Digital Twin Challenges and Opportunities for Nuclear Fuel Manufacturing Applications

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Abstract

There have been a number of digital twin (DT) frameworks proposed for multiple disciplines in recent years. However, there is a need to develop systematic methodologies to improve our ability to produce DT solutions for the nuclear fuel industry considering specific requirements and conditions exclusive to the nuclear fuel manufacturing cycle. A methodology tailored for nuclear fuel production is presented in this paper. Due to the nature of the chemical processes involved in fuel manufacturing, we highlight the importance of using a combination of physics-based and data-driven modelling. We introduce key technologies for DT construction and the technical challenges for DT are discussed. Furthermore, we depict typical application scenarios, such as key stages of the nuclear manufacturing cycle. Finally, a number of technology issues and research questions related to DT and nuclear fuel manufacturing are identified.

Keywords: Digital Twin, Physics-based Modelling, Data-driven Modelling, Manufacturing, Nuclear Fuel

2022 MSC: 00-01, 00-10

1. Introduction

Modern industry requires the use of advanced manufacturing techniques and operations utilising smart technologies that allow for interoperability among organisations, assets and the people involved in the process. The advent of modern technologies is leading industry to focus on the inter-connectivity of automation, machine learning, real-time data monitoring and control. The challenge is to create manufacturing processes that need to be observed or controlled remotely from an environment that may not be accessible easily by human operators, while having the capability to test and improve the quality of the product, service or process without incurring in high prototyping costs.

The idea of digital twinning originated as a virtual representation of an engineering system, to better understand what was designed versus what was produced, with the purpose of closing the gap between design and execution [Grieves (2014)]. This formal definition, as shown in Fig. 3, encompasses three primary elements: (a) a physical object in a physical space; (2) a virtual object in a virtual space; and (3) the data link between the two spaces.

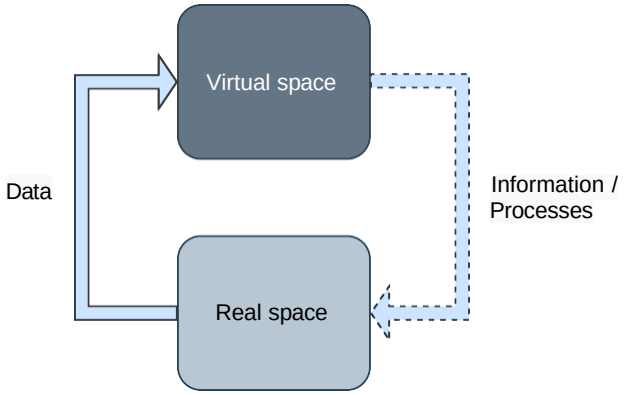

Figure 1: Twinning between the physical and virtual spaces. Adapted from Jones et al. (2020).

The concept of virtualisation spread quickly when NASA started to develop systems and mechanisms that needed to be monitored and manipulated in space,

an environment where operating conditions are difficult to reproduce or unavailable during the design phase. They started to develop virtual prototypes that could be tested before being sent to space or even before physical manufacturing. After a number of iterations testing the virtual prototype, and only after making sure the prototype could reach the required specification, the manufacture of a device was started [Glaessgen and Stargel (2012)].

DT technology has been discussed widely as a key game changer in advancing Smart Manufacturing and Industry 4.0 initiatives. A significant advantage of DT technology is the availability of data gathered from different domains in the manufacturing value chain to derive time-sensitive decisions [Lim et al. (2020); Fukawa and Rindfleisch (2023)]. However, it is argued that most DT industrial approaches are ad-hoc solutions where DTs are expected to be used once or a few times within a limited time-frame associated with a particular project. Major industrial corporations such as Siemens, General Electric, Bosch and Ansys. offer DTs solutions and infrastructure based on their own experience in manufacturing of products and services. However, there is a need for a systematic and unified DT methodology, in which DTs could be used/reused over time in multiple coordinated applications [Qamsane et al. (2021); Johansen et al. (2023)].

