Digital twin of nuclear waste management facilities

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Abstract

We describe the functions and features of a prototype digital twin developed to support effluent management from a facility undergoing decommissioning. The concept of a digital twin is fairly recent and there are relatively few descriptions of digital twin frameworks in the open literature. Moreover the application to decommissioning is novel and challenging due to the dynamic nature of the process and the large uncertainty. It has been recognized that digitalization of knowledge across the life-cycle could deliver significant benefits to the nuclear industry; Successful decommissioning projects require improved process reliability therefore reducing risks associated with schedule and cost whilst ensuring operations are undertaken safely. The digital twin consists of the integration of numerical models that cover the operation of the asset. These models simulate from a system level description of scheduled operations and process flows of waste material extending down to chemical models that can account for changes in speciation and solubility as a function of process conditions. Statistical tools have been developed to calculate the uncertainty in plant data and this can be propagated through to the predictions. The digital twin has been developed within a modern enterprise server bus framework with a web based front end. Back-end services are scalable and have been designed to take advantage of high performance distributed computing to accelerate model solution.

Keywords: Digital Twin, Uncertainty quantification, chemical process engineering.

1 Introduction

Nuclear decommissioning is a strategic goal of the United Kingdom to achieve the end state of all historic nuclear sites by 2125, [1]. These sites include the 1st Generation Magnox fleet of nuclear reactors and the associated recycling facilities at Sellafield site. These 1st generation facilities were not built with decommissioning in mind and this contributes to the relatively high cost relative to today's operating 2nd and 3rd generation plant where lessons have been learned.

The Magnox Swarf Storage Silos (MSSS) are a facility that is currently operating on Sellafield site and is undergoing a process of decommissioning. The facility was established as a temporary storage facility for waste materials, principally fuel cladding and miscellaneous solids wastes, from military and civilian reprocessing operations. These materials are stored under water to minimise the hazard associated with oxidation and secondary benefit of radiation shielding. The building is aging and the structural integrity represents a significant risk; as such the facility is a priority for decommissioning. A simplified description of the process will involve the removal and safe storage of solid wastes. Radioactivity has leached from the solid wastes into the cover water. Furthermore further liquid wastes will be generated through evaporative top ups and washing of waste grabs. These liquid wastes will also be removed and they will be discharged through a treatment plant which will remove radioactivity before discharge to sea. The first operations to remove and replace radioactive liquors, liquor activity reduction (LAR), have already started, with the first phase completed. From next year, solids wastes retrievals will begin. Over the next two decades, significant quantities of waste will be retrieved from these silos by mechanical grab and transferred to waste boxes. Liquors within the waste silos and additional liquors generated in operations containing potentially hazardous levels of radioactive species will be treated.

Planning the retrievals process is challenging because no plans were drawn up for how waste would be taken out of the building when it was built in the 1960s. Inventory records were kept but it is unknown how the waste has changed after several decades of storage and so it is difficult to predict what will arise when waste is retrieved. The strategy adopted by the programme is to undertake early phase operations in a cautious manner (leading phase) to gather information during early retrievals (learning phase), and this knowledge allows acceleration of the decommissioning in later phases. Digitalization of the information management has the potential to extract as much useful information as possible from retrievals to improve predictions of how the plant will operate in later years. A digital twin representation of the real world asset is required to capture this learning to lead future operations.

2 Introduction to digital twins

The origin of the concept of a digital twin is uncertain. Early references to the concept can be found in NASA and aerospace technology roadmaps, [2], [3]. The role of digital twins in the nuclear industry has been argued by [4]. A digital twin is a framework capable of predicting the most important variables of a physical asset. It is built from a number of components which are integrated into a single powerful tool that enables the end user to predict the outcome of scenarios based on changing process variable. At the core of the digital twin are phenomenological relationships, which can be mechanistic models or data driven models that predict the values of outputs as a function of the inputs. As the digital twin is a representation of a real world operating plant, vehicle or building it is implicit that there will be some coupling of the framework to data obtained from the system. The tight integration of data and model allows the twin to learn from the behaviour of the operating plant. The final part of the picture is data required to validate the phenomenological models. This data can be acquired from commissioning or laboratory experiments and is used to establish the credibility of the models. Credibility is obtained from quantifying the uncertainty and therefore it is useful to couple within the digital twin mathematical models to quantify uncertainty in both the model (epistemic or systematic uncertainty in the phenomenological model) and the plant data (aleatoric or statistical uncertainty).

