The current time of the simulation is checked against the value of the simulation end time (*T*).
    a. If $t < T$, time is incremented by one year and the loop restarts.
    b. If $t = T$ the simulation ends.

Inside the offer loop, the following operations are performed for each mine in the simulation, starting with the first mine ($n = 1$). The loop is visualized in Figure 11:

1. The mine is checked for availability. Any mine not currently able to operate in the given year is unavailable.
    a. If the mine is not available, skip to the next mine.
    b. If the mine is available, proceed to step 2.
2. The mine is checked for operation in the previous time step.
    a. If the mine operated in the previous time step, go to step 3.
    b. If no uranium was produced by the mine in the previous time step, proceed to step 4.
3. The E_2 of the mine is check against the current market price.
    a. If E_2 is greater than or equal to the market price proceed to step 5.
    b. If E_2 is less than market price the mine enters temporary shutdown and the model restarts at step 1 with the next mine.
4. If the mine did not operate in the previous time-step, the current market price is checked against the mine's E_1.
    a. If E_1 is greater than or equal to the market price, a new mine is opened and the model proceeds to step 5.
    b. If E1 is less than the market price, the loop restarts with the next mine.
5. The mine is flagged to produce uranium during the current time step.
6. A check is made to determine if the current mine is the last mine in the simulation (n = N).
    a. If true, the loop ends.
    b. If false, the loop is restarted with the next mine in the list.

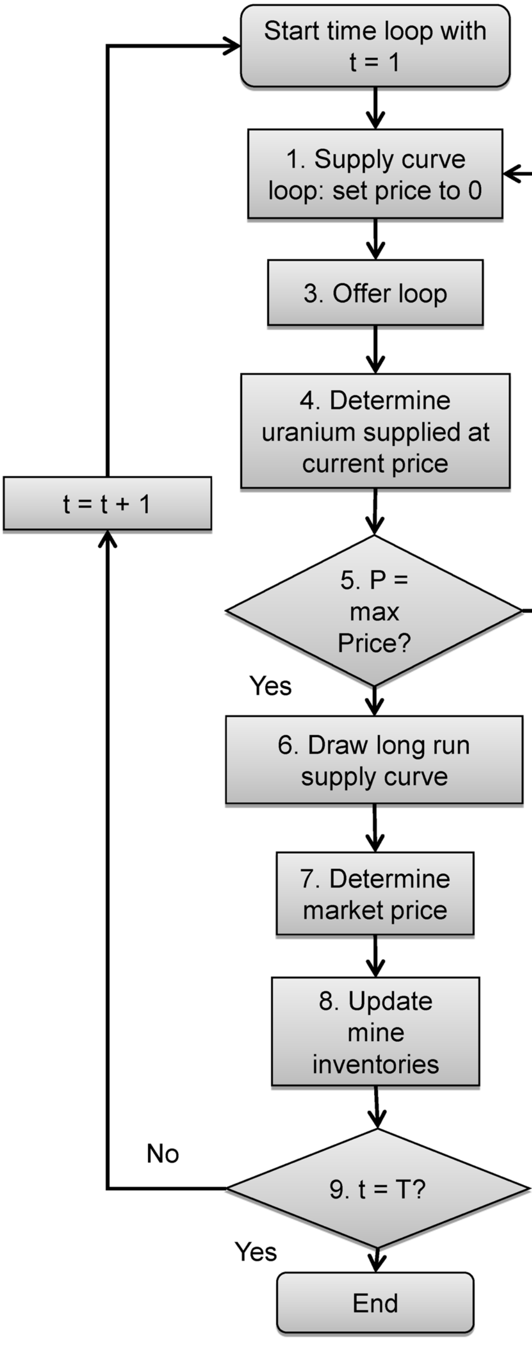


Figure 10. The main time loop algorithm.

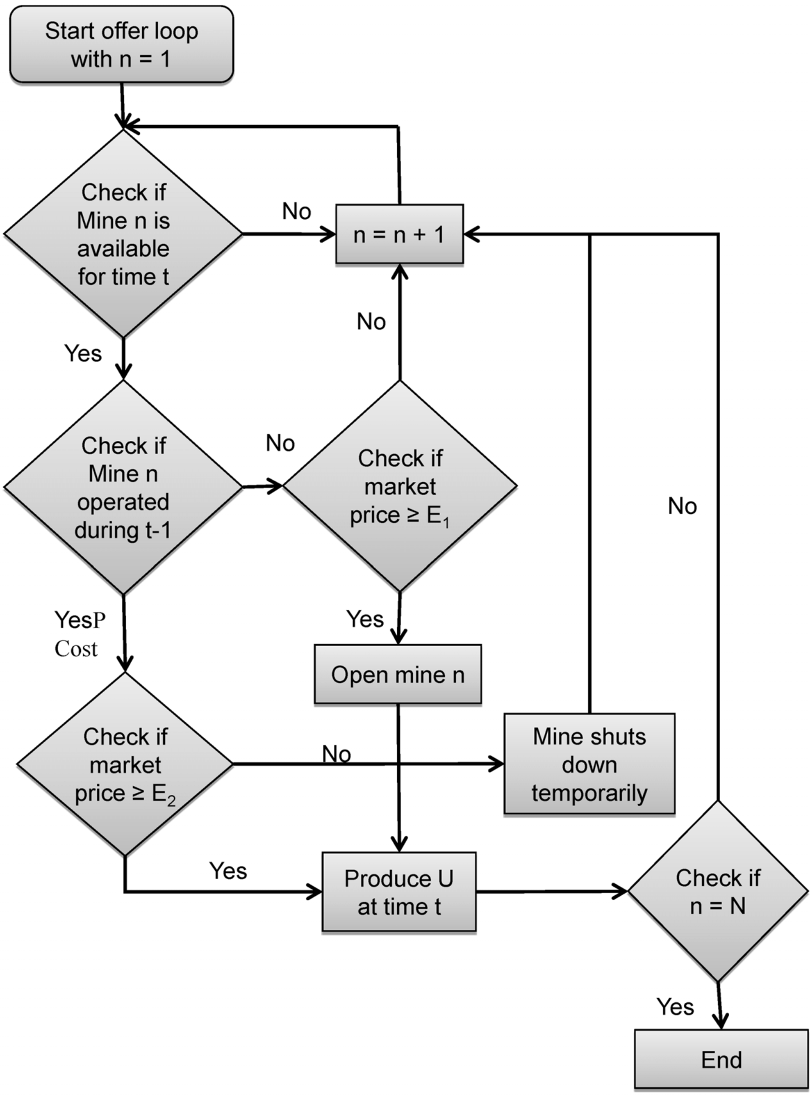


Figure 11. Uranium mine operation decision making event chain.

8.2. Uranium mine agent with profit accumulation and time delay function

The profit accumulation and time delay function are an extension of main operation decision event chain described in previous section and displayed in Figure 11. In certain U market conditions the natural U price can fall and stay relatively low for several years. In such case we introduce the loss minimization logic, which allows keep open U mine under the long run market exit price and use accumulated profit to cover marginal costs. U mine will bankrupt when all accumulated profit is used and a market price is under the long run market exit price. In such case the model will try to open U mine once again after several years (depends from the model configuration), if the market conditions will satisfy U mine economic parameters. In such case the annual profit calculation logic will start calculation from reopening year. The opening and reopening time delay will reduce the supply since uranium producers will enter the market slower when the conditions are favorable. Their tolerance to continue operating is based on their accumulated profits. The excess liquidity are high enough to cover operation and maintenance (OM) costs and keep mine open until market conditions become more favorable. This will make the market much more volatile than modelled in a mine-based U market clearing model and resemble the actual market behavior more realistically. We assumed, that reopening delay time simulate U property ownership change and related legal issues and mine relicensing. However, the time delay function did not include additional costs that are related to U mine reopening.

The enhanced decision making is applicable in each simulation time step, where the model calculates annual profit or losses based on actually sold U amount by current market price. In case if U mine was working with the profit, certain share will be paid out to shareholders, other part will be diverted to the special accumulated profit fund. We will use a dividend payout ratio of 55% which was the average payout ratio for the mining industry in 2012 (Canadian Nuclear Safety Commission, 2007). It has to be noted that the exact value of the payout is irrelevant and rather the sensitivity of the payout ratio to economic value is analyzed.

In Figure 12 the accumulated profit calculation algorithm is shown.

1. For each mine in the simulation, starting with the first mine (n = 1), module is finding accumulated profit calculation start time.
2. Checks if accumulated profit calculation time is less than current time period.
   a. If $T_{st} < T$, continue with a sold quantity check in the time period T_{st}.
   b. If $T_{st} => T$, continue with accumulated profit check.
3. Check, if quantity that is sold by the calculation period market price, can cover mine's running costs (OM).
   a. If running costs is covered, calculate profit.
   b. If running costs is not covered, calculate loses.
4. Sum annual profit or loses in the time period T_{st} taking into account dividend payments.
5. Increase valuation time step $T_{st.}$
6. Check if a mine is not operating with losses in the financial lifetime.
   a. ACC > 0, in the current calculation period mine is working with profit; ACC calculate for the next period.
   b. Continue with the suspended operation check.
7. Check if U mine operation was suspended due to bankruptcy.
   a. U mine is not bankrupt, continue calculation for next time period.
   b. U mine is in bankruptcy, exit from accumulated profit calculation loop.

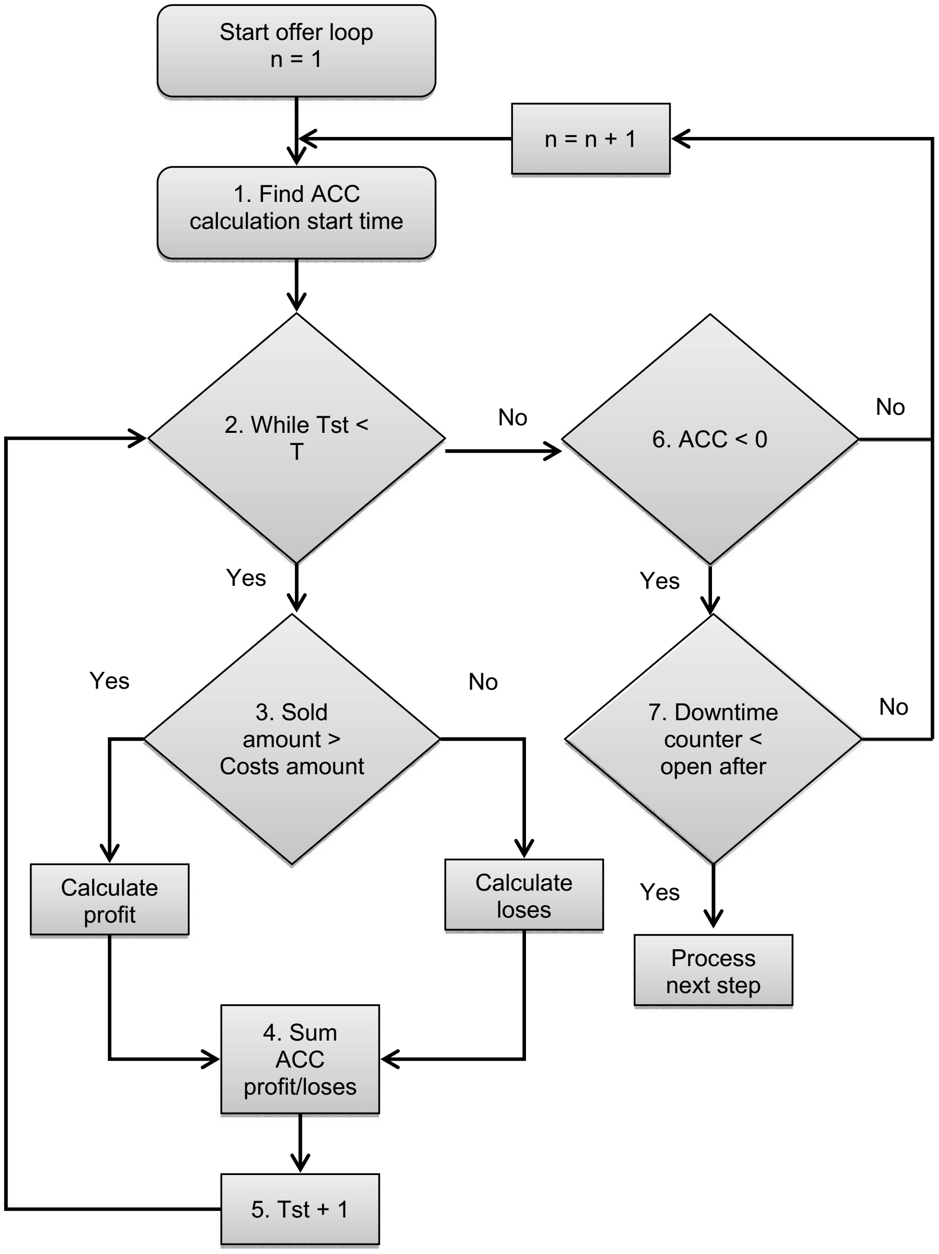


Figure 12. Uranium mine accumulated profit event chain.

9. ECONOMICAL EFFECT EVALUATION IN A MINE BASED URANIUM MINING MARKET CLEARING MODEL

The features added to the model, i.e., profit accumulation and decision delay functions makes model more realistic and the economic value of these changes can be measured and compared to the mine-based market clearing model results. By default, a mine-based U market clearing model does not take into account uranium mine licensing issues and other operational activities, allowing for new mines to open, reopen or shut down instantly. The time which is needed to reopen the mine is closely related to the economic and regulative environment and often is not solely dependent on the producer's decision. The profit accumulation function simulates ability to distributes some of the earnings back to investors and retains rest of the earnings for the future needs to cover mine fixed costs such as maintenance and labor costs whenever the marginal costs are below the average total costs.

The time delay will reduce the supply since uranium producers will enter the market slower when the conditions are favorable. Their tolerance to continue operating is based on their accumulated profits. The excess liquidity is high enough to cover operation and maintenance (OM) costs and keep mine open until market conditions become more favorable. This will make the market much more volatile and resemble the actual market behavior more realistically. The latter is also presented in Figure 13. In an ideal market where supply and demand are ideally matched the price would always stay the same over time if no shocks occur in the marketplace. This is reflected as scenario S* on the chart. The line S_1 represents a case where U mines enter or exit the market whenever market price is favorable to mines. The line S_2 reflects the case with time delay and profit accumulation function so miners will constantly over- and underreact to current situations causing more volatility in the marketplace.