Given that the primary objective of a DT is to create a virtual representation or model of a physical process, this technology has proven useful in numerous major industries. The present work explores the advantages of employing this technology in nuclear fuel manufacturing, an industry facing several challenges that DTs are highly likely to help overcome. The adoption of a DT, in general terms, to aid nuclear fuel manufacture offers the potential for a wide variety of benefits.

Nuclear power projects are capital-intensive, making them economically challenging compared to other forms of energy generation [Rothwell (G.); Hansen (2019)]. Reducing costs is a continual focus in the industry [Rabl (2013)]. Similarly, the enrichment process, aimed at increasing the concentration of ^{235}U, can be both energy-intensive and expensive [Lahoda (2004)]. Ongoing research

is focused on developing more efficient and cost-effective enrichment methods [Nishizawa et al. (1998); Seko et al. (1990)], where DTs can be employed to test these new approaches inexpensively.

Managing and disposing of spent nuclear fuel is a significant challenge. Long-lived radioactive isotopes present in spent fuel require secure storage solutions to prevent environmental contamination [Bruno and Ewing (2006); Gauld et al. (2017)]. Processes operated in parallel to those depicted in a digital representation might provide an additional way in which fissile material quantities are assessed and accounted for, particularly in the context of safeguards [Woo (2012)], and could reduce uncertainties on quantities such as material unaccounted for.

Implementing a closed nuclear fuel cycle, where spent fuel is reprocessed and recycled, faces technical, economic, and socio-political challenges. Nuclear power can face public opposition due to concerns about safety, radioactive waste, and the perceived potential for nuclear accidents [Havl´ıcek (2019)]. Overcoming these concerns is crucial for the expansion of nuclear energy [Havl´ıcek (2019); Ganda et al. (2016)]. Digital parallels of nuclear processes might also allow for greater optimisation concerning the quantities of reagents used, thereby improving efficiency, whilst reducing cost and waste [Atz and Fratoni (2023)].

Obtaining regulatory approval for new fuel cycle technologies and reactor designs can be a lengthy and challenging process [Sauter (2009); Heffron (2013); Hogselius (2009)], potentially hindering innovation and development. Over time, where learning concerning the specific features of a process by means of DTs, concerning such factors as hold-up and wear [Strobel et al. (2023)] might take years to acquire, comparison of the DT operation with the real system could highlight departures from accepted performance much earlier. This could aid maintenance, allow for improvements to the process design and prevent significant periods of reduced operation [Zhong et al. (2023); van Dinter et al. (2022)]. In the future, DTs of existing process architectures could be adapted and scrutinised before an advanced plant is built, on the basis of these developments, complementing the development and use of test rigs and prototype process infrastructure [Song et al. (2022); Edwards et al. (2023)]. Understanding the

roles and distinctions between digital plans and DTs is crucial, especially in fields such as manufacturing where they play significant roles in project management and optimisation. Digital plans are primarily used for design, visualisation, and communication during the pre-construction or pre-production phases. DTs, nevertheless, serve operational purposes, offering insights into real-time performance, monitoring, and optimisation throughout the asset's lifecycle.

Significant effort in DT research has been focusing on the connection between the real and virtual spaces. Grieves (2014) state that global manufacturers today either work with the physical product or with the virtual product, missing a deep meaningful understanding of the interaction between the two products. Lin et al. (2021) claim that DTs provide reasonably useful behaviour adjustments based on feedback from the physical part. However, such adjustments are deterministic, and thus lack flexibility and adaptability. To address such problems, an extended concept, evolutionary digital twin (EDT) was proposed. With an EDT, a more precise approximated model of the physical world could be established through supervised learning [Lin et al. (2021)].

The present article highlights the importance of combining both physics-based and data-driven modelling approaches for nuclear applications (Section 2). We introduce key technologies and typical application scenarios, such as the stages of the nuclear manufacturing cycle (Appendix A). We introduce a DT methodology tailored for nuclear fuel production, and use it to discuss relevant technical challenges (Section 3). Finally, a number of technological issues and research questions related to DT in the context of nuclear fuel manufacturing are identified (Section 4).