2.1 Origin of a digital Twins for MSSS liquor waste management

To plan decommissioning operations we need to know how much waste is to be treated, what the waste consists of, when it needs to be treated and what other wastes need treating at the same time that will compete for the finite capacity in the treatment plants. To assist planning, models are developed to understand the uncertainty associated with each aspect. Models are developed in computer software and simulations are carried out where the inputs are varied to quantify the uncertainties. Data is gathered from both the real world asset and laboratory experiments to first parametrise and then validate these models. A key part of the solution is to ensure that this information is then made available to those who need it to make decisions.

In decommissioning we have the problem that the process is inherently not steady state as over the lifetime of the operation we want to achieve an end state of zero output and the waste arising varies with the type of operation being carried out. Therefore we must use tools for modelling the dynamics of the system as we progress from an operational (where outputs reflect normal operations) to fully decommissioned state (with zero or close to zero outputs). Process operations can be both discrete (grabbing some waste and transferrin it to a box) and quasi-continuous (batched transfer of radioactive liquor from the silos to treatment plant and continuous processes such a liquor evaporation). It can also be important to consider additional variability due to the availability of resources and failure rates of plant equipment. We can add to this complexity the dynamic changes in the system chemistry which in turn impacts on our ability to process the effluent. All of these processes require different types of model and the usual practice is to develop independent models in software specifically optimally designed for the purpose of solving a particular type of real-world problem.

When considering the performance of the decommissioning process as a whole, we need to understand how the outputs of the various models link together. Standard practice within the industry is to exchange data via a quality assured process of written reports which have been assessed technical peer review. However this process is inefficient in that only a limited amount of data can be interpreted and passed to the next model. This limits the quantity and fidelity of the solution that can be interpreted by the decision maker. Once the need to exchange data is determined there is an obvious next step to consider how the models themselves can be integrated into a digital twin to improve performance and enhance the quality assurance on the exchange of data. The adoption of a digital twin widens the stakeholders that need to interact with each model establishing a need for a simple, easy to use interface so that those who need to access the inputs and outputs can do so.

3 Methodology

3.1 Existing and planned components of the digital twin framework

The software architecture is based on a Service Oriented Architecture where information (and models) is broken down into discrete blocks such that one service only deals with one particular type of data. A central service register tracks where services and versions are located. At present an event management system has not been implemented as there is currently only the need to implement a limited number of pre-defined operations. The components of this architecture are described in more detail in the following sections. The services are presented to the end user via a web interface with industry standard security protocols. Each of the services is implemented using micro-server architecture with dynamic load balancing and parallel distributed computing enabled. The service is deployed on a high performance distributed computing architecture, which includes scheduler execution services to manage simulation throughput of sensitivity and uncertainty quantification calculations.

3.2 Source data and data management

The first task is to identify the temporal nature of the data which reflects its behaviour in-service through to decommissioning. Historic data refers to the liquor inventory data from tipping records and sample data acquired during early phase of the operations. We have the highest degree of confidence in the data acquired in the more recent time periods (within the last ten years) as we can be sure of the quality of the data and analytic records are stored in a digital format. Finally, there is considerable potential to acquire new data during retrievals and capturing this data is a key part of the learning process that is to be followed.