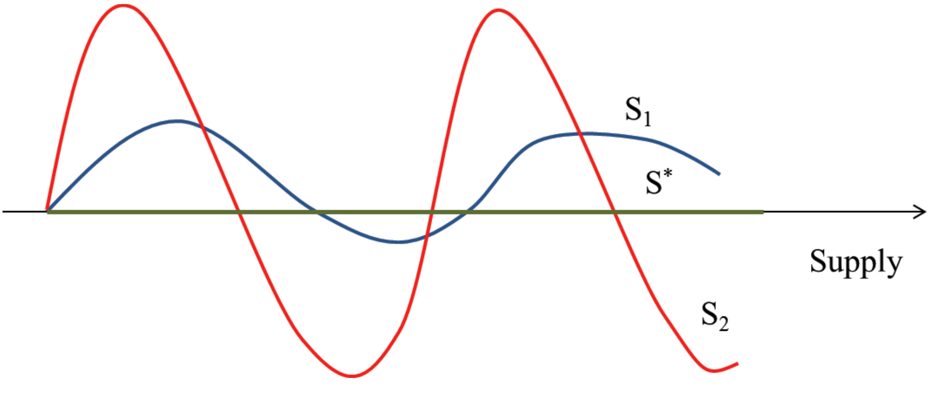


Figure 13. Uranium market supply curves

9.1. Profit accumulator model effect on an individual uranium mine

Operational decisions are based on the current market price and accumulated profits. If the current market price exceeds marginal costs the producer is operational. If the current market price (P) is below marginal costs per unit (MC) the producer can stay operational until the producer is able to cover the losses from producing the anticipated quantity (Q) with accumulated profits (П). Accumulated profits are defined as:

$$\prod = \prod_{t-n} \times R + \cdots + \prod_{t-1} \times R, \tag{18}$$

where R demounts the share of retained earnings and n stands for the number of periods included in the model, whereas 1-R reflects the share of earnings that are distributed to shareholders. Hence the condition for operating is the following:

$$\prod - Q \times P \geqslant 0. \tag{19}$$

If the company is unable to continue production, it will shut down its operations instantly until the current market price exceeds production costs per unit. At that time a decision will be made to reopen the mine. Reopening the mine takes time and is dependent on the time required for obtaining operating licenses, hiring personnel and restarting other operations (T) (PwC, 2013). Such a behavior leads to over and underreacting in the marketplace. The economic logic is illustrated on Figure 14.

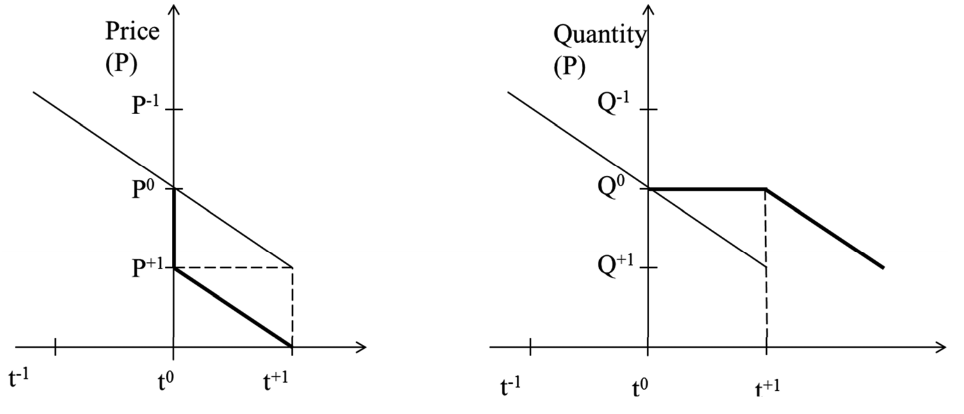


Figure 14. Individual uranium mine production regulation

Whereas in mine based market clearing model the miners would reduce the amount of production to Q^{+1} or even 0 if the price were below the marginal cost or production price P^0 then in the model with profit accumulation logic built in the miner keeps the production rate the same at period t^{+1} causing the miner to overproduce. This leads to increased supply in the marketplace causing prices to drop from P^0 to P^{+1}.

9.2. Economic value and price dynamic calculation

The introduction of profit accumulation model and time delay in reopening the mines is expected to increase volatility in the market. The profit accumulation model assumes that companies will stay in operation even if their production costs per unit are higher than the current market price. Changes in the current market price decrease new mines entering the market. When new producers enter the market the supply curve shifts to the right and price decreases from P_1 to P_2, quantity increases from Q to Q_* as is shown in Figure 15. Since mines do not shut down instantly which would instantly reduce supply and make the supply curve shift to the left again the quantity stays the same (or increases if new producers would enter the market) until the producers run out of accumulated profits.

When individual mines go bankrupt the supply curve starts shifting to the left (slowly) but if there are enough producers operating in loss the number of bankruptcies increases suddenly and the supply curve makes a sudden shift to the left causing price to increase suddenly. Price increase allows less efficient producers to become profitable again and mines make the decision to reenter the market. Because there is a time delay a lot of producers enter the market at the same time causing sudden increase in supply and sudden drop in the price leading to new wave of bankruptcies.

This leads to much higher volatility on the market compared to conditions where producers can enter and exit the market instantly and make decisions based on current market price.

A number of different scenarios are analyzed where two variables – share of profits and time delay – and their sensitivity are analyzed based on the economic value of the scenario compared to base scenario. The economic value (EV) is defined as the total change in market value of the produced uranium. We can calculate the economic value for a certain time period according to the formula:

$$\mathrm{EV} = P_1 \times Q_* - P_2 \times Q_*. \tag{20}$$

The economic value is positive when the total market value of the produced uranium increases and negative when the market value of produced uranium decreases. In that sense EV is that change in market value.

The value of EV depends on the steepness of the demand curve near the current equilibrium price. The steeper the demand curve near the current equilibrium price the bigger is the price decrease and smaller the change quantity. With steep demand curve the EV is negative. Since we expect the demand to be relatively rigid the demand curve is steep – price changes don't significantly increase or decrease consumption since demand is relatively non-elastic. Hence scenarios that include bigger price changes are expected to have more significant impact on the economic value.

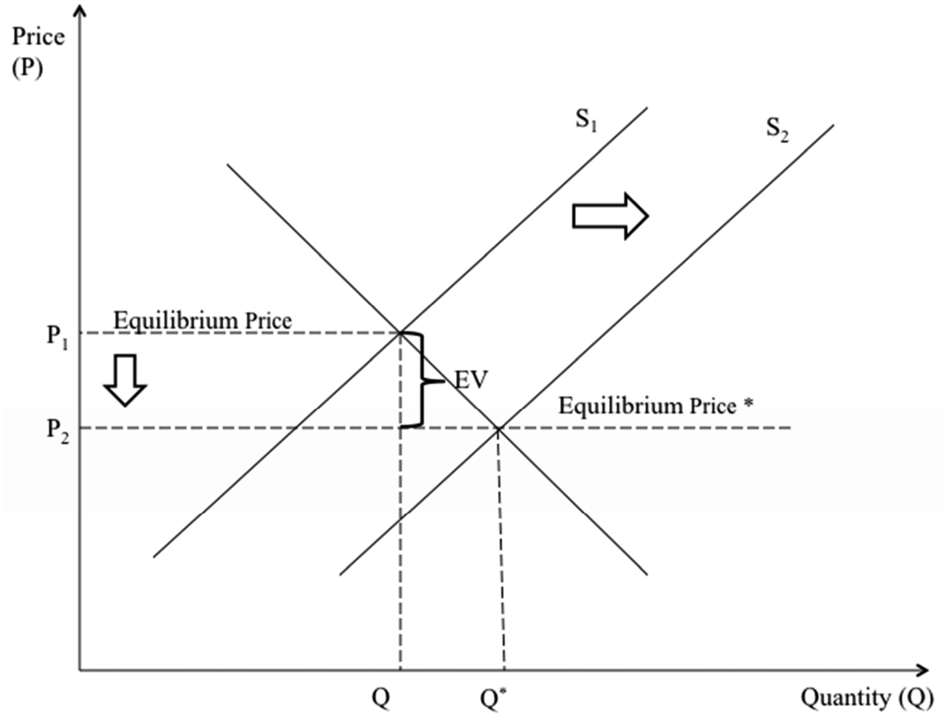


Figure 15. Market price and supply changes

10. AN OPTIMAL NFC EVALUATION WITH MASS EQUILIBRIUM MODEL (BASED ON PUBLICATION III)

Previous sections outlined possibility to simulate individual U mines decision making strategy and focused only on front-end nuclear fuel cycle. This section will present an autonomous dynamic decision-making tool in a nuclear fuel cycle simulator, which verifies optimal NFC bases on the expected cost of electricity (CoE) as the simulation driving factor. In the most of the NFC simulators such as VISON, GENIUS or NFCSim must be manually specified certain NFC to be simulated, or total produced energy demand for nuclear power and a target NFC with specific reactor's technologies allowed to be built subject to satisfaction of material balance model. (Schneider et al., 2003;Schneider et al., 2005; Oliver 2009). A mine-based uranium market clearing model does not focus on an actual NFC, but tries to satisfy NU demand which is determined with predefined growth rate.

A key capability of the model described here is to solve optimization task and find optimal NFC based upon objective criteria. Such capability is achieved by issuing automatic reactor technology building. Based on optimization aim, defined by the multi-criteria objective function, the agents might make certain technology deployment decision. In principle, any objective function representing a combination of different criteria, for example, the costs of electricity, natural resource consumption reduction, nuclear materials proliferation risks minimization, can be defined. Later the reactor build decision can be based upon optimization problem solving. In a real life, the highly nonlinear nature of the constraints imposed by the time-dependent material balance, that compose the objective function, cause decision-making very difficult to by implemented. This section demonstrates generalized autonomous decision making approach that is based on minimization of cost of electricity (CoE) alone. However there are no limits to extend the objective function with multiple criteria. A nuclear fuel cycle and cycle economy simulation tool VEGAS is used to find optimal reactor technology mix. The tool is written in Java™ programming language (Juchau et al., 2011). VEGAS uses traditional present-value levelized cost of electricity (LCOE) analyses to calculate reactor and fuel cycle costs. In VEGAS each defined reactor is described with capacity (MWe) and lifetime, along with other economical parameters. The tool assumes that each reactor will always serve out their complete lifetime operating at their full capacity. VEGAS is built to compute individual nuclear reactor input and output mass flow in each simulation time step, avoiding from overhead to track individual fuel batches isotopic composition. Such approach is acceptable, when calculation is applied over a long period and the aim is simulate many reactors and different technologies. VEGAS tracks nuclear materials in entire simulation period and consider required cooling time of spent fuel to meet safety and technical requirements for reprocessing. Whenever VEGAS detects energy supply deficit, it tries to deploy new reactor to meet the specified energy demand. Since the tool simulates entire reactor lifetime, then is highly likelihood that some nuclear reactors burn fuel which made of reprocessed spent fuel of other reactors and will not be able to operate because of fuel shortages. Such behavior leads the simulator to roll back simulation clock in time when the most recent reactor of the type with the fuel shortage was built and replacing it with a different type of reactor and other fuel. This rolling back algorithm is repeated until the simulation is finished at defined simulation period and all reactors being fully operated in entire simulation time. Before the improvements the simulation was designed in a way that it added new facilities based on time-dependent build priorities specified by user. The main concept how VEGAS works is to ensure that reactor is always operation in entire lifetime. It relies on predefined user scenery as to when and how to begin deploying new technologies. In addition to the predefined technology mix the user could manually determine economically attractive scenarios.

Optimization based upon nuclear fuel cycle cost ideally includes a degree of foresight. The full mathematical optimization would require complete foresight of many economic parametrs, but that is arguably not a realistic depiction of how agents make decisions. In a real life agents also make decisions which include some degree of freedom. In VEGAS NFC simulator decisions will be made on the basis of the CoE-minimising equilibrium fuel cycle. Any combination of reactor types can meet the equilibrium fuel cycle condition which means that at least one hard material balance constraint must be satisfied. An equilibrium conditions is described by a specific reactor technology deployment ratio.

As example can be given fuel cycle with light water reactors (LWR) and low-conversion ratio fast neutron reactors. Such fuel cycle has equilibrium of ~2.5 MWt of LWRs deployed/MWt of fast reactors deployed. (OECD Nuclear Energy Agency, 2002). This equilibrium state means that to satisfy material balance constraints the fast neutron reactors are fissioning the transuranic elements at the same rate as they are being produced in the LWRs. This simulation approach requires finding the equilibria state for all possible nuclear fuel cycles depending from technology mix. Currently are many commercially available nuclear reactor technologies and in the foreseeing time even more technologies are likely to become available. Even to find an equilibrium fuel cycle become challenging if many of the technologies are made available to the simulation and each technology is a member of different fuel cycle. Once equilibrium state is achieved then the CoE for each equilibrium cycle may be calculated. Later on build decision can be based on newly acquired equilibrium conditions. The equilibrium costs might also have time dependent stochastic nature since the composition of CoEs includes multiple criteria, such as uranium price, labor costs etc. Thus, this simulation approach can track the changes in the targeted equilibrium by adjusting technologies and react to uranium price changes. As well the simulator can switch between fuel cycle types – from once-through to a closed fuel cycle (OECD Nuclear Energy Agency, 2002; Shropshire et al., 2009).

10.1. Nuclear fuel cycle tree

A simplified NFC model is allowed to consist of up to three types (tiers) of reactors hierarchically reprocessing each other's fuel. The model represents both nuclear fuel cycles, i.e., once-through and closed. In VEGAS, the composition vector for nuclear reactor fuel has 4 lumped components: uranium (U), plutonium (Pu), minor actinides (MA) and fission products (FP), but the approach proposed here generalizes to more finely resolved composition vectors. A flowchart for such an NFC is illustrated in Figure 16, which shows how reactors are assigned to a tier based on if and what they are capable of reprocessing. Tier 0 usually means a thermal neutrons spectrum reactor burning uranium fuel where belongs most of current nuclear reactors. The Tier 1 denotes plutonium burning reactors while tier 2 is represented by transuranic (TRU) element burning reactors, possibly capable of reusing their own reprocessed spent nuclear fuel (SNF). The SNF from a reactor can be either sent to waste or be reprocessed to fuel the next tier reactors, or in the case of tier 2, to fuel itself (Pelakauskas et al., 2013).