2. Background

In recent years, special attention has been given to the creation of DTs and their applications, encompassing an important number of domains, such as manufacturing, aerospace, healthcare, satellite networks, intelligent transportation and smart cities [Jones et al. (2020); Wanasinghe et al. (2020)]. Despite the pos-

itive advantages provided by DTs, there are no survey reports focusing on this technology applied to the nuclear fuel manufacturing industry. Some reports explore the promising utilisation of DTs in the design and construction of nuclear reactors [Kochunas and Huan (2021); Lin et al. (2021); Bowman et al. (2022)]. However, the manufacturing processes involved in the creation of nuclear fuel are entirely different from the reactor designs. In other words, DTs deployed for nuclear energy generation are significantly different from DTs proposed for manufacturing of the fuel required by the reactors.

Due to their high applicability in any industrial sector, DTs are a significant technology trend, where the incorporation of machine learning / artificial intelligence techniques enrich DT significance and research potential [Rathore et al. (2021)]. Wu et al. (2021) have explored the connection between DTs and their physical counterparts, where physical objects and virtual twins can communicate, collaborate, share information, complete tasks with each other, and form an information sharing network by connecting multiple DT nodes. This concept is called Digital Twin Network (DTN). Autiosalo et al. (2021) propose an open-source server solution called Digital Twin Web, software that follows a similar structure to the World Wide Web and which allows digital distribution of twin documents as effortlessly as possible using a web browser. Users with no experience in programming or server administration can create a public and free-of-charge instance of the software intended to be deployed as a server for DT implementations.

A new concept, Digital Twin Data (DTD) was introduced by Zhang et al. (2022). Since data are a core driver for DTs, a DTD approach simply defines physical entity-related data, virtual model-related data, service-related data, domain knowledge, fusion data, and connection data [Tekinerdogan (2023)]. This approach demands specific data requirements in terms of data gathering, interaction, universality, mining, fusion, iterative optimisation, and on-demand usage. Another DT framework is based on the System Development Life Cycle (SDLC) process that establishes (1) the specific requirements of a DT, (2) an understanding of the manufacturing process within the operation of the DT,

and (3) the object-oriented aspects of the DT to achieve scalability, re-usability, interoperability, interchangeability and extensibility [Qamsane et al. (2021)]. This framework serves as a procedure for good practice in DT development as it provides guidelines across the DT life-cycle. Other recent work has focused on the deployment of autonomous control systems into new nuclear reactor designs with DT technology. An analysis for DTs for nearly autonomous management and control systems (NAMAC) was reported by Lin et al. (2021). For this approach, DTs are used to extract information from the NAMAC's knowledge base to support decision-making in reactor control and management during all modes of plant operations. This data-driven approach identifies nonlinear relationships within the complex reactor system and the supporting real-time operations for the evaluation of uncertainty quantification.

Kochunas and Huan (2021) propose that, for nuclear power applications, DT development should rely on mechanistic model-based methods to leverage the considerable experience and understanding of these systems. Model-free techniques can be adopted subsequently to selectively, and correctively, augment limitations in the model-based approaches. Both forward and reverse uncertainty quantification and their optimisation are also analysed to facilitate decision making in support of the physical asset operating in an uncertain environment. This work in particular focuses on DTs that can be deployed in the design of nuclear reactors. Rasheed et al. (2020), Bárkányi et al. (2021) and Kochunas and Huan (2021) state that surrogate models in DTs are suitable for linking together physics-based modelling, data-driven modelling, and hybrid solutions. Fig. 2 shows a simple approach to hybrid modelling. This work shows that the use of surrogate models has advantages. Even though they are black-box type models, they clearly reflect some of the physics involved in the system. Once the models have been trained, they become stable for making prediction inferences, uncertainties can be bounded and estimated and they are less susceptible to bias. This study shows how the surrogate model types that have been applied for different DT applications are implemented based on: neural networks, support vector machines, radial basis functions, linear

regression, polynomial functions, Gaussian process regression, power series expansions, fuzzy models, state space models, Monte Carlo and Kalman filters [Papacharalampopoulos (2020); Lin et al. (2021); Bárkányi et al. (2021)].