We have developed a data management system to both store the liquor data which is based on a SQL database for storing the analytical data and MongoDB database for storing documents, which includes simulation outputs. When connecting different physical and temporal scales, we need to consider how data from one scale can be extrapolated (coarse-grained or interpolated) to another. For a decreasing granularity of the data, we can apply statistical methods to either spatially or temporally average the data. For an increasing granularity of data we need to apply interpolation to fill in the gaps between 'coarse-grained' data measured over a long time scale and data required at a 'fine grained' level. If this data was not measured, it must be artificially generated (interpolated) in a realistic and representative manner. A statistical analysis functionality developed in R-shiny provides these interpolation functions. We have analysed the data from the liquor activity reduction operations and have determined its effectiveness. A linear trend was fitted to the data with functions in ggplot2. The confidence interval was determined from the t-distribution with P=95%. The effectiveness of the operation can then be determined by comparing the slopes of the fit to an extrapolation using radioactive decay (eq. 2). The results from a typical analysis are shown in figure 3, overlaid with the results of a simulation from the current development version of the digital twin.

Implementation of extrapolation and interpolation are described in the following section and are limited to specific cases where codes are coupled: extrapolation is only currently only applied to the experimental data trending and interpolation is currently only used to reduce the number of calls to PHREEQC from the process model.

3.3 Models and outputs

Going beyond the data management the design of the digital twin is that of a hierarchy of coupled multi-scale and multi-physics models that together capture the key phenomenological properties of the asset. Individual models can be placed into categories based on the spatial and temporal resolution of the underlying physical models:

3.3.1 Chemical and physical underpinning

Thermodynamic and kinetic models representing the changes in chemical species within the effluent. Physical (chemical) models represent particulate interactions at very small spatial and temporal resolutions (lengths in nm, time steps hours and timescales in years with temporal resolution of fractions of seconds). Also represents mechanistic models of physical processes like settling of colloidal suspensions and bulk flow of liquids through pipes and transfer lines. The key phenomenological properties of the effluent arising from decommissioning operations are the solubility of species that can challenge downstream treatment plants and the potentially in future we can model the formation of mobile slow-settling or colloidal materials that can similarly be transported via pumps and transfer lines. Chemical reactions between the remaining solids and the liquors could result in the release of activity which in future will be captured in the phenomenological models.

The development of a purely mechanistic model to predict speciation and solubility of legacy wastes is an unsurmountable challenge due to the chemical complexity of the system and a paucity of information of the source terms (detailed chemical knowledge of the waste inventory). Data is readily available for the concentration of species in solution obtained from sampling and chemical analysis on up to a daily basis, and extending back to the 1970's (though less frequently) when waste was still being deposited. Trending of this data can be used to predict the change in concentrations over time. We have integrated a tool set developed in the R statistical language within the digital twin framework to undertake trending analysis of the input data. This can compute the trends over time to compute the release rates of activity from current operations. As decommissioning progresses we can analyse the emerging data to update the correlations as required.

The challenge comes when identifying limiting cases, for example where the concentration of a species assumes a nominally constant value. We have therefore derived a hybrid approach where mechanistic models developed in PHREEQC are used to capture the solubility/ speciation behaviour at the point where a step change occurs, for example the limit of solubility. The solubility of species is determined by the solubility product; this is an equilibrium reaction that expresses the concentration of the ions in solution and in the solid product in terms of an equilibrium coefficient. The effective concentration (or activity) of species in solution is corrected for the excess free energy of mixing via Pitzers method,[5]. The materials in the silos are continuously slowly changing due to reactions such as corrosion. However we can use this approach by assuming that the principle of local thermodynamic equilibrium applies due to the large difference between the silo heterogeneity (which is macroscopic) with the thermodynamic principle of heterogeneity (which is microscopic). Fundamental chemical data is managed in a database and has been critically assessed to determine its suitability for this specific application.