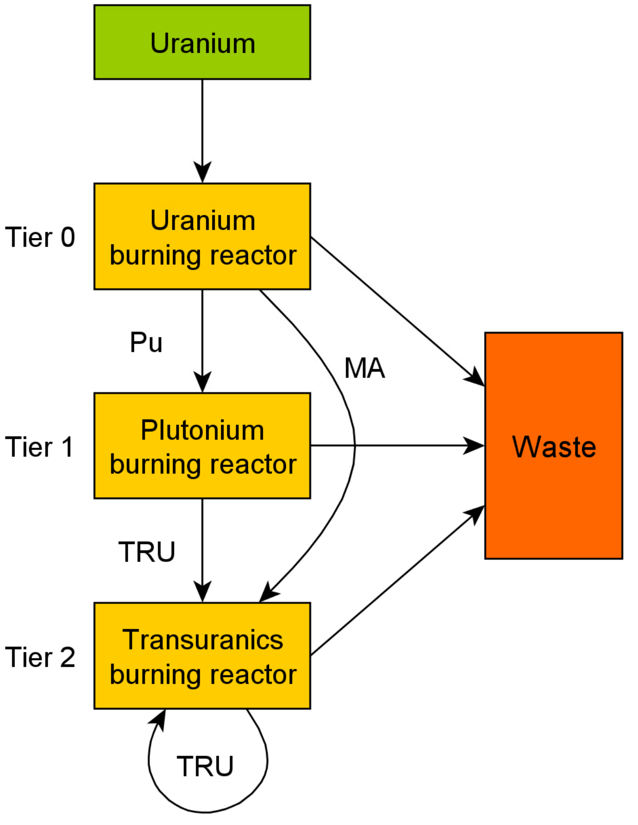


Figure 16. A Typical NFC flowchart

10.2. Nuclear fuel cycle equilibrium calculation

For all possible combinations of reactor types, the mass equilibrium model calculates the relative throughput of materials in each NFC facility based on defined charge and discharge compositions for each reactor type. The tier 0 is a primary technology with which all other technologies must work in equilibrium to consume the generated plutonium or transuranic materials.

To carry out calculation of mass flow equilibrium for a technology mix that is identified in the previous section, the technologies is categorized by all possible NFC types:

1. Once-through fuel cycle (includes tier 0 only). Currently describes existing nuclear reactor fleet in the world, which represents LEU burners and CANDU reactors.
2. Pu recycling scenario (tier 0 and tier1). This NFC includes MOX fuel burners;
3. TRU recycling scenario (tier 0 and tier 2; or tier 0, tier 1 and tier 2, or tier 2 only for a breeder reactor).

The mass equilibrium calculation process is described in the next equations and is repeated from autonomous dynamic decision making in a nuclear fuel cycle simulator methodology. Input natural uranium mass is found from equation 21 which calculates uranium needed as feed for the enrichment process per kilogram of product:

$$F = P\frac{x_p - x_w}{x_f - x_w}, \qquad (21)$$

where F – number of kilograms of feed material, P – number of kilograms of product enriched, x_w – weight fraction of ^{235}U in the waste, x_p – weight fraction of ^{235}U in the product, x_f – weight fraction of ^{235}U in the feed material.

Input and output composition recipes are used to obtain the tracked heavy metal (U, Pu and MA) mass streams at equilibrium for each flow shown in Figure 17. The recipes along with other parameters of the reactors selected for the test case are given in Table 4 and are taken from (OECD Nuclear Energy Agency, 2002). Refer to Figure 17 for definitions of mass flows and symbols used in this section. The input U fuel mass, M_0, is initially normalized to 1 kg. The remainder of this section outlines the calculation of the masses M_1 and M_2 of tier 1 and 2 reactor fuel per unit mass of tier 0 reactor fuel. The M_1 stream is calculated according to:

$$M_1 = M_0 y_{Pu,0} + \frac{M_0 y_{Pu,0} x_{U,1}}{x_{Pu,1}}, \qquad (22)$$

where $y_{Pu,0}$ – output Pu mass fraction from tier 0 reactor, $x_{U,1}$ – uranium input fraction in tier 1 reactor, $x_{Pu,1}$ – Pu input fraction in tier 1 reactor.

The TRU burner reactor (tier 2) fuel mass may be limited by the availability of either Pu or MA. The MA available to the tier 2 reactor, m_{MA}, comes from the reprocessed tier 1 fuel and tier 0 reactors' MA that bypassed tier 1:

$$m_{MA} = M_1 y_{MA,1} + M_0 y_{MA,0}\,, \tag{23}$$

where $y_{MA,1}$ – output MA fraction from tier 1 reactor, $y_{MA,0}$ – output MA fraction from tier 0 reactor.

The mass stream M_2 calculation in the case when the TRU burner reactor is limited in its deployment by availability of MA and does not reprocess its own fuel is described in equation 24:

$$M_2 = m_{MA} + \frac{m_{MA} x_{U,2}}{x_{MA,2}} + \frac{m_{MA} x_{Pu,2}}{x_{MA,2}}\,, \tag{24}$$

where $x_{U,2}$ – uranium input fraction in tier 2 reactor, $x_{MA,2}$ – MA input fraction in tier 2 reactor, $x_{Pu,2}$ – Pu input fraction in tier 2 reactor.

When TRU burners reprocess their own fuel and are MA-limited, M_2 is given by:

$$M_2 = \frac{m_{MA} + \dfrac{m_{MA} x_{U,2}}{x_{MA,2}} + \dfrac{m_{MA} x_{Pu,2}}{x_{MA,2}}}{1 - \dfrac{y_{MA,2}}{x_{MA,2}}}\,, \tag{25}$$

where $y_{MA,2}$ – output MA fraction from tier 2 reactor, $x_{MA,2}$ – MA input fraction in tier 2 reactor.

When the TRU burner reactors reprocess their own fuel and are Pu-limited, M_2 is given by:

$$M_2 = \frac{M_1 y_{Pu,1} + \dfrac{M_1 y_{Pu,1} x_{U,2}}{x_{Pu,2}} + \dfrac{M_1 y_{Pu,1} x_{MA,2}}{x_{Pu,2}}}{1 - \dfrac{y_{Pu,2}}{x_{Pu,2}}}\,, \tag{26}$$

where $y_{Pu,1}$ – output Pu mass fraction from tier 1 reactor, $x_{U,2}$ – uranium input fraction in tier 2 reactor, $x_{Pu,2}$ – Pu input mass fraction in tier 2 reactor, $y_{Pu,2}$ – output Pu mass fraction from tier 2 reactor. Whichever of the constraints (Pu limited or MA limited) leads to the smaller value of M_2 is the actual limiting constraint.

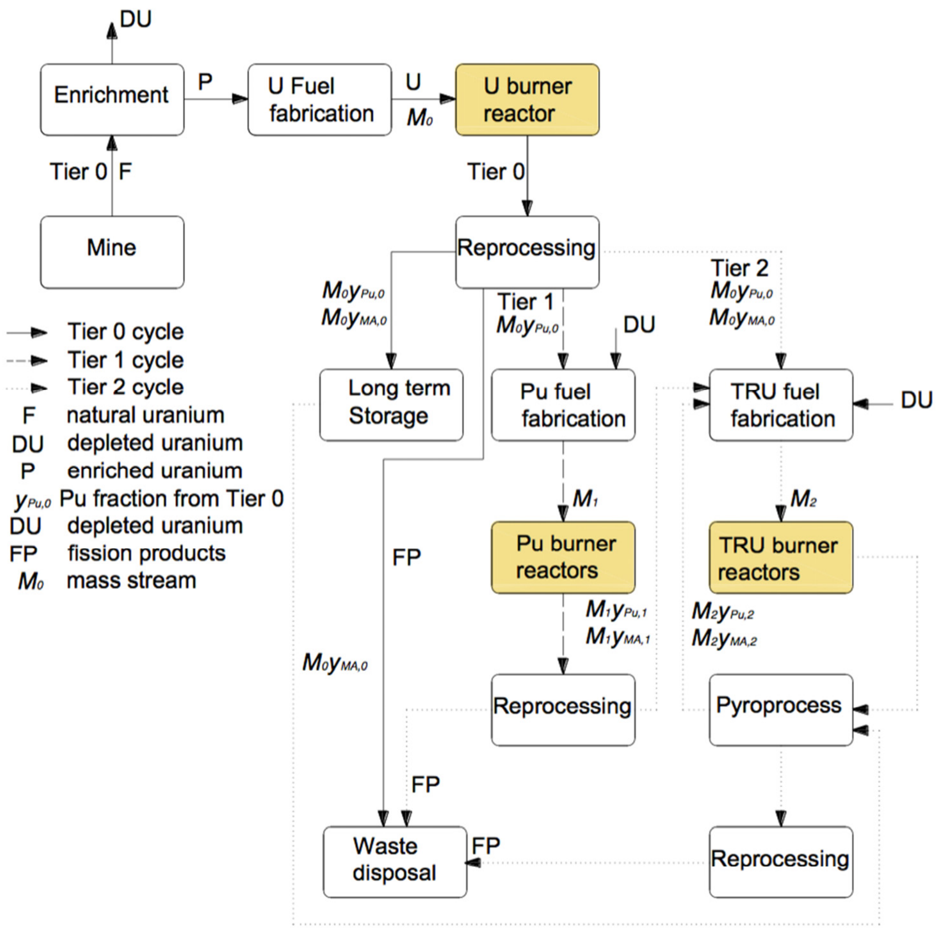


Figure 17. Equilibrium mass flows through a generic three tier NFC. Solid line arrows show the flow of uranium fuel, dashed arrows show the flow of Plutonium fuel and dotted arrows show the flow of TRU fuel.

Table 4. Parameters of the nuclear reactors selected for the test case. The current fleet approximates the mix of Pressurized Water Reactors (PWR) and Boiling Water Reactors (BWR) currently operating in the USA. APWR-UOX is an Advanced Pressurized Water Reactor burning uranium Oxide fuel. SFR is a Sodium Cooled Fast Burner Reactor.

Reactor name	Current fleet	APWR-UOX	SFR
Tier	0	0	2
Plant size (MWe)	900	1450	600
Thermal efficiency (%)	35	35	42
Availability (%)	90	90	85
Input U enrichment (%)	4.2	4.9	0.25
Input U mass fraction, x_U	1	1	0.669
Input Pu mass fraction, x_{Pu}	0	0	0.291
Input MA mass fraction, x_{Ma}	0	0	0.0398
Output U mass fraction, y_U	0.93595	0.92466	0.5931
Output Pu mass fraction, y_{Pu}	0.01110	0.01194	0.24769
Output MA mass fraction, y_{Ma}	0.00129	0.00160	0.030
Minimums cooling time (years)	4	4	4
Can reprocess SNF from	–	–	SFR, APWR-UOX

10.3. Cost of electricity calculation

The methodology for costs of electricity calculation is taken from autonomous dynamic decision making in a nuclear fuel cycle simulator. The cost of electricity (CoE) calculation consists of 3 major components: reactor construction (RC), operations and maintenance (OM) and fuel cycle costs (FCC), and is given in equation 27. Reactor construction costs reflect yearly reactor construction loan payments. OM costs represent all the services required to assure normal operation of the reactor. FCC includes all the costs related to fresh and spent fuel.

$$CoE = RC + OM + FCC \tag{27}$$

The RC part of the CoE can be expressed in units of \$/kWh as:

$$RC = \frac{K}{E_y} \frac{r}{1-\left(\frac{1}{1+r}\right)^{T_0}} \tag{28}$$

where K is the total capital investment cost in \$, E_y is the yearly energy production in kWh/year, r is the invest rate of capital in units of 1/year and T_0 in years is the number of years in the repayment period. K is related to the overnight construction cost by:

$$K = \sum_{i=1}^{T_C} \frac{C_O}{T_C} (1 + r)^i \tag{29}$$

where C_O is the overnight construction cost in \$ and T_C is the construction period in years.

The OM part of the CoE in units of \$/kWh is expressed as:

$$OM = \frac{Cy_{O\&M}}{E_y}, \tag{30}$$

where $Cy_{O\&M}$ is the yearly total operations and maintenance cost in \$/year and E_y is the total yearly energy production in kWh/year.

The FCC in units of \$/kWh is:

$$FCC = \frac{\sum_{i=1}^{N_{steps}} UC_i M_i (1 + r_i)^{T_i}}{E}, \tag{31}$$

where M_i is the process mass flow in kg or separative work units (SWU) associated with the production of E kWh of energy, UC_i is the unit cost in \$/kg or \$/SWU, r_i is the discount rate associated with that process in 1/year and T_i is the lag or lead time of the cost with respect to a reference time in years.

In this particular case the only cost input allowed to vary with time is the cost of natural uranium (NU). While other costs are fixed, NU price growth is described by a model proposed in the 2011 Massachusetts Institute of Technology (MIT) assessment of the NFC (Massachusetts Institute of Technology, 2009):

$$\left(\frac{C_U}{Cr_U}\right) = \left(\frac{U}{Ur}\right)^{\theta} \tag{32}$$

in which C_U is current cost of NU in \$/kg, U is the total amount of uranium extracted until the current time, Ur is the cumulative amount of uranium extracted up to some reference time, Cr_U is the production cost of NU at that reference time and θ is the growth coefficient. The values of θ are 0.11 for the

50% cumulative probability density function (CPDF) percentile, which corresponds to the median case, and 0.29 for the 85% CPDF percentile corresponding to the conservative choice (Juchau et al., 2011).

10.4. Reactor building decision making model

Initially VEGAS were built in a way that simulation was driven by predefined user's parameter selection. The simulator code is extended with addtion to select lowest cost equilibrium NFC strategy and issue dynamic reactor build order. Figure 18 shows the computation algorithm. Dynamic decision making is based on the yearly CoE analysis for equilibrium nuclear fuel cycle and allows simulation of nuclear technology competitiveness given that uranium costs are not constant over time.

The NFC simulation tool VEGAS takes annual electricity demand growth rate, which is predefined for simulation and current nuclear reactor fleet retirement rate as inputs for certain region. Annual demand growth rate is expressed as a function of time as given by:

$$D(t) = P(t_0)[1 + growth]^{Y(t)}, \qquad (33)$$

where $P(t_0)$ – installed capacity at time t_0; *growth* – growth rate; $Y(t) = t - t_0$ – time after start of simulation.