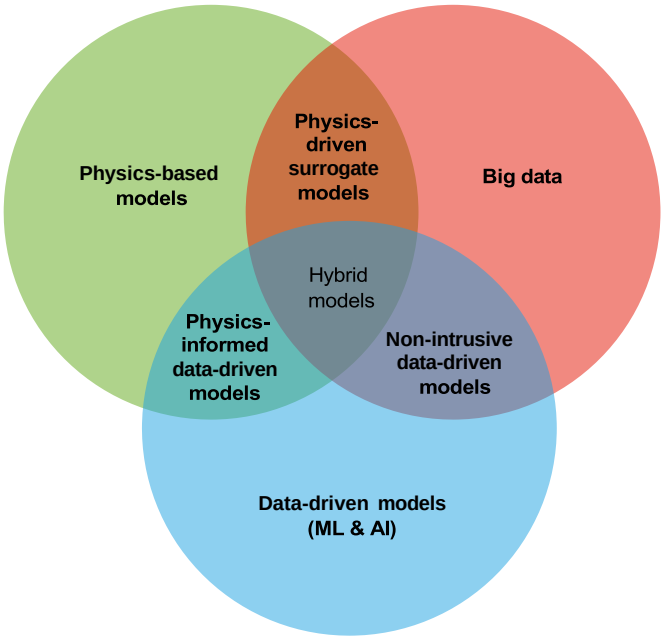

Figure 2: Hybrid analysis and modelling [Rasheed et al. (2020); B´ark´anyi et al. (2021)].

The main reasoning behind applying surrogates in DTs is that their computational requirements are significantly smaller than other simulation process such as Finite Element Analysis (FEA) or Computational Fluid Dynamics (CFD). Two issues with the application of surrogate models have been identified: (1) the significant amount of data needed for model building and (2) the need of continuous maintenance over the whole life cycle of the model. An alternative approach to improving computational efficiency for surrogate models is the application of models based on sets of physics-based equations or sets of differential equations that describe a well-known process or system. Successful implementations of DTs will require trust in the models, trust in the data, and trust in the algorithms used to update the model based on the data. When all

the aforementioned elements are present, a system defined in the physical space can be replicated successfully in a virtual space [Wright and Davidson (2020)].

In the context of manufacturing, Bao et al. (2019) define three types of DTs: product DT, process DT and service DT. The inter-operation mode among these DTs are presented and combined to execute operations between product, process and resource using the Automated Markup Language (AutomationML). This standard aims to converge the physical space and the virtual space in the workshop or factory for predicting manufacturing outcomes.

3. Defining Digital Twins for Nuclear Fuel Manufacturing

3.1. Reaction kinetics

Based on our current understanding of the primary processes involved in nuclear fuel production (see Appendix A), it is evident that many of the stages in nuclear fuel manufacturing can be modelled as a series of chemical processes. By modelling the chemical interactions of the elements involved in each reaction, it is feasible to use the kinetics of the reaction as a basis for the creation of a DT. Reactor kinetics is the study of processes that control the time-dependent behaviour of a chemical reactor. The chemistry involved in the nuclear fuel manufacturing cycle plays a crucial role in the generation of nuclear energy [Nash and Braley (2011)]. A chemical process is represented mathematically as the change in the concentration of its reactants or products with time [Smith and Konings (2020)]. A two-component chemical reaction is described by the balance equation

$$aA + bB \rightarrow cP, \tag{1}$$

where A and B represent the reactants and C represents a product of the reaction. The coefficients a, b and c in reaction 1 represent the stoichiometric ratios of each component in the reaction. The rate of appearance or disappearance of these chemicals are related to each other by the rate equation

$$r_L = -\frac{\sigma}{\rho} r_R, \tag{2}$$

where L and σ represents a chemical and its stoichiometric coefficient on the left hand side of reaction 1; R and ρ represent a product and its stoichiometric coefficient on the right hand side of reaction 1. The negative sign indicates that the rate of appearance of a chemical on the right is proportional to the rate of disappearance of a chemical on the left. The reaction rate expressions describe the rate of a reaction to concentrations of the reactants and products, with each concentration expressed with an order. For the general reaction 1, the reaction rates can be expressed as