The PHREEQC model can be used to determine whether a measurement exceeds the limit of solubility of the species. If the measured value exceeds the solubility limit, then either excess quantity of a species is present as a third phase (colloidal); or the measurement is suspect. At equilibrium, the concentration of a substance in solution is given by the distribution constant, the ratio of the concentrations in the solid and aqueous phases (eq. 1). Currently we can only measure the concentration in solution however we can assume that the solids concentration is effectively constant as it is in large excess and is based on the inventory. To obtain k_D, we used the solution data where we can assume the concentration is constant (at equilibrium) then apply eq. 1.

$$k_D = \frac{[A]_{solid}}{[A]_{aq}} \tag{1}$$

A further mechanistic process that can be captured is radioactive decay. Many of the important radiotoxic species have short half-lives and the change in concentration of these over time can be accounted for. The half-life is computed from a simple 1st order exponential decay expression for the amount of substance N remaining, the integral form being:

$$\log \frac{N}{N_0} = -kt \tag{2}$$

The effectiveness of liquor dilution on the radioactivity of the waste can be calculated as the ratio of the slope of the measure radioactivity data over 1st order decay constant, k, which is related to the half-life of the radionuclide.

3.3.2 Unit operations/ component models

Conservation models for mass, energy and phase changes in chemical species evaluated over the physical scales of filtration, pipes, settling tanks, etc. over length scales equal to the real physical dimensions of these vessels and time-scales up to those of the typical residence times within the vessels (lengths from centimetres to meters, time steps in minutes and timescales from seconds to months).

For the MSSS process unit operations are the individual silos, transfer lines and discharge tank. The models are developed on a compartment by compartment basis which reflects the known inventory and chemical analysis of each compartment. Each compartment group typically has hydraulic connectivity and these results in common liquor chemistry until such time as retrievals have progressed to the point where liquor levels fall below the connectors. Both the compartment model and the chemical process dynamic model are developed in the gPROMS software and language. As the chemistry of the waste is linked to the compartment, we have directly integrated the chemical model developed in PHREEQC with the compartment model. This coupling is implemented in a C++ object interface to deliver high performance. However, calling PHREEQC results in a computational overhead that could be problematic if running a simulation over the whole lifetime of planned retrievals (25+ years.) and so the model has been optimised in this respect with interpolation used to minimise external calls.

3.3.3 Process models

Conservation models for mass, evaluated over the physical scales of connected unit operations (sequences of vessels, pipes etc. in either series or parallel) over length scales representing the components of a chemical plant or series of plants (Lengths from metres to 100s of metres, time steps in hours and timescales from days to decades). The process model is set up to represent the transfer operations associated with the planned decommissioning choreography.

The process model computes dynamically the changes in silo inventory as a function of planned retrieval operations. Each of the silo models is close-coupled within the process flowsheet and the gPROMS model describes mathematically the mass flow of materials between them. Mass balance equations are computed to calculate the volume change and the activity change as liquor is transferred between the compartments and to the discharge. The general form for activity A of soluble species i is

$$\frac{dA_{(aq)i}}{dt} = \sum Ain_{(aq)i} + L_{(aq)i} + R_{(aq)i} - \sum Aout_{(aq)i} \tag{3}$$

For radioactive species an additional decay term (eq.2) is added to the RHS of eq. 3. The reaction term covers the rate of change of species that are known to undergo chemical reactions. For reactions we can assume the reaction is limited by k_D or by solubility, determined from the PHREEQC model and the limiting value is chosen. Release fractions, which define the quantities released during retrieval operations, are also determined from k_D. As these cannot be known for future operations, they will need to be fitted to plant data once these operations actually start. The leach rates, L, are determined by the rate of reaction, which are assumed to be instantaneous in most cases. For some species, we adjust the rate constant minimising the sum of squares of the error until the model prediction closely matches the measured trend. Currently the activity balance for 29 chemical species is tracked in the model and 8 reactions are modelled. We also apply balance equations of a form similar to eq. 3 for the mass of solids in the silos and volume of liquors, both of which change over time depending on the operations being carried out (for example a waste grab removes solid waste, and a liquor top-up adds water to the silos to increase the volume).