VEGAS issue dynamic build orders for the simulation in every simulation time period, which is one year. The uranium price is calculated at the start of every time step. This is then used to calculate the CoE of every possible equilibrium fuel cycle for that year, which allows them to be evaluated and the cheapest one to be identified.

As is displayed in the algorithmically scheme in the Figure 18, then the next step of the simulation creates build orders for the current year using the reactor technology mix of the cheapest equilibrium state. If the requirements for energy demand is satisfied for the current time loop, no new build orders are issued. However, if demand is not met, additional reactor build orders are issued in the technology ratio of the current lowest cost equilibrium NFC.

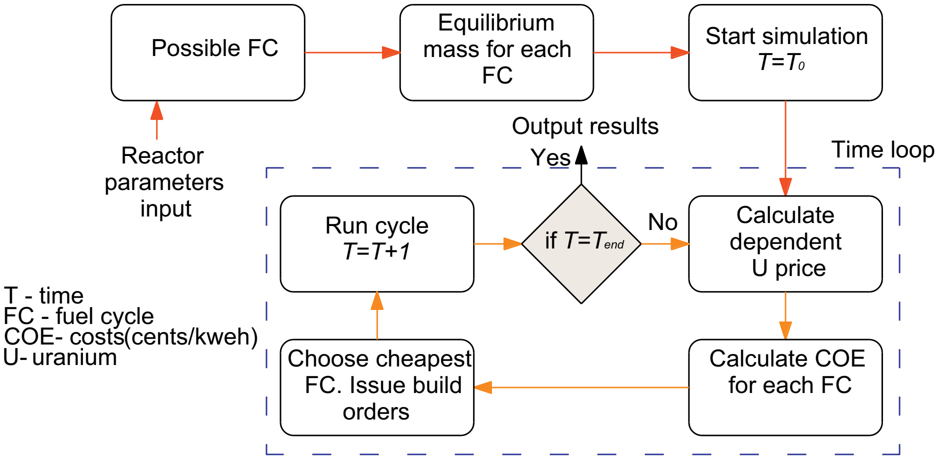


Figure 18. The NFC simulator computation algorithm. The possible NFCs with their corresponding equilibrium masses are determined once at the beginning of the simulation. This data is then used to find the cheapest NFC on a yearly basis.

11. RESULTS AND DISCUSSION

The result section will illustrate a mine-based market clearing model decision algorithm for a simple scenario characterized by a limited number of uranium mines and constant LEU demand and depiction for world scenery. It also will demonstrate decision time delay and accumulated profit function effect on a U market price. The second section includes improved NFC model VEGAS test case to illustrate how the new decision making model switches between different reactor technologies as the equilibrium electricity cost changes over time.

11.1. A mine-based uranium market clearing model configuration and test

The test case is designed to illustrate the decision algorithm for a simple scenario characterized by a limited number of uranium mines and constant LEU demand. The simulation runs from 2010 to 2030 under a fixed annual reactor fuel demand of 6790 t/year of 4.5% enriched U and 3390 t/year of natural U to supply CANDU and other NU-fueled reactors. These values are representative of world reactor fuel demand in 2010 and will be used again in a full-scale scenario of world production and demand is presented as well as in a time delay test case. As additional simplifications for this test case, the enrichment price is fixed at \$100/SWU and no secondary supplies of U are made available. Table 4 contains information about total reserves, annual U extraction rate, production costs, year from which each mine is available to enter production and mining method.
The simulation test case aims to demonstrate:

1. mine opening decisions based on market price;
2. the effect of supply capacity changes on short and long run market prices;
3. competition effects where a lower-cost U mine becoming available displaces other U mines from the market;
4. mine opening decision time delay effect evaluation;
5. accumulated profit function effect on a uranium market price.

Table 5 lists the properties of the five mines included in both demonstration cases. Recall that the uranium production cost table entry is the cost, in \$/kgU, if the mine produces at its reference annual extraction rate. The amount actually produced every year by each mine depends on the market-clearing price as described in the previous section. In this test case, mine E is a large and inexpensive U producer with a production cost of 50 \$/kgU at its reference capacity 30,000 tU/year. Unlike the other mines, mine E has a large uranium reserve that will not be exhausted during the 2010–30 period. Of the other mines, A, B and C feature progressively higher costs and will open in succession if demand warrants it. Mine D cannot open earlier than 2018, but its low reference production cost, 60 \$/kgU, may cause the U market price to decrease and might push some other U mine out of the market.

Table 5. Primary uranium supply data

U mine	Total Reserves & Resources tU	Reference Annual Extraction Rate tU/year	Year Available	Reference Cost $/kg U	Mining Method
A	150,000	15,000	2009	75	ISL
B	300,000	15,000	2009	100	ISL
C	200,000	20,000	2009	120	UG
D	150,000	15,000	2018	60	ISL
E	10,000,000	30,000	2009	50	UG

To illustrate the sensitivity of the results to the shape assigned to the individual supply curves, the test case is carried out for three values of the (P_2, Q_2) lowest-cost production point which was described previously. The Q value is the quantity at which the marginal cost of producing the next unit is minimized, while P is the marginal cost at that quantity. Table 6 lists the P_2 and Q_2 values studied. They are normalized against the reference cost and quantity respectively, so that $P_2 = 0.5$, $Q_2 = 0.5$ means that the mine's marginal cost is minimized at 50% of its reference production level, and at that level its MC is 50% of the reference value. Hence changing the P and Q coefficients alters the slope and shape of the supply curve as shown in Figure 19. The steeper the supply curve for $Q > 1$, the costlier it is for the mine to produce additional uranium beyond its reference annual capacity. This reflects the need to make short term investments in additional equipment and labor.

Table 6. Individual supply curve coefficients

No.	Q_2	P_2
1	0.8	0.5
2	0.7	0.5
3	0.5	0.5

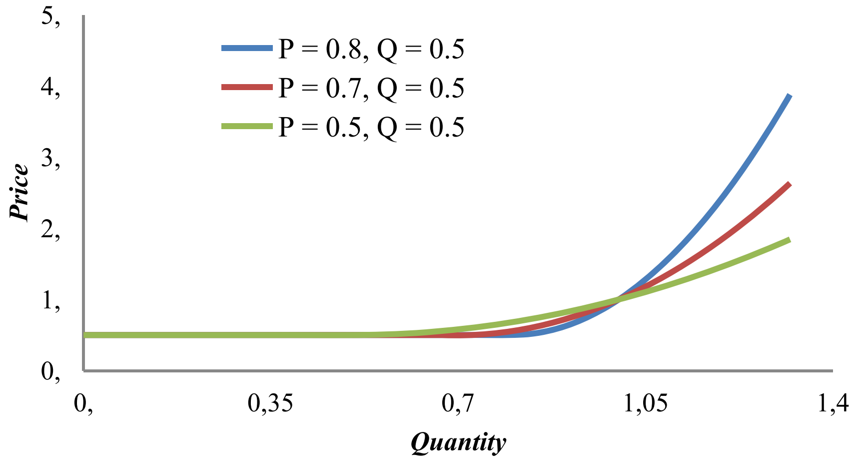


Figure 19. The individual supply curve with different coefficients

In the Table 7 is combined profit accumulation model configuration for each test case. In this case data of Q value (quantity at which the marginal cost of producing the next unit) and P (the marginal cost at that quantity) are normalized against the reference quantity and cost respectively, so that Q = 0.5 and P = 0.7, meaning that the mine's marginal cost is minimized at 50% of its reference production level, and at that the level of its MC is 70% of the reference value.

Table 7. U mine profit accumulation model configuration

Scenario/ configuration	openAfterYears *	defStartTime**	profitIndex***
1	5	2	55
2	3	2	55

* Allows to restart U mine operations after bankruptcy in fixed time period, if market conditions satisfy individual U mine's economic characters
** Accumulated profit calculation start time for each of the individual U mines
*** Sets the share of profits that is paid to the shareholders (in percentage). The other part of the profit will be redirected in the accumulated profit fund.

11.1.1. Mine opening decisions tests case results

Figure 20a–c shows the uranium supply mix for the three supply curve calibrations presented in the test case. The general trends are similar: the two lowest-cost mines, A and E, initially provide all supply. In order to do so, they both produce somewhat more uranium than their reference capacity annually. Figure 21 shows the uranium price evolution for each calibration. It can be seen that the uranium price is initially above $75/kgU, the reference production cost for mine A, for all three calibrations. However, only for the steepest calibration (P = 0.5, Q = 0.8) does mine B enter into production as well. This is because at this calibration mines A and E cannot increase production far beyond their design values without incurring sharply increasing costs. Therefore, in this case mine B can profitably enter into production if it produces somewhat less uranium than its reference capacity (hence at somewhat lower than its reference $100/kg U cost).

Regardless of calibration, in 2018 low-cost mine D becomes available and is entered into production. This causes the price of uranium to drop, but not so far as to drop below mine A's long- term shutdown price. Therefore, A continues to operate until its supply is exhausted. For the case where mine B had already entered the market, though, it chooses to enter short term shutdown when mine D opens. Only after mine A is exhausted does it become feasible for B to again enter the market. In all cases, after D is exhausted, the market clearing price rises as mines B and E are operating since B has substantially higher costs than D.

This demonstration case illustrates the effect of the individual firm supply curve elasticities. It is possible to affect firms' decision-making by modifying their supply curves. The original model of (Schneider et al., 2013) was in-flexible in the sense that each mine could only produce at its reference capacity and cost.

This misses the flexibility mines have to respond to changes in price by expanding or reducing production. Although not evident from the plots, the rollback algorithm prevented mine "C" from opening shortly before inexpensive mine "D" became available in 2018. Mine "C" features somewhat higher ope-rating costs than "B" but would have been profitable had "D" not appeared.

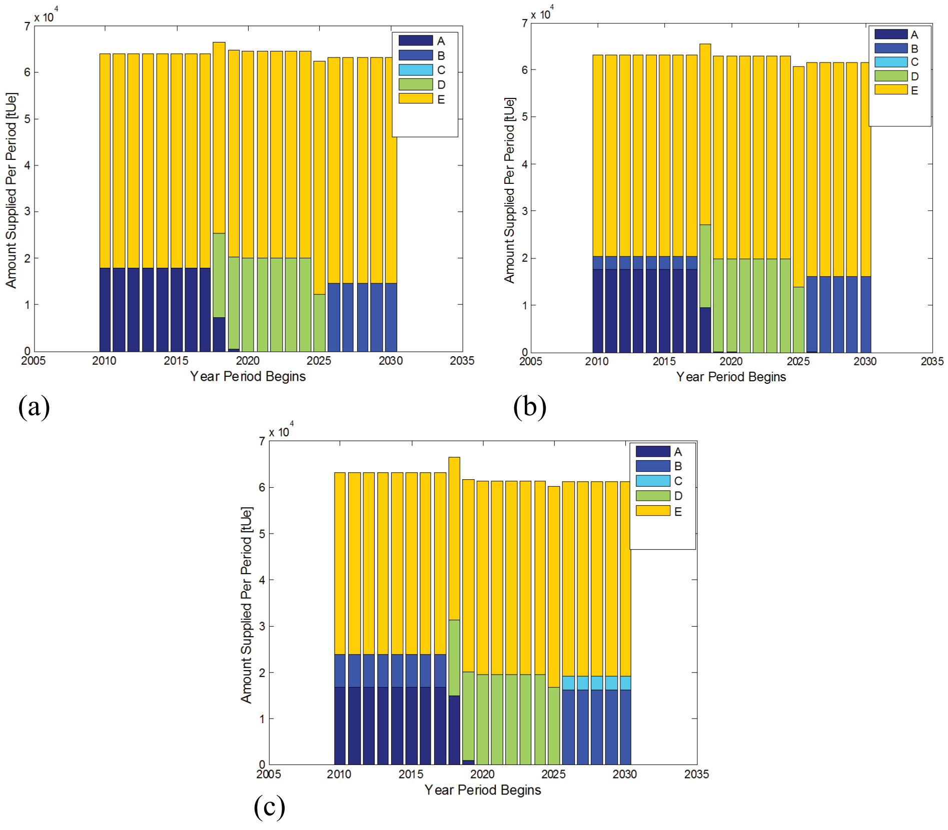


Figure 20. Amount supplied per period with coefficients: (a) $Q = 0.5$, $P = 0.5$; (b) $Q = 0.7$, $P = 0.5$; (c) $Q = 0.8$, $P = 0.5$.

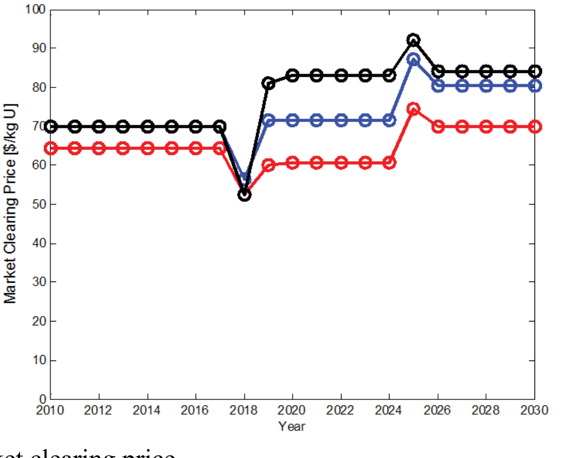


Figure 21. Market clearing price.

11.1.2. Mine opening decisions world case results

The world case scenario utilizes the reference-case uranium and enrichment industries described in (Schneider et al., 2013) and summarized here. As Table S1 shows, the reference scenario does assume that weapons grade plutonium, down blended highly enriched uranium (HEU), and stocks of natural uranium will be available as secondary sources of supply and that re-enrichment of stored depleted uranium continues. Other global parameters used in the reference scenario are given in supplements in the Table 3. This case assumes a 2.6% annual LEU fuel demand growth from its 2010 value. Enrichment plant capacities follow the schedule given in Table S2; in addition, all enrichment plant capacities are assumed to grow at a rate equal to that of LEU demand, an average of 2.6% per year, in each year after 2018. In the world case, the coefficients in the individual mines' supply curves were chosen to be $P_1 = 0.7$, $Q_1 = 0.7$. The world case results are illustrated in Figures 22–27. NU and SWU consumption both increase in proportion to overall demand growth, as can been seen in Figures 22 and 23. NU usage, though, is seen to grow at an average annual rate of slightly less than 2.0%, while SWU use grows at an annual rate of 3.6%. This difference arises because the price of uranium (Figure 24) is seen to rise through the simulation period, while the price of SWU (Figure 25) falls. The decline in the SWU price can be attributed to oversupply as well as completion of the transition away from diffusion to cheaper centrifuge technology. As the SWU price falls, the optimal tails enrichment (Figure 26) trends downward as well. By shifting to lower tails assays, consumers are substituting NU for SWU. Note that the SWU price and consumption, NU price and consumption and optimal tails are coupled to one another and are derived in calculations that take place in each year of the simulation.