$$r_A = \frac{dC_A}{dt} = -k_1 C_A^{\alpha} C_B^{\beta}, \tag{3}$$

$$r_B = \frac{dC_B}{dt} = -k_2 C_A^{\alpha} C_B^{\beta} \tag{4}$$

and

$$r_P = \frac{dC_P}{dt} = k_3 C_P^{\varphi}, \tag{5}$$

where C_A, C_B and C_P represent the concentration of reactant A and B and product C respectively. Here, k_1, k_2 and k_3 are rate constants which are not a function of concentration. It can be seen from expressions 3, 4 and 5 that reaction 1 becomes a nonlinear differential system that can be solved for any concentration C which has reacted by time t [Scholz and Scholz (2014)]. The solution will depend on the experimentally-determined reaction rates k and exponents α, β and φ. In many elementary reactions the exponents are of order zero, one or two. However, in more complex processes, fractional orders also occur [Rodin and Egan (1989)].

As identified previously in the literature, the creation of a DT can be facilitated through the utilisation of a physics-based model. This approach aligns with the methodology proposed and detailed in the next section.

3.2. Methodology

The creation of DT solutions for nuclear fuel manufacturing processes will involve considering the following steps. This approach is grounded in a general methodology that holds applicability across diverse manufacturing industries [Qamsane et al. (2021)]. Fig. 3 illustrates this methodology in a graphical representation, demonstrating the process in a non-linear or non-sequential manner, allowing for more complexity and flexibility in presenting relationships and connections between various phases of the DT implementation. Each stage in the methodology is explained in the list below.

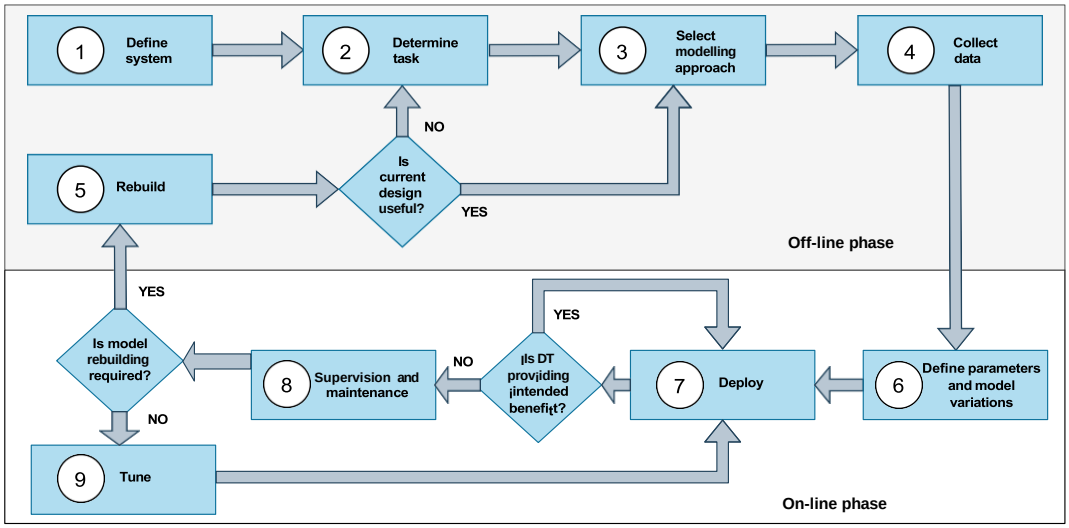

Figure 3: A Methodology to implement DT solutions for manufacturing systems. Adapted from [Qamsane et al. (2021)].