Interpolation between model scales is currently only applied to the linking of the PHREEQC chemical model and the gPROMS process model. Calling the PHREEQC model at every timestep would be prohibitively expensive over the run-time of the simulation, and so it is called based on schedule and linked to specific operations. The log form of a 1st order rate equation, where the rate constant is either assumed to be constant and large or is back fitted as discussed earlier, is used to numerically scale the error in the process model to bring the prediction in line with the PHREEQC prediction.

3.3.4 Operational Research (OR)

Conservation models for mass and usually other physical constraints (availability of manpower etc.) evaluated over a series of connected plant flowsheets (length and time-scales identical to the process models). Some processes are simplified to increase the range of process variables that can be modelled.

This models the retrieval operations as a function of resource constraints and ultimately provides the input to the process model. The system model is developed in FlexSim from Saker Solutions. The process model is developed to match the operations modelling in the OR model, with the additional overlay of the chemical changes as included through the silo model. Ultimately it is the OR model that provides decision makers with information on what decommissioning schedule is achievable. The two way exchange with the process chemical models assures that this is not limited by chemistry.

3.3.5 Uncertainty Quantification

Deterministic simulation of the impact of variable uncertainty on the simulation outcome computed for an individual campaign (months) or over the decommissioning schedule as a whole (years) in order to obtain a probabilistic outcome for the discharge profile for liquid effluent.

To understand the importance of the sensitivity of the performance of downstream plants we need to evaluate the propagation of uncertainty of the feed liquors and eventually also to understand the impact of model uncertainty. The distribution of variable uncertainty can be obtained from a top-down analysis of the liquor chemical analysis using the R functionality that has been built into the digital twin. To undertake sensitivity analysis and eventually uncertainty quantification we plan to integrate the COSSAN-X software with the gPROMS model. We have already demonstrated the potential of this technique for effluent treatment in published work [6]. This will enable multi-variate sensitivity studies to quantify the uncertainty in the outputs.

Figure 1: 3D Render of the Magnox Swarf Storage Silos (Source: Sellafield Ltd, original video on ITV.com). The OR model described in 3.4.4 uses 3D visualisation to demonstrate potential bottlenecks in decommissioning activities. The image shows three of the silos which contain a mix of solid debris, settled solids and liquid wastes. The digital twin has been designed to support operations for the removal and treatment of the liquid waste.

4 Conclusions

We have presented a short technical description of a framework for a digital twin of silo decommissioning. The development process of the system architecture is being delivered in several phases, with the database and statistical functionality already implemented and the current work programme integrating the process model service into the architecture. This work will continue in line with the commencement of the next phase of retrieval operations with the approach evolving as the availability of data increases. Value has already been demonstrated with the individual twin components already used to support key decision milestones and the capability we will develop will mitigate against schedule delays, contributing to the saving millions over the lifetime of the plant decommissioning. One of the ways this will be achieved will be to put the tool in the hands of decision makers allowing for real-time analysis of current and planned operations.

Key challenges that have been overcome in this project include collaborative working between teams, across different organisations, which have traditionally focused on solving problems within their own discipline. Further collaboration will be necessary to implement features on the current roadmap, particularly uncertainty quantification. The tools produced to date have been used to support key decisions and as the technology evolves, widening the stakeholder interaction then we will gain further tangible benefits against the current decommissioning challenge. One of the key learning points from this programme has been in the value of data. From an analysis of the quantity of historic data available from which to construct a digital twin, it is clear that increased knowledge of past operations would greatly assist decision making today. It is important for industry to re-evaluate the value and need for data given the continued rise of digital technologies.