As mentioned, the SWU price is seen to decline from $160/SWU in 2010 to $90/SWU in 2020 even as annual SWU consumption increases by 44%. As existing U mines exhaust their resources and close, new mines open pushing marginal costs and hence prices above $100/kg. As the market price approaches $120/kg U, it becomes worthwhile for several new mines to come online, stabilizing the NU price by the mid-2020s.

Figure 27 illustrates the supply and demand curves giving rise to the market clearing condition in one arbitrarily selected year, 2025. The x_w values noted on the demand curve are the U-235 mass fractions in the enrichment tailings corresponding to the indicated locations on the demand curve. The sloping demand curve illustrates the tradeoff between NU and SWU, as points with lower x_w values rely more heavily on enrichment and less heavily on NU purchase to meet enriched uranium fuel demand. The lower the x_w value, the more expensive NU would have to be in order to make that tails enrichment optimal. Steps and plateaus in the supply curve, which starts from (0,0) at lower left, indicate the marginal cost of the next unit of NU produced as a function of the NU price. It is important to note that since this model exactly satisfies the enriched U fuel requirements each year, with no option for utilities, enrichers, producers and other market players to build up or draw down inventories or engage in speculation, the model cannot predict spot price excursions such as the one that took place at the end of the decade of the 2000 s. Instead, it is a tool for predicting longer-term price trends, especially in the face of policy decisions or changes in primary or secondary U or SWU supplies.

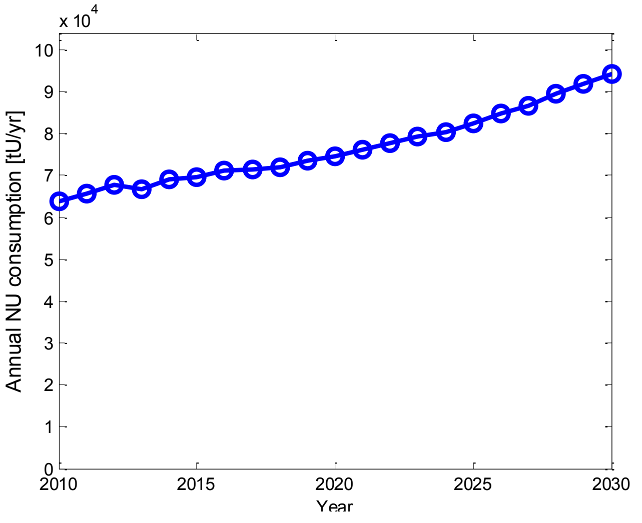


Figure 22. Annual NU consumption.

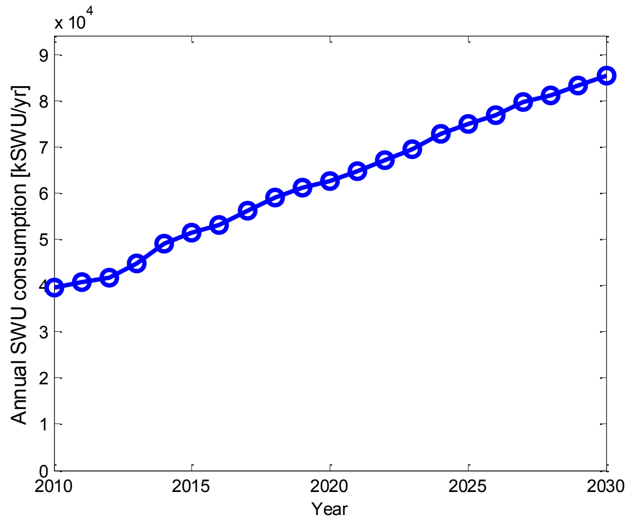


Figure 23. Annual SWU consumption.

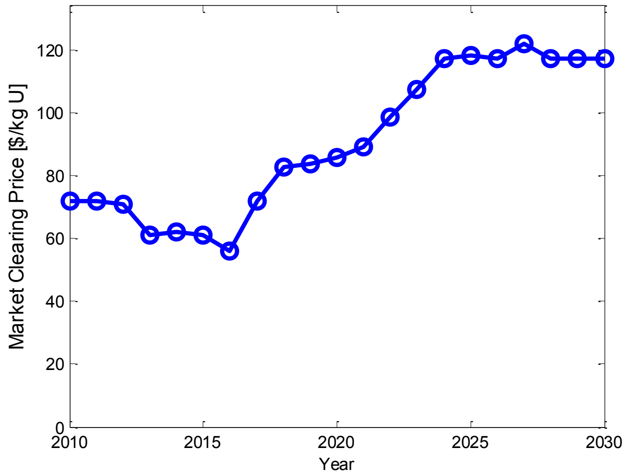


Figure 24. Market clearing uranium price.

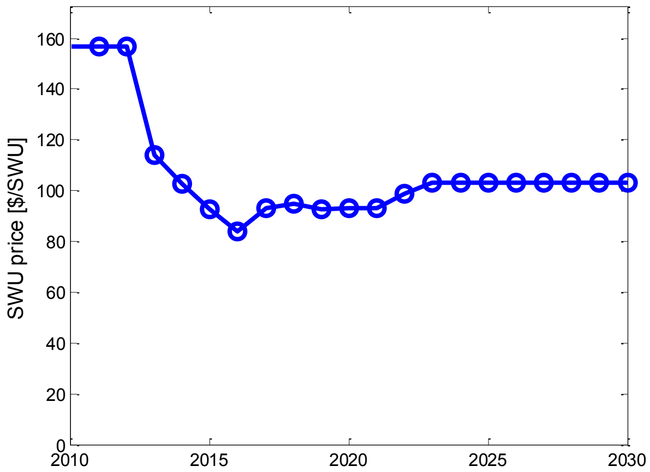


Figure 25. SWU price.

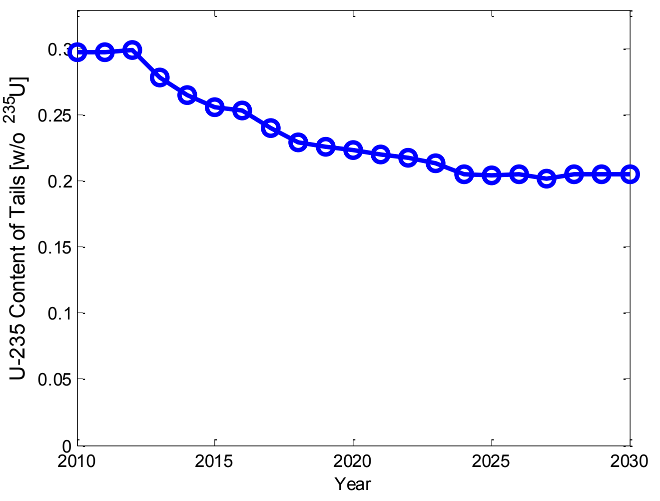


Figure 26. The tails enrichment.

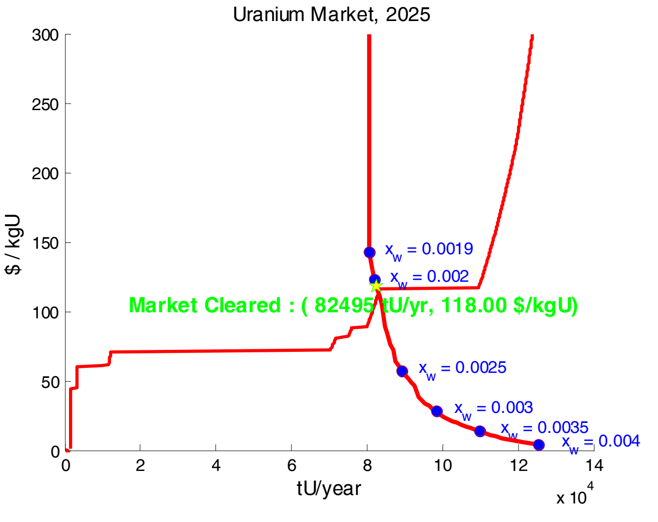
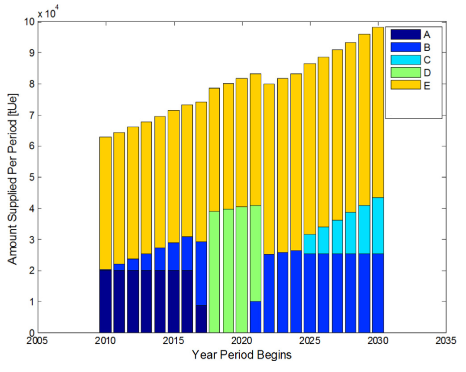


Figure 27. Uranium market supply and demand curves in 2025.

11.1.3. Time delay and accumulated profit simple tests case

Figures 28 and 29 represents in the previous section described test case with five U mines and P = 0.5, Q=0.7 coefficients, and 2.6% annual LEU fuel demand growth. In Figure 28 we see, that in 2018 low-cost mine D becomes available and is entered into production, causing the price of uranium to drop. U market price is below mine B's long-term shutdown price therefore B leaves the market. Only after mine D is exhausted does it become feasible for B to again enter the market. Due to growing NU demand in 2025 U market price exceeds mine C's short-run break-event point and C enters the market, which causes a price drop.

We see that U mines are operating whenever U market price satisfies requirements and can start operation instantly. Such conditions give smaller effect of U market price volatility as it can be seen in Figure 29.



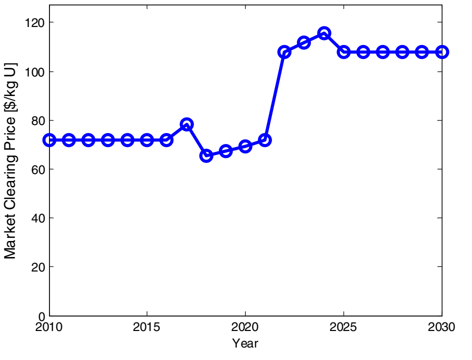
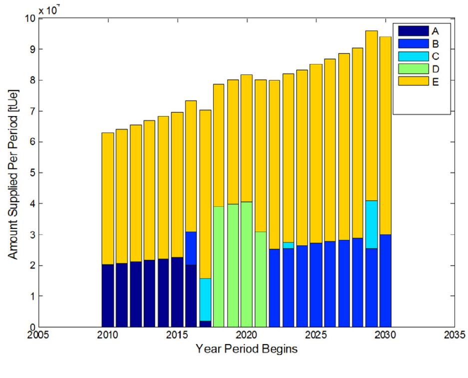


Figure 28. Amount supplied per period **Figure 29**. Market clearing price

Figures 30 and 31 represents test scenario 1 from the Table 6 with activated time delay effect and profit accumulation function with the same data setup and P, Q coefficients. In the results we can see that in a year 2017 U mine A runs out of uranium and U mine C is opened. In 2018 U mine D is opened, because D is available for production and is cheaper compared to the C. That mean that mine C will be closed in year 2018, because NU market is filled with cheaper uranium. In the same year the NU market price falls to 65.3 $/kgU. Starting from year 2020 the mine D runs out of uranium and market price is growing. In a year 2022 U mine B is opened according to the configuration, which says that the bankrupted mines can be reopened only after five years. In year 2023 uranium market price forecast exceeds 120 $/kgU and mine C is opened. Meanwhile the U enrichment industry reacts on the price change and in year 2023 NU consumption decreases as well as U235 content of tails decreases. This reaction leads to U mine C being shut down on the same year. In a year 2029 U market price is high enough and mine C is reopened and a year later closed because U production cannot cover production costs.



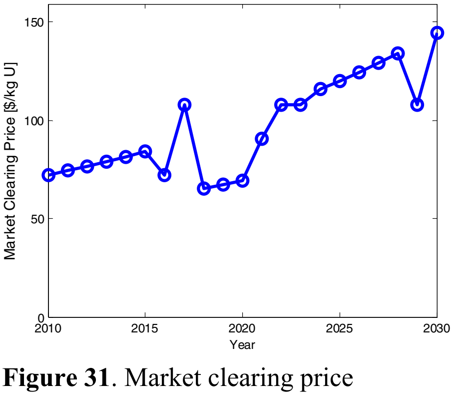


Figure 30. Amount supplied per period **Figure 31**. Market clearing price

The test scenario 2 from the Table 6 is presented in Figures 32 and 33. In this case U mines can be reopened 3 years after closure. Such scenario gives bigger price volatility as it can be seen in Figure 31. In Figure 32 we see that initial NU demand satisfies U mines A and E. In the year 2014 U mine B was opened and closed in the same year, which causes small U price drop. In 2017 mine A exhausted U reserves and mine C start production. But in 2018 low-cost mine D becomes available and is entered into production, causing the price of uranium to drop and mine C leave the market. In 2021 mine D exhausted U reserves and mine B start production, which cause U market price slow increment and B cannot cover U production costs therefore B leave the market in the same year. In a year 2022 we can see U market price peak, because model has mine start time delay, therefore mine C start production only in 2023. In the year 2025 mine B start production and push out from the market mine C, because mine B's U costs cheaper compare to mine C. Mine C tries to start production again in 2028. But as a result C causes U oversupply and U price drop therefore C leave the market.

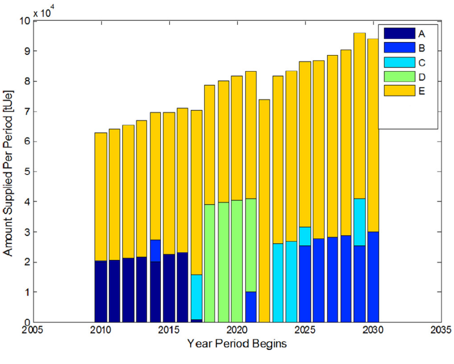


Figure 32. Amount supplied per period

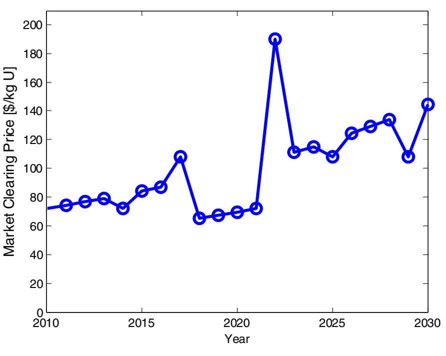


Figure 33. Amount supplied per period

The previously described a real-world test cases are compared with the accumulated profit regime switched on in scenarios 1 and 2. And with the accumulated profit calculation function on. Figures 34 and 35 represents the results from the first scenario and Figure 36 and 37 represents results from the second scenario. In Figure 39 we can see that market price is growing faster and accedes 230 $/kgU. Meanwhile in the second case (Figure 37) when mines can be reopened after 3 years, price is not growing so fast and can be seen bigger price volatility.