3.3. Off-line development phase

1. **Define system:** Definition of the physical system or manufacturing process to be represented as a DT. This initial phase involves planning to assess whether there is a need to enhance a specific aspect of the manufacturing process. It aims to determine whether a DT solution can address the identified need. During this phase, problems within the manufacturing facility are pinpointed, and potential solutions are proposed. In situations where implementing a solution directly in the physical space is impractical, for reasons such as financial constraints preventing production halts, a parallel representation of the physical environment can be employed. This allows for improvements or optimisations to be explored without disrupting the ongoing process, especially during the development phase [Bao et al. (2019); Bárkányi et al. (2021); Bowman et al. (2022); Fukawa and Rindfleisch (2023); Grieves (2014); Jones et al. (2020); Lim et al. (2020); Lin et al. (2021); Wright and Davidson (2020)].
2. **Determine task:** Determination of the DT task or purpose (e.g., monitoring and optimisation, predictive maintenance, real-time decision-making, automated control, and responsiveness). This phase involves identifying the specific goals of the DT application. Typically, the overarching objectives include enhancing the economic efficiency of the entire process, improving manufacturing efficiency, optimising the proportion of production time dedicated to value-added activities, or ensuring consistency in the quality of the final product [Wanasinghe et al. (2020); Garc´ıa et al. (1989); Grieves (2014); Qin and Badgwell (2003); Wu et al. (2021); Zhang et al. (2022)]. Quantitative assessment and evaluation of historical data are essential in gaining insights into the relevant issues that the DT aims to address. To achieve a comprehensive understanding of the data, considerable expertise and knowledge of the manufacturing problem are necessary. Input and insights from domain experts are invaluable during this phase, aiding in the collection of additional perspectives on data collection. For

example, this step facilitates the identification of useful versus non-useful data, establishes criteria for data trustworthiness, determines which data to utilise, specifies features to extract, and addresses considerations such as data handling or data manipulation [Qamsane et al. (2021)].

3. **Select modelling approach:** The selection of a suitable modelling approach (whether physics-based, data-driven, or hybrid) is contingent upon the knowledge available about the system or process. Given that most processes involved in nuclear fuel manufacturing are highly automated, a substantial amount of data were collected routinely using advanced technologies such as Supervisory Control and Data Acquisition (SCADA) and Failure Mode and Effects Analysis (FMEA). These processes often entail the transformation of chemical elements (e.g., converting uranium hexafluoride into uranium dioxide) or the physical enhancement of elements (e.g., uranium enrichment). In light of these considerations, a hybrid modelling approach proves advantageous. This is particularly beneficial, given that all chemical interactions within the fuel cycle have been studied, characterised, and documented extensively in the past [Atz and Fratoni (2023); Ganda et al. (2016); Havl´ıcek (2019); Kang et al. (2008); Nash and Braley (2011)]. As discussed in Section 3.1, the equations derived from reaction kinetics can serve potentially as a foundational element for a hybrid model. This approach integrates real-time sensor data from the physical system, provided it is available in real-time, offering a comprehensive and dynamic representation of the manufacturing processes.
4. **Collect data:** After defining the DT models, the next step involves the collection of data from the physical system. It is imperative to gather an appropriate quantity and quality of data, tailored to the chosen modelling approach. As mentioned earlier, these manufacturing activities leverage professional tools for data collection, integrated seamlessly with digital manufacturing and DTs. Technologies such as Big Data and Cloud Computing are already inherent components of these processes [Qi and Tao (2018); Kkarchenko (2018); Wanasinghe et al. (2020)]. As illustrated in

Fig. 3, the data collection step is positioned as an offline element in this proposed methodology. This strategic placement stems from the acknowledgment that, in scenarios where no historical data is available for assessing the prerequisites of a DT, establishing a setup for physically acquiring data takes precedence before the implementation phase.

5. **Rebuild:** The necessity to rebuild a DT solution may arise if the current design fails to produce the expected results, as defined in step 2. However, as depicted in Fig. 3, the evaluation of the current solution occurs at the end of the on-line phase, following the deployment of the proposed off-line solution. Consequently, establishing an iterative nature for the proposed methodology, this rebuilding step is positioned in the offline phase. This is because this step requires a revision of the DT modelling approach, where even a redefinition of the DT task or purpose may be necessary if the current design yields unsatisfactory results [Wanasinghe et al. (2020); Garc´ıa et al. (1989); Grieves (2014); Zhang et al. (2022)].