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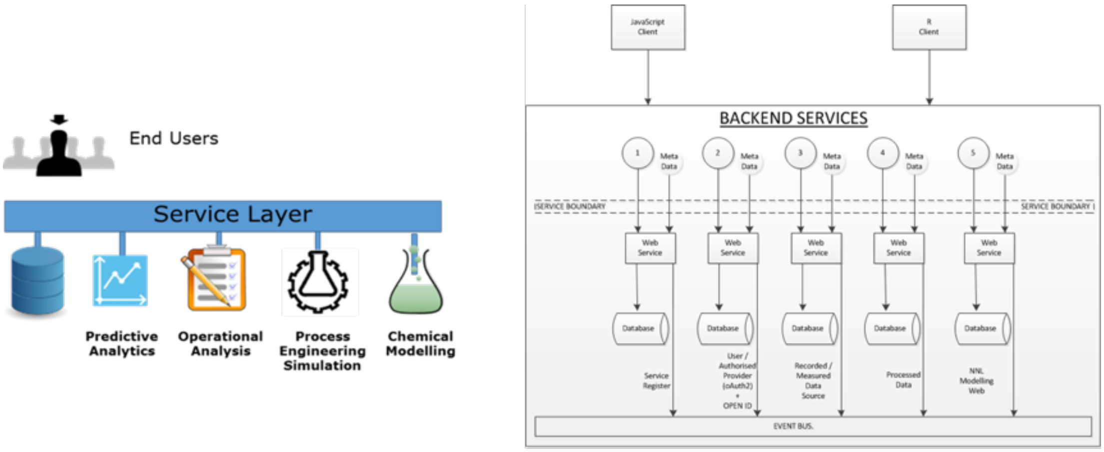

Figure 2: Schematic of the service oriented architecture of the digital twin framework. Showing the high level components (left) and the service Oriented Architecture (right). The R service is integrated as a client and the process model is integrated as a web service (NNL Modelling Web) as part of the High Level Architecture. A more detailed description of the architecture is presented in section 3.3 and 3.4.

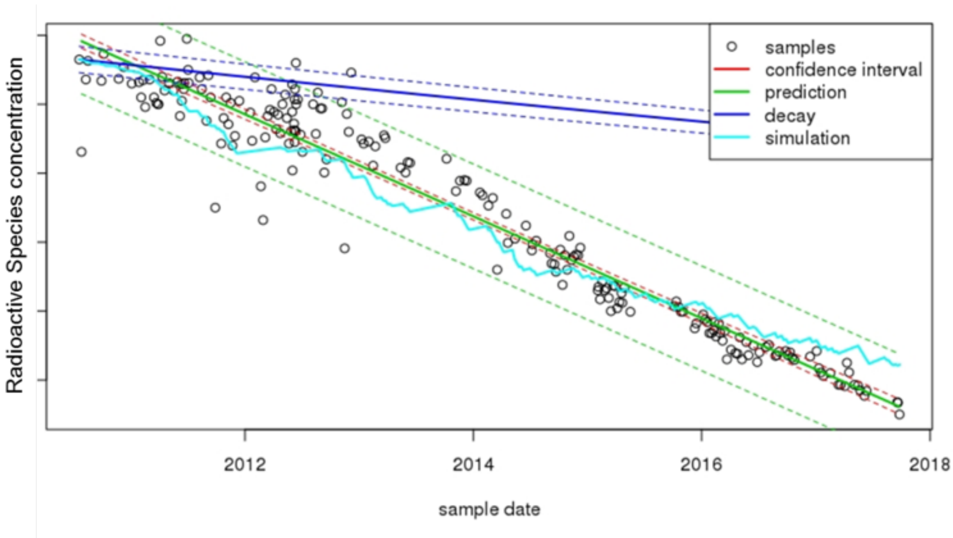

Figure 3: Results of the trending analysis showing the decreasing silo radioactivity with the commencement of decommissioning operations. Sample points are shown as filled circles and the linear fits to the trend and the radioactive decay prediction are shown. Due to the fact that these results represent a work in progress other specific details have been omitted. The simulation (light blue) is the result of the combination of the PHREEQC chemical model coupled with the process simulator (as described in sections 3.4.1-3.4.3). The model prediction falls within the confidence interval and represents a step towards validation and acceptance of the model.