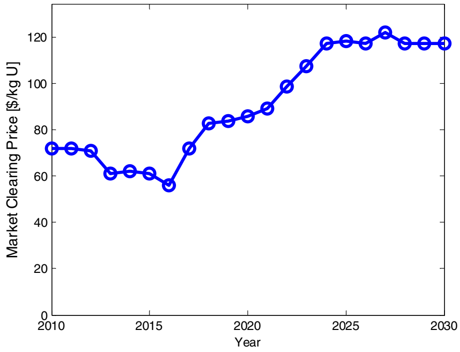


Figure 34. Market clearing price. Replica data.from the reference model.

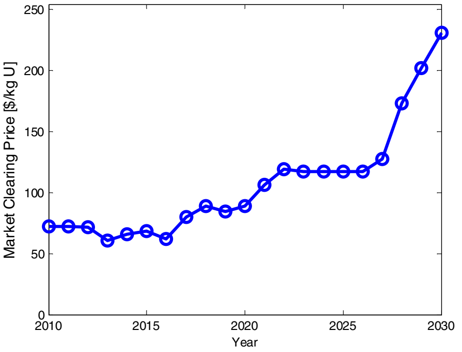


Figure 35. Market clearing price.

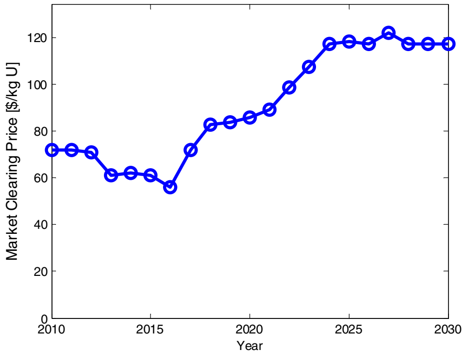


Figure 36. Market clearing price. Replica data from the reference model.

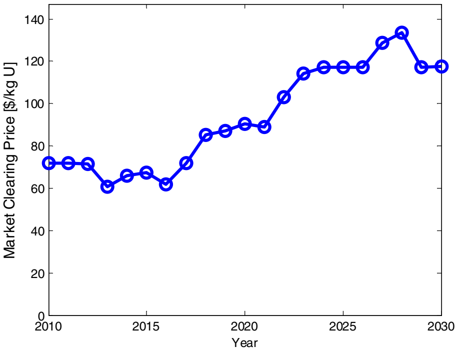


Figure 37. Market clearing price.

11.1.4. Time delay and accumulated profit world case results

The world case test conditions are described in the previous sections. With a mined-based market clearing model in which the time delay and profit accumulation functions are activated was tested such hypotheses. Firstly, we expected that the changes in the model would lead to reduction of supply and overall tougher conditions for uranium producers also reflected in higher market clearing price for uranium. Secondly, we expected the market price to be much more volatile.

We can estimate the change to overall supply by calculating the economic value for each different scenario and time period and find the cumulative economic value for each scenario by summing the economic value across years. The Table 8 presents such summarized economic value for different scenarios where two parameters are analyzed for sensitivity. The length of the delay in restarting operations in years is presented in columns and the share of retained earnings is presented in rows.

Table 8. Economic value calculation for each scenario

Share of retained earnings / Year	1 year	2 years	3 years	4 years
10%	11 897 625	12 377 002	15 250 552	17 411 760
20%	11 905 403	12 419 416	15 250 552	17 411 760
30%	11 905 403	12 401 042	15 250 552	17 411 760
40%	11 848 800	12 419 416	15 193 949	17 411 760
50%	11 905 403	12 419 416	15 250 552	17 411 760
70%	10 714 392	12 419 416	8 949 970	11 111 179
90%	11 905 403	12 419 416	15 250 552	17 411 760

As can be seen from the Table 8 for all scenarios the economic values are positive which means the prices in average are higher with a marketplace where decision making is delayed and the process for reopening a mine is time consuming. We see that the longer the delay, the higher the prices are in the market on average. This is because prices are more volatile and a lot more companies shut down their operations and reopen the mine with a delay causing larger fluctuations in the market. We also see that share of retained earnings does not have a significant effect on the economic value. We will separately analyze volatility by analyzing whether prices are more volatile. The results are illustrated in the Table 9.

Table 9. Price volatility

Share of retained earnings / Year	1 year	2 years	3 years	4 years
10	32.23*	31.80*	32.30*	33.30*
20	32.24*	31.82*	32.31*	33.30*
30	32.24*	31.81*	32.31*	33.30*
40	32.20*	31.82*	32.27*	33.30*
50	32.24*	31.82*	32.31*	33.30*
70	24.89	31.82*	24.96	26.40
90	32.24*	31.82*	32.31*	33.30*

* standard deviation

As can be seen from the Table 8 the standard deviations are much higher than in the case of base scenario where standard deviation is 23.05. The standard deviations are statistically significantly different from the base scenario with a confidence level of 0.9. The Microsoft Excel was used in performing the F-test for comparison of variances. This means that introducing delay to the model has significantly increased the volatility of Uranium price. We also see that volatility increases with longer delay. The share of retained earnings at 70% was not statistically significant and difference in results requires further research. Generally, the results are similar and share of retained earnings is not a factor in price variance. We also see that share of retained earnings does not have a significant effect on the standard deviation of the price.

Hence, we can confirm that the changes made in a main-based market clearing model resulted in higher market price and more volatile prices in general resulting in tougher conditions for miners to operate. This means that by reducing the time that is needed to reopen the mine one can increase efficiency on the market and make the market much more stable. This also results in overall lower prices and higher efficiency.

11.2. An optimal NFC evaluation test

The test case is created to demonstrate how VEGAS decision making model switches between different reactor technologies and nuclear fuel cycles as the equilibrium electricity cost changes over time. However the test case demonstrates scenery with only includes two available reactor technologies, the model is capable of perform a switch between possible NFCs which is also easy to observe and simple to explain. The chosen test case simulates the USA nuclear reactor fleet and considers the possible adoption of fast spectrum reactors. In the test simulation only two reactor types where made available, but adding additional reactors to the simulation will not significantly impact performance. Such simplification was performed to easily verify results and algorithm correctness. Additional available reactor technologies might lead to many switching points and due to the system being rather inert and taking a while for the switch to become apparent because of the long operational life of the reactors, these points can become very hard to identify. Therefore, only two reactor technologies were used in the simulation to keep the results easy to analyze.

The test case conditions are taken from autonomous dynamic decision making in a nuclear fuel cycle simulator. The test scenario approximates the current USA nuclear reactors fleet with capacity 100 GWe and is set to increases by 0.8% every year (U.S. Department of Energy, 2010; U.S. Department of Energy, 2012). Initially the capacity is made up entirely of “current fleet” reactors with their assumed parameters listed in Table 10. This fleet begins retiring in 2010 at a constant rate and is completely offline by 2030. This is a faster retirement than expected, but it permits a more rapid transition to next-generation reactors. As the reactors are decommissioned and unfulfilled capacity becomes available, the simulator chooses the currently cheapest equilibrium NFC when deciding which reactors to build.

The reactors available to the simulation are listed in Table 10. Advanced Pressurized Water Reactors (APWR-UOX) represent Generation III+ and LWRs and have been selected due to their high likelihood of being built in the USA. Sodium Cooled Fast Burner Reactors (SFR), were chosen because of their ability to recycle their own SNF and the relatively advanced state of maturity. Plutonium fueled tier 1 reactors were not used in order to keep the model as simple as possible. While the Technological Readiness Level (TRL) functionality has also been implemented, it was not used for the same reasons of keeping the model simple.

Since the current fleet reactors are inferior to the APWR-UOX technology, they are only used for the beginning of the simulation, effectively leaving two options to choose from: the APWR-UOX only, and the APWR-UOX – SFR recycle scenarios. All reactors built during the simulation have a lifetime of 60 years.

Table 10. Nuclear reactor fuel cycle costs for the test case in 2009 US Dollars (Shropshire et al., 2008)

Service	**Price in USD**
U mining and milling \$/kg(U_3O_8)	106 (initially)
Conversion to UF_6 \$/kg(U_3O_8)	10
Enrichment \$/SWU*	155
PWR fuel fabrication \$/kg_{IHM}	250
Fresh fuel transportation \$/kg_{IHM}	50
Reactor operation and maintenance \$/kWh/y	68
SNF storage \$/kg_{IHM}	300
SNF transportation \$/kg_{IHM}	50
Reprocessing \$/kg_{IHM}	1120
SNF disposal \$/kg_{IHM}	500
HLW vitrification \$/kg_{IHM} in HLW**	480
HLW storage \$/kg_{IHM} in HLW	100
HLW disposal \$/kg_{IHM} in HLW	1600
APWR-UOX construction costs \$/kW_e overnight	3500
SFR construction costs \$/kW_e overnight	3850

* SWU – separative work unit.
** HLW – high level radioactive waste

The financial discount rate was set to 7 % per year. The costs including taxes for various NFC services are listed in Table 10. Uranium mining and milling costs were the only ones to change with usage. The parameters used for these calculations were an initial reference amount of 600 000 tons in 2009, an approximation of the total amount of U that was required to fuel all the reactors in the USA up until this year, a growth exponent of 0.5 and an initial cost Cr_U of \$106/kg. For purposes of calculating the NU price from equation 33, it is assumed that the uranium consumption rate in the rest of the world remains proportional to that of the USA. While the exponent value is rather large, it allows switching to an NFC with reprocessing on the basis of cost alone within the simulation time frame.

11.2.1. NFC evaluation results

The installed electricity generation capacity by technology type is shown in Figure 38. The black solid line represents the total demanded electricity generation capacity in GWe while the other colors represent the generation capacities from their respective reactors technology as listed in the legend. These sum to the total generation capacity. The current USA nuclear fleet reactors start retiring in 2010 and will finish in 2030. From the beginning the APWR-UOX only NFC is cheaper compare to SFR reactors, therefore all newly constructed reactors are APWR-UOX type. As illustrated in Figure 39, 1.93 million tons of uranium are used by the represented USA fleet (6.95 million tons around the world) over the 100-year simulation and by 2050 uranium price has increased from \$106/kgU to \$160/kgU. At this point reprocessing the spent fuel for use in SFRs becomes cheaper under the optimistic, illustrative SFR capital cost assumption shown in Table 10 and the model switches to the APWR-UOX – SFR NFC. Therefore, SFR type reactors begin appearing in the simulation output. Because of limited capacity demand growth and slow APWR-UOX reactor retirements rate the SFR are slow to reach the equilibrium state. Only when the first APWR-UOX reactors built in 2010 started retire, then in 2070 does the transition speed increase for switching to SFR reactors and slowly approaching the equilibrium state by 2090.

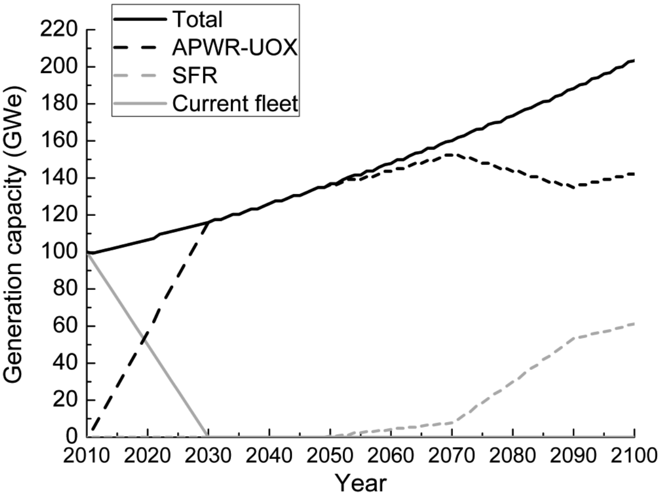


Figure 38. Generation capacity results by reactor type. Technology switching begins at 2050 followed by two transitional stages, the first due to limited total capacity growth and no decommissioned reactors and the second as APWR-UOX reactors are decommissioned. By 2090 the system approaches an equilibrium state.

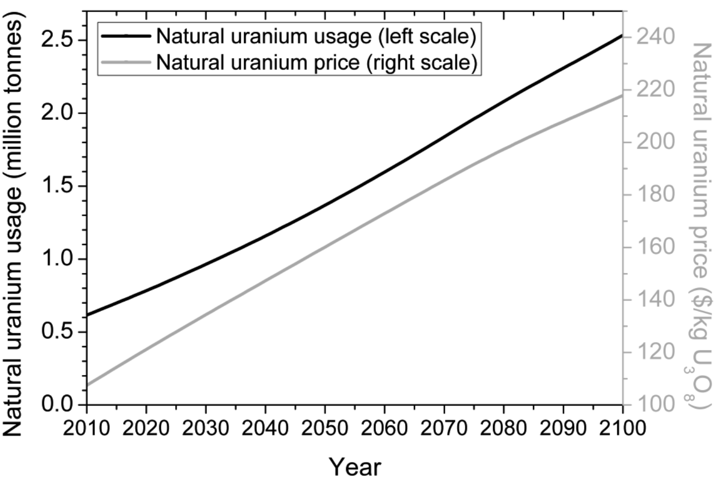


Figure 39. Natural uranium price and utilization

The cost of electricity results of the simulation was plotted in Figure 40. The solid black curve represents the CoE of the test case simulation with dynamic switching. The solid grey curve and the dashed black curve plot the CoE of the two equilibrium NFCs calculated by the simulator. The decision to switch to the APWR – SFR NFC is made as the latter two lines cross in 2050.