3.4. On-line deployment phase

6. **Define parameters and model variations:** This preparatory step is crucial and must be completed before moving on to the implementation of the model(s) and the determination of the model parameters, along with the establishment of a robust model validation strategy. The reason behind this activity is to ensure a solid foundation for the subsequent deployment phase of the methodology. Considering the aforementioned versatility of hybrid approaches in deploying DT solutions for nuclear fuel fabrication, a range of possibilities exists. These approaches, as discussed in Section 2, draw inspiration from practices applicable to various industries [Wanasinghe et al. (2020); Garc´ıa et al. (1989); Grieves (2014); Qin and Badgwell (2003); Wu et al. (2021); Zhang et al. (2022)]. By leveraging hybrid models, which combine physics-based and data-driven elements, the methodology gains flexibility and adaptability. A pivotal aspect of this step involves the seamless integration of the DT solution into the opera-

tional framework. This integration is designed to harness run-time data, enabling the DT to assess dynamically the system and provide valuable recommendations. The utilisation of real-time data not only enhances the accuracy and relevance of the DT but also empowers it to respond effectively to dynamic changes in the manufacturing environment. As a result, this integration serves as a proactive measure, aligning the DT with the real-time intricacies of the fabrication process and ensuring its efficacy in offering timely insights and recommendations [Bao et al. (2019); Bárkányi et al. (2021); Fukawa and Rindfleisch (2023); **?**); Qin and Badgwell (2003); Wu et al. (2021); Zhang et al. (2022)].

7. **Deploy:** The deployment of a DT is a complex process demanding a comprehensive, multidisciplinary approach that incorporates domain expertise, seamless technology integration, and effective communication among diverse stakeholders. Each deployment is inherently distinct, tailored to the specific characteristics and requirements of the physical system or process represented by the DT. Leveraging insights gained from past experiences in nuclear sites, establishing a dedicated DT for nuclear fuel fabrication necessitates careful consideration of critical elements. This includes securing adequate computational resources, seamless integration with existing IT systems, the development of an intuitive user interface and visualisation tools, robust security measures, adherence to regulatory compliance standards, and more [Fukawa and Rindfleisch (2023); Glaessgen and Stargel (2012); Johansen et al. (2023)]. Each of these aspects contributes to the successful implementation and operation of the DT in the context of nuclear fuel fabrication. As depicted in Fig. 3, evaluating the deployment of a DT solution is straightforward. In instances where the intended benefits are not realised, the deployment task may need to be repeated, having addressed or resolved issues previously, until the desired outcomes are achieved.
8. **Supervision and maintenance:** Supervise and maintain the deployment of the previously proposed offline solution. Continuous oversight

of the DT within the application environment and ongoing assessment of model quality are indispensable aspects of the maintenance stage. To ensure optimal performance, a systematic approach is established for the con- tinuous monitoring of the DT operations [Jones et al. (2020); Kochunas and Huan (2021)]. Regular updates and maintenance activities for both the DT models and data sources are crucial to uphold accuracy and rel- evance over time. At this stage, potential modifications to the model parameters or structure may be necessary [Lin et al. (2021)]. Similar to the preceding step, an evaluation of the DT's performance may reveal the need to rebuild and improve the solution or simply fine-tune the existing one.

9. **Tune:** Tuning the proposed DT involves adjusting its parameters or configurations to optimise performance and enhance accuracy in representing the physical system. The first step is to evaluate how effectively the DT captures and predicts the behaviour of the physical system. This assessment includes considering feedback from end-users or stakeholders who may highlight any discrepancies between the DT's predictions and the actual system behaviour [Wanasinghe et al. (2020); Wu et al. (2021)]. Next, it is important to examine critically the parameters and configurations of the DT model to identify areas for improvement. This evaluation aims to determine whether adjustments to these parameters could lead to enhanced accuracy and better alignment with the real-world system. Once potential adjustments are identified, the tuned DT needs validation. This involves assessing its performance using historical data or separate datasets not used during the initial model development. Tuning is often an iterative process; therefore, after making adjustments, it is crucial to repeat the evaluation, validation, and testing steps to assess thoroughly the impact of changes. Documentation and communication play a key role in the tuning process. Finally, for long-term effectiveness, the performance of the tuned DT must be monitored over time. This ongoing assessment helps ensure that the model remains accurate and aligned with changes in

the physical system, providing a reliable representation over the course of its deployment [Wanasinghe et al. (2020); Wu et al. (2021); Rathore et al. (2021)].