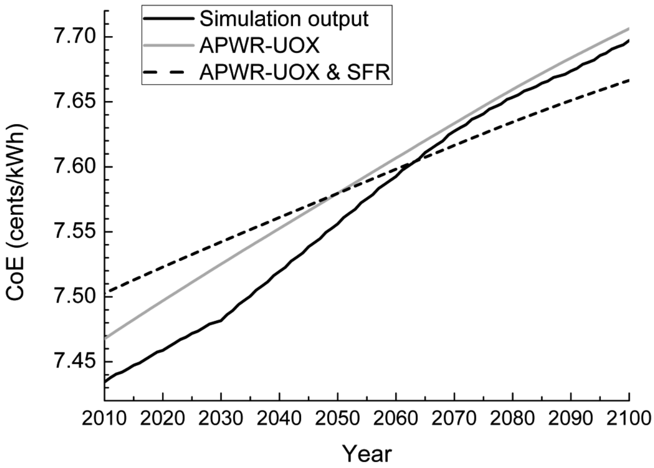


Figure 40. Cost of electricity results for the test case. The solid black curve represents the actual results of the dynamic switching-enabled test case simulation and the other curves illustrate the CoE for their corresponding static simulations.

As can be seen in the Figure 40, then the actual CoE calculated with the dynamic decision tool never match to equilibrium fuel cycle calculation with predefined user's input. For example, until 2050 the actual results calculated with the dynamic switch are lower than the APWR-UOX equilibrium results. Such calculation differences is due to the fact that discharged fuel in the case that transitions to SFRs is stored for decades prior to reprocessing, whereas it almost immediately pays a disposal cost in the APWR-UOX case. As the actual spent nuclear fuel reprocessing is not performed until fuel is required for SFRs, the fuel reprocessing costs are effectively reduced due to the 7% financial discount rate. This would require a more appropriate financial model that would discount back-end costs like reprocessing and disposal at a lower rate and this effect would be less significant factor to the cost of electricity. In the case of a constant equilibrium state of APWR-UOX and SFR reactors which start from 2090 full reprocessing costs are covered shortly after spent fuel is discharged, and the simulation output will converge with the APWR – SFR equilibrium CoE as fuel interim storage costs diminish. From the results it is clear that needed additional time to switch between technologies and fuel cycles.

12. CONCLUSIONS

The thesis is focused on NFC numerical modelling and advanced approach testing in an existing models. An agent-based modelling concept was implemented and tested in a uranium market clearing model. An autonomous dynamic decision making approach was tested in the VEGAS NFC model. The work conducted within this study is summarized in next points:

1. A mine-based uranium market clearing model demonstrates an approach to model the behavior of autonomous entities – uranium mines, within a simulation of part of the nuclear fuel cycle. Such approach allows creating an advanced, more realistic stochastic model in which entities act independently, focusing only on profit maximization. Based upon their unique characteristics, the entities uranium mines made yearly decisions to commence or continue production, or alternatively to enter into short-term or permanent shutdown. The decisions were based upon the economic theory of individual firms with unique supply curves participating in a competitive market. Individual startup and permanent shutdown decisions were myopic in the sense that they took into account only the state of the market in the year they were taken. Therefore, a rollback algorithm was implemented if a mine was found to enter a permanent shutdown condition before it had produced all of its reserves. This algorithm returns the simulation to the year in which the mine was opened and undoes the decision. In that sense, the rollback algorithm replicates firms' ability to project future market behavior when weighing the costs and benefits of entering an industry. The thesis leads to a methodology governing decision-making entities inside a nuclear fuel cycle simulator. A similar algorithm can be envisioned to drive the construction of other fuel cycle facilities as well as power reactors. But it can generalize to entities whose objective is other than maximization of profit. For instance, the decision to construct reactors whose purpose is to burn down transuranic elements may not be driven only by economic considerations. Yet these reactors face a condition similar to the one that led to the rollback algorithm that was demonstrated in this paper for uranium mines. A mine, initially profitable, might later become unprofitable so that its owner would have been better off never having opened it in the first place. Similarly, a transmuter reactor that might have an adequate supply of transuranic fuel at the time it was constructed could face in absence of fuel later on. Within the environment of the fuel cycle simulator, one way to tell whether unfavorable conditions of either type will arise the only way if the simulator is highly complex or nonlinear is to run the simulation clock forward. In both cases, the rollback strategy resolves the unfavorable condition, although it must be noted that this alone does not guarantee that the final outcome of the simulation is in any sense optimal. Nonetheless, the approach represents a step toward autonomous decision making within nuclear energy system models.
2. Improved decision-making strategy with time delay and profit accumulation function of an individual U mine gives more flexibility to model the dif-

ferent regulators conditions. In it important to note, that the model does not assume that regulations might differ in each country or region, but such scenery can also be simulated. The results show that the improvements made to the model made the conditions much tougher for miners to operate in, causing the prices in the market to increase on average. It is also possible to confirm that the improvements also increased volatility. However, the impact of retained earnings proved to be insignificant and did not have a significant effect on the economic value of the scenarios. This means that even if all the profits are retained, the price changes are significant enough to wipe out all profits in a short period of time. We found that delay in decision making is very significant. Hence, we can conclude that the longer it takes for miners to reopen their mines the greater inefficiency this creates, leading to higher prices and more volatility in the market. Better regulations can reduce the time that is needed to reopen mines, whether it is related to a more efficient licensing procedure, more flexible labor laws or other relevant regulations. If the regulator of the market was able to create an environment where miners can quickly exit and re-enter the market then this would lead to market efficiency, lower average prices and more stable prices.

3. The autonomous decision-making tool test case shown that the simulator is able to issue dynamic reactor building orders for different equilibrium fuel cycles, which is based on NFC economic characteristic and uranium price dynamic. The possibility of NFC simulator to issue autonomous building decisions based on performance metric has been demonstrated. In this particular case was demonstrated approach of issuing building order based on the costs of electricity minimization. However the current test case only included 2 types of reactors, the list could be expanded to include many possible reactor types. The extended version of VEGAS simulator could be a useful tool for quickly determining the feasibility and costs of various NFCs. In addition such simulation approach could be applied to a more complex NFC simulator. The work can be used to support more complicated NFC simulations where user's defined build order might not guaranty the best results. The simulator is capable to issue reactor technology deployment orders in the ratio of the targeted least-cost NFC. The model could achieve quicker convergence in the target NFC if the build order "overshoots" the target, e.g. by constructing a greater-than-equilibrium share of high-tier reactors until the equilibrium ratio is reached or even surpassed. The simulator can violate material balance constraints by deploying extra reactors. To solve this problem VEGAS take the computationally expensive step of rolling back in time and reissuing build orders. The current simulation approach uses present value costs analysis within the decision metric. But in a real life technology deployment decisions are taken on the basis of current and discounted future costs. In order to make model more precise the CoE metric would need to include a time-dependent U price forecast. The improved decision metric would condition each year's build decisions on the expected discounted CoE over the new reactors' lifetime.

SUPPLEMENTS

Table S1. Secondary sources

Name	Amount (tonnes U or Pu*)	Enrichment (wt% ^{235}U)	Maximum annual rate (tonnes/yr)	Year avail-able	Cate-gory
Purchase Agreement HEU	100	90	25	2010	HEU
Surplus HEU	417.1	90	13.9	2014	HEU
Surplus WGPu	68	N/A	3.4	2020	Pu
DU-enrichment step A	291,432	0.19	14,572	2010	DU
DU enrichment step B	322,804	0.24	16,140	2010	DU
DU enrichment step C	226,025	0.29	11,301	2010	DU
DU enrichment step D	254,303	0.34	12,715	2010	DU
DU enrichment step E	40,147	0.39	2,007	2010	DU
DU enrichment step F	27,379	0.44	1,369	2010	DU
DU enrichment step G	1,103	0.49	55	2010	DU
DU enrichment step H	3,023	0.54	151	2010	DU
DU enrichment step I	244	0.59	12	2010	DU
DU enrichment step J	591	0.64	30	2010	DU

Table S2. LEU demand.

Enrichment supply growth*	**2010**	**2011**	**2012**	**2013**	**2014**	**2015**	**2016**	**2017**	**2018**	**2019**	**2020 and beyond**	**Type**	**SWU Cost**
Name	kSWU/yr	kSWU/yr	kSWU/yr	kSWU/yr	kSWU/yr	kSWU/yr	kSWU/yr	kSWU/yr	kSWU/yr	kSWU/yr	kSWU/yr		$/SWU
USEC ACP	0	0	0	0	1,000	2,400	3,800	3,800	3,800	3,800	3,800	C	103
URENCO NEF	1,180	2,360	3,540	4,720	5,900	5,900	5,900	5,900	5,900	5,900	5,900	C	63
Areva Eagle Rock	0	0	0	0	1,100	1,100	2,200	2,200	3,300	3,300	3,300	C	75
Eurodif Besse II	0	1,250	2,500	3,750	5,000	6,250	7,500	7,500	7,500	7,500	7,500	C	62
Brazil Resende	0	0	0	0	0	120	120	120	120	120	120	C	160
Urenco Capenhurst	5,000	5,000	5,000	5,000	5,000	5,000	5,000	5,000	5,000	5,000	5,000	C	70
Urenco Almelo	3,800	4,150	4,150	4,500	4,500	4,500	4,500	4,500	4,500	4,500	4,500	C	73
Urenco Gronau	2,200	2,200	2,200	2,775	3,350	3,925	4,500	4,500	4,500	4,500	4,500	C	84
JNFL Rokkasho	150	150	300	450	600	750	900	1,050	1,200	1,350	1,500	C	93
Tenex UEKhK	9,800	9,800	9,800	9,800	9,800	9,800	9,800	9,800	9,800	9,800	9,800	C	35
Tenex EKhZ	5,800	5,800	5,800	5,800	5,800	5,800	5,800	5,800	5,800	5,800	5,800	C	40
Tenex SKhK	2,800	2,800	2,800	2,800	2,800	2,800	2,800	2,800	2,800	2,800	2,800	C	48
Tenex Angarsk	2,600	3,600	3,600	4,600	4,600	5,600	5,600	6,600	6,600	7,600	7,600	C	53
USEC Paducah	8,000	8,000	4,000	0	0	0	0	0	0	0	0	D	163
Eurodif Georges Besse	11,300	9,417	7,534	5,651	3,768	1,885	0	0	0	0	0	D	157
CNNC Heping	400	400	400	400	400	400	400	400	400	400	400	D	129
CNNC Hanzhong	500	500	500	500	500	500	500	500	500	500	500	C	107
CNNC Lanzhou	500	500	500	500	500	500	1,000	1,000	1,000	1,000	1,000	C	89

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ARCHIMEDES

SUMMARY

Development of computational model for nuclear energy systems analysis: natural resources optimisation and radiological impact minimization

Many countries are struggling to limit greenhouse gas emissions and focus on carbon-free energy sources, and therefore nuclear energy is a subject of continuing debate to enhance the worldwide energy production mix and cover the base load requirements. Evaluation of uranium supply in a market and resource optimization context is needed to inform decisions impacting the long-term development of nuclear power and warn policy makers about possible uranium market supply-side volatilities and to help choose the technology mix. The aim of this work is to demonstrate and test advanced simulation methods and conceptual ideas to enable realistic fuel cycle simulators and develop a supporting tool for decision makers. Additionally, this work facilitates the selection of the most favorable nuclear fuel cycle, using optimization with respect to multiple criteria save natural resources, minimize the impact of high level radioactive waste on nature, to and decrease nuclear material proliferation risks.

Below are explained several separate tasks and stages which have been addressed during this study:

1) The nuclear fuel cycle is a complex system with a series of industrial processes involving the production of electricity from uranium, plutonium and other fissile materials in nuclear power reactors. The first part of the work is focused on the front-end nuclear fuel cycle which includes uranium mining and milling, enrichment services and nuclear reactors. Nuclear reactors are designed to run on a specific nuclear fuel, which cannot be substituted in a short period and any change requires large investment. Therefore, fuel requirements must be satisfied in the short run.
2) Nuclear fuel cycle numerical models are intended to simulate the evolution of cycles over a period of time and then to provide output data relevant to the input parameters. Currently there are several nuclear fuel cycle simulation codes available, but usually simulators are designed only for one specific target. Nearly all nuclear fuel cycle simulation codes can be divided into two groups – codes which track material movement in discrete fuel batches and codes which do not. Nuclear fuel cycle simulation tools can easily become complex, and any new simulation can require significant effort as well data analysis. There are situations where validation can become almost impossible. Most previous simulation tools work on arbitrary data and simulate only a possible event horizon but do not predict prices, costs or other economic criteria.
3) In this work, a mine-based uranium market clearing model is built upon databases of primary and secondary uranium resources as well as enrichment facilities. The model derives market-clearing conditions by locating the intersections between the annual supply and demand curves, also considering the

effects of secondary supplies including highly enriched uranium down-blending and the sale of natural uranium inventories. Therefore, the model incorporates the coupling between the uranium and enrichment markets. Each uranium mine in the core database has unique characteristics including total uranium reserves, earliest feasible opening date, capital and operating costs, and other parameters which are fixed. These parameters are the same in every time period, as long as the mine still possesses the uranium reserves it can produce. The uranium mine production decisions of each mine are determined based on the short-run market price. To make operational decisions based on the short-run market price, the model uses representative mine cost structure and assumes the same relative distribution of capital, operating, and decommissioning costs. Hence these costs are obtained by scaling the costs for the reference mine by the ratio of unit costs. The short run market supply curve is defined as the horizontal sum of the individual mines' supply curves. The demand curve creation mechanism involves finding the natural uranium price for which each tails weight fraction would be cost-minimizing when natural uranium and conversion costs are all incorporated.

4) The agent-based modelling concept is widely used in energy systems modelling and other fields to model individual agents' behavior in an ecosystem where each agent solves an optimization task and makes individual decisions. A mine-based uranium market clearing model uses a cycle type agent-based modelling approach. An individual agent can represent a large uranium mine, which has significant effect on the uranium market share. Therefore, such agents have a weight fraction on the natural uranium market and individual decisions can affect market price. During each year of the simulation, the market clearing model uses decision tree criteria to determine whether each mine will operate. It then must decide how much uranium the mine will contribute to the total amount supplied across the industry. The model has built-in profit accumulation and time delay functions to make the model more realistic and volatile to external factors – such as mining policy changes and natural disasters.

5) By default, a mine-based uranium market clearing model does not take into account uranium mine licensing issues and other operational activities, allowing for new mines to open, reopen or shut down instantly. The time which is needed to reopen the mine is closely related to the economic and regulative environment and often is not solely dependent on the producer's decision. The time delay will reduce the supply, since uranium producers will enter the market more slowly when the conditions are favorable. This will make the market much more volatile and resemble the actual market behavior more realistically. When new producers enter the market the supply curve shifts to the right and price decreases. When individual mines go bankrupt, the supply curve starts shifting to the left (slowly), but if there are enough producers operating in loss, the number of bankruptcies increases

suddenly and the supply curve makes a sudden shift to the left, causing price to increase suddenly.

6) The VEGAS – a nuclear fuel cycle and economy simulation tool, which verifies optimal nuclear fuel cycle is based on the expected cost of electricity as the simulation driving factor. A key capability is to select which type of reactor to build based upon objective criteria. Optimization based upon cost ideally includes a degree of foresight. True mathematical optimization would require complete foresight, but that is arguably not a realistic depiction of how agents make decisions. In the VEGAS nuclear fuel cycle simulator, decisions are made on the basis of the costs of electricity minimising equilibrium fuel cycle. An equilibrium fuel cycle can be defined for any combination of reactor types and represents a state in which at least one hard material balance constraint is met. It is characterized by a specific deployment ratio of the member types. There are many nuclear reactor technologies already available and even more are likely to become available in the future, so even the task of finding the equilibrium is challenging, if many of the technologies are made available to the simulation.

Main highlights of this work include development of a mine-based uranium market clearing model, which demonstrates an approach to model the behavior of autonomous entities – uranium mines. Furthermore, an important achievement is the autonomous decision making tool, which illustrates that the model is capable of dynamically issuing building orders for different equilibrium fuel cycles, based on fuel cycle economics and uranium price evolution.

SUMMARY IN ESTONIAN

Loodussäästliku tuumkütuse tsükli modelleerimine ja analüüs optimaalseks tooraine kasutuseks ja radioloogilise mõju vähendamiseks

Paljud riigid püüavad piirata kasvuhoonegaaside heitkoguseid ja püüavad keskenduda süsinikuvabadele energiaallikatele, mistõttu on tuumaenergia jätkuva arutelu teema, et laiendada kogu maailma energiatootmise segmenti ja katta baaskoormuse nõudeid. On vaja hinnangut turul pakutavatele uraanitarnetele ja vastavat ressursside optimeerimise konteksti, tegemaks otsuseid, mis mõjutavad tuumaenergia pikaajalist arengut, ning hoiatab poliitikakujundajaid võimalikest uraaniturul toimuvatest muutustest, et aidata teha tehnoloogilisi valikuid. Käesoleva töö eesmärgiks on demonstreerida ja katsetada arenenud simulatsioonimeetodeid ja kontseptsioone, et luua realistlikumaid kütusetsüklite simulaatoreid ja seeläbi luua otsusetegijatele vajalik abivahend. Lisaks lahendab töö optimeerimisparadigma, leidmaks soodsaima tuumakütusetsükli tehnoloogia, mis aitab säästa loodusvarasid, suudab minimiseerida kõrgetasemelist radioaktiivsete jäätmete mõju loodusele ja vähendades tuumamaterjalide levikust tulenevat ohtu.

Selgitame järgnevalt eri ülesandeid ja probleemipüstitusi, et näidata vajadust täiustatud simulatsioonilähenemisviiside järele:

1) Tuumkütusetsükkel on kompleksne tööstusprotsesside järgnevuste süsteem, koosnedes mitmest etapist eesmärgiga toota elektrienergiat uraani, plutooniumi ja muude lõhustuvate materjalide lõhustamisel tuumareaktorites. Töö esimene osa on pühendatud tuumkütuse esimesele tsüklile, mis hõlmab uraani kaevandamist ja freesimist, rikastamisteenuseid ja tuumareaktoreid. Tuumareaktorid on loodud töötama teatud konkreetse tuumkütusega, mida ei saa lühikese aja jooksul asendada ning mistahes muudatusteks on vaja suuri investeeringuid. Seetõttu tuleb esmatähtsalt rahuldada vajadus etteantud tuumakütuse järele.
2) Tuumkütuse tsükli arvutuslike mudelite eesmärgiks on modelleerida eri tsüklite arengut mingi ajaperioodi jooksul, et seejärel genereerida relevantseid väljundandmeid vastavalt etteantud sisendparameetritele. Hetkel leidub mitmeid tuumkütuse tsükli modelleerimise simulatsiooniprogramme, kuid tavaliselt on need simulaatorid kavandatud vaid ühe konkreetse eesmärgi jaoks. Peaaegu kõik tuumkütusetsükli simulatsiooniprogrammid võib jagada kahte rühma – programmid, mis järgivad materjali liikumist diskreetsete kütusekogustena ja teised, mis seda ei tee. Tuumkütusetsükli simulatsioonitööriistad võivad kergesti muutuda keerukaks ja iga uus simulatsioon võib tähendada märkimisväärset jõupingutust kui ka andmeanalüüsi, samas kui tulemuste valideerimine võib osutuda peaaegu võimatuks. Enamus simulatsioonitööriistu töötavad suvaliste andmete korral ja modelleerivad vaid võimalikke sündmuste väljavaateid, kuid ei prognoosi hindu, kulusid ega muid majanduslikke kriteeriume.

3) Kaevanduspõhine uraaniturgude arveldusmudel põhineb esmaste ja sekundaarsete uraaniressursside andmebaasidel ning rikastamisrajatistel. Mudel näitab turgude arveldustingimusi, leides iga-aastase pakkumise ja nõudluse kõverate vahelisi seoseid, võttes arvesse ka sekundaarse tarne tagajärgi, sealhulgas kõrgrikastatud uraani segusid kui ka looduslike uraanivarude koguseid. Tänu sellele hõlmab mudel uraani ja rikastamiseturgude ühismõjusid. Iga uraanikaevanduse kohta on tuumik-andmebaasis unikaalsed karakteristikud, sealhulgas uraanivarude koguhulk, vareseim võimalik avamise kuupäev, kapitali- ja tegevuskulud ning muud fikseeritud parameetrid, mis ajas ei muutu, eeldusel et kaevandusel on veel uraanivarusid mida toota. Uraani tootmise otsused tehakse iga kaevanduse puhul lähtuvalt hetke turuhinnast. Operatiivsete otsuste tegemiseks lähtuvalt lühiajalisest turuhinna prognoosist kasutab mudel kaevanduskulude tüüpstruktuuri eeldades sarnast kapitali, käitus- ja sulgemiskulude suhtelist jaotumist. Tänu sellele saadakse antud kulud skaleerides tüüpkaevanduse vastavad näitajad ühikuhindadega etteantud kaevanduses. Lühiajalise turupakkumise kõver on defineeritud kui üksikute kaevanduste pakkumiskõverate horisontaalne summa. Nõudluse kõvera loomise mehhanism hõlmab loodusliku uraani hinna leidmist, mille puhul iga fragmendi osakaal oleks minimaalne, kaasates nii loodusliku uraanimaagi kui ka selle ümbertöötlemise kulud.
4) Agendipõhine modelleerimise kontseptsioon on laialdaselt kasutusel energiasüsteemide modelleerimisel kui ka teistes valdkondades, et modelleerida üksikute agentide käitumist ökosüsteemis, kus iga agent lahendab optimeerimisülesande ja teeb iseseisvaid otsuseid. Kaevandustel põhinev uraani turumudel kasutab tsükli-tüüpi agendipõhist modelleerimisviisi. Üksikagent võib esindada suurt uraanikaevandust, mis mõjutab märkimisväärselt uraani turuosa. Seetõttu on sellistel agentidel kaalukas osa loodusliku uraani turul ja individuaalsed otsused võivad mõjutada turuhinda. Simulatsiooni iga aasta kohta kasutab turukontrollimudel teatud otsustuspuu kriteeriume, et määrata kindlaks, kas iga konkreetne kaevandus töötab või mitte. Sellele järgneb otsus, kui palju uraani antud kaevandus turule panustab kogu tööstusharu lõikes. Lisaks on mudelisse sisse ehitatud kasumi akumulatsiooni ja ajatamise funktsioon, et muuta mudel realistlikumaks ja volatiilsemaks sõltuvalt välistest teguritest – nagu näiteks kaevanduspoliitika muudatused, võimalikud loodusõnnetused jne.
5) Vaikimisi ei võeta kaevanduspõhise uraaniturgude arveldamise mudelil arvesse uraanikaevanduste litsentsimisega seotud küsimusi ega muid kaasnevaid toiminguid, mis võimaldavad uute kaevanduste avamist, taasavamist või viivitamatut sulgemist. Kaevanduse taasavamiseks vajalik aeg on tihedalt seotud majandusliku ja regulatiivse keskkonnaga ning see ei sõltu ainult tootja otsusest. Selline viivitus vähendab pakkumist, kuna uraanitootjad sisenevad turule soodsamate tingimuste tekkimisel alles teatud viivisega. See muudab turu tunduvalt muutlikumaks ja sarnasemaks tegelike turgude käitumisele. Kui turule sisenevad uued tootjad, kaldub pakkumise kõver paremale ja toimub hinnalangus. Kui üksikud kaevandused pankrotistuvad,

hakkab pakkumiskõver pöörduma (aeglaselt) vasakule, kuid kui on palju kahjumis tootjeid, kasvab järsult ka pankrottide arv ning pakkumiskõver teeb suure nihke vasakule, mille tagajärjeks on järsk hinnatõus.

6) VEGAS – tuumkütuse tsükli ja majanduslike faktorite modelleerimistööriist, mis teeb kindlaks optimaalse tuumkütusetsükli põhialused lähtuvalt simultsiooni juhtivast tegurist – elektrienergia oodatavast maksumusest. Võtmeomaduseks on võime teha valikut, mis tüüpi reaktorit ehitada lähtuvalt objektiivsetest kriteeriumitest. Kulupõhine optimeerimine sisaldab ideaaljuhul ka tulevikuvaadet. Puhtmatemaatiline optimeerimine eeldaks täielikku ennustust, kuid see ei ole tõenäoliselt realistlik kirjeldus agentidele otsustetegemiseks. VEGAS-e tuumkütusetsükli simulaatoris tehakse otsuseid elektrienergia kulude põhjal, minimiseerides tasakaalu-kütusetsüklit. Reaktoritüüpide mis tahes kombinatsiooni jaoks saab määrata tasakaalu-kütusetsükli, mis kujutab endast olukorda, kus täidetud vähemalt üks tugevatest materjali tasakaalu piirangutest. Seda iseloomustab spetsiifiline liikmestüüpide kasutussuhe. Praeguseks juba eksisteerib mitmeid erinevaid tuumareaktoritehnoloogiaid ja tõenäoliselt lisandub neid tulevikus veelgi, mistõttu isegi tasakaalu leidmise ülesanne osutub parajaks väljakutseks modelleerimisel, kui kasutusele võetakse palju erinevaid tehnoloogiaid.

Kaevanduspõhine uraaniturgude arveldusmudel demonstreerib lähenemisviisi, kus modelleeritakse uuraanikaevandusi autonoomselt käituvate üksustena. Autonoomne otsustusvahend näitab, et mudel suudab dünaamiliselt väljastada ehitustellimusi erinevate kütuseahela tasakaalude korral, mis põhinevad kütusetsükli ökonoomikal ja uraanihindade arengudünaamikal.

PUBLICATIONS

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Publications

1. **Auzans, Aris**; Teder, Allan; Tkaczyk, Alan H. (2016). Time Delay and Profit Accumulation Effect on a Mine-Based Uranium Market Clearing Model. Nuclear Engineering and Design, 310, 154–162, 10.1016/j.nucengdes.2016.09.031.
2. **Auzans, Aris**; Schneider, Erich A.; Flanagan, Robert; Tkaczyk, Alan H. (2014). A Mine-Based Uranium Market Clearing Model. Energies, 7 (11), 7673–7693, 10.3390/en7117673.
3. Pelakauskas, Martynas; **Auzans, Aris**; Schneider, Erich A.; Tkaczyk, Alan H. (2013). Autonomous dynamic decision making in a nuclear fuel cycle simulator. Nuclear Engineering and Design, 262, 358–364, 10.1016/j.nucengdes.2013.04.033.
4. Pelakauskas, Martynas; **Auzans, Aris**; Schneider, Erich A.; Flanagan, Robert R.; Tkaczyk, Alan H. (2012). Reprocessing delay and capacity limitation effects on transuranic waste inventory. American Nuclear

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5. **Auzans, Aris**; Schneider, Erich A.; Flanagan, Robert; Tkaczyk, Alan H. (2014). Uranium market clearing individual mines decision making model. PGMO together with the COST Action “Mathematical Optimization in the Decision Support Systems for Efficient and Robust Energy Networks”, Paris, France 2014.
6. **Auzans, Aris**; Teder, Allan; Tkaczyk, Alan H. (2015). Nuclear Fuel Demand Effect on the Front-end Uranium Market. 12th international Conference of Young Scientists on Energy Issues CYSENI-2015, Kaunas, Lithuania, May 27–28, 2015.
7. Pelakauskas, Martynas; **Auzans, Aris**; Schneider, Erich A.; Tkaczyk, Alan H. (2015). Autonominis branduolinio kuro ciklo simuliatorius. Lithuanian National Physics Conference. Vilniaus universitetas, 89., Vilnus, Lithuania, 2015.
8. **Auzans, Aris**; Teder, Allan; Tkaczyk, Alan H. (2016). Regional regulation effect on the Uranium market price. CYSENI 2016, Kaunas, Lithuania, May 27, 2016.
9. **Auzans, Aris**; Tkaczyk, Alan H.; Teder, Allan (2016). The Global Uranium Bank Effect on Uranium Market Clearing Price. Workshop on Optimization Challenges in the Evolution of Energy Networks to Smart Grids, Coimbra, October 27–28, 2016.
10. **Auzans, Aris**, Teder, Allan; Tkaczyk, Alan H. (2017). Front-end uranium mining market evaluation using a uranium market clearing model with a rules-based challenge approach. Activities for Mathematical Optimization in the Decision Support Systems for Efficient and Robust Energy Networks Final Conference, Modena, Italy, 29.03–01.04, 2017.
11. **Auzans, Aris**; Tkaczyk, Alan H. (2017). A Deep Learning Concept in the Agent Based Uranium Market Clearing Model. III. FINEXCA Workshop. Competition and Finance in Natural Resource Markets, Szczecin, Poland, June 9–10, 2017.
12. **Auzans, Aris**; Tkaczyk, Alan H. (2018). Uranium Economics: Mining Market Modelling with a Mine-Based Uranium Market Clearing Model. The University of Latvia, Riga, Latvia, February 26–27, 2018.

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