4. Opportunities

The adaptability of DTs to specific industries, processes, or systems enables organisations to adopt them as tailored solutions, emphasising specific possibilities for the nuclear fuel industry. To demonstrate the potential of DTs in fostering innovation, efficiency, and strategic decision-making, positioning the nuclear fuel industry for success in a technology-driven landscape, various opportunities and challenges have been identified.

4.1. Standardisation

Data collection is a crucial aspect of DTs. However, field-collected data often lacks a standardised format. Various commercially-available data integration platforms from different vendors adhere to distinct standards and methods for presenting data. Furthermore, existing datasets are decentralised frequently, stored in separate locations, and not linked to a common database [Qamsane et al. (2021); Johansen et al. (2023)]. These challenges pose a significant obstacle when integrating previously collected data and real-time data into a unified data analytics process. Consequently, the need arises for an intermediate custom tool capable of converting data from both proprietary and open access sources into a standardised format that the DT can comprehend.

Therefore, no standard DT approach has seen broad adoption because they are largely tool-based or framework-based [Qamsane et al. (2021)]. The absence of a standard in data representations for DT, coupled with the multitude of available frameworks for DT development, introduces challenges to deploying DTs in real manufacturing settings. Additionally, there is a lack of systematic techniques that leverage well-known research approaches to achieve scalable, reusable, and interoperable DT solutions in the real manufacturing world.

While industries are gradually embracing solutions from recognised digital service providers (refer to Section 1), the approach to DT solutions varies significantly across different industries. Nonetheless, it is plausible that a solution for the nuclear fuel cycle will adopt a framework similar to the one illustrated in Fig. 3. Once a modelling framework is selected and developed, the final solution will manifest in a software-defined manner, operating on a dedicated computing system either locally or in the cloud (refer to Fig. 4).

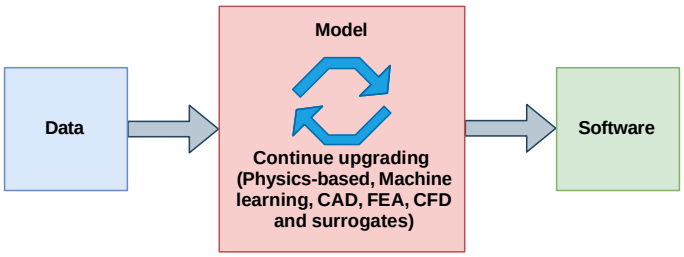

Figure 4: Software-based DT solution. Adapted from Wu et al. (2021).

A recently published report, outlined in [Kung et al. (2022)], offers a comprehensive overview of ongoing global standardisation efforts in DTs, along with the involved organisations. The report, compiled by a dedicated group, maps international standards and classifies related documents extensively, identifying originating bodies and industrial domains. It emphasises the existence of numerous documents supporting DT technologies, covering aspects such as modelling, security, protocols, and data formats. Additionally, the report provides guidelines that aid developers and users of DTs, potentially serving as a foundational basis for standardising DT technology across industries.

It is a priority that a standard for DT development be adopted to facilitate interaction with commercial tools and software tools developed within the nuclear fuel sector. Furthermore, a standard can support integration with physically-sensed data and their extended reality counterpart [Kochunas and Huan (2021); Touran et al. (2017)]. In fact, the reason for success of deployed technologies in the nuclear industry is arguably a reliance on standardisation.

Whilst the industry generally demands standardised solutions, currently there is no standard exclusively focusing on digital twinning. The ISO/DIS 23247-1 standard [ISO/DIS (2022)] provides limited information on DT frameworks. Moreover, it provides no specific guidance for implementing DT solutions nor is this standard specifically tailored for any industry, including nuclear.

4.2. On-line uranium enrichment assessment

In nearly every industrial process, including product design, product performance, process planning, assembly line, task-scheduling, and resource allocation, optimisation is required. As an emerging technology, digital twinning provides a direct pathway to optimisation with considerably less effort than with no digital virtualisation. However, careful consideration of the chosen DT methods and the underlying feature set will be essential for better optimisation of the results.

In terms of uranium enrichment, a number of off-line methods exist to determine enrichment of uranium throughout the manufacturing process of nuclear fuel [Park et al. (2012)]. The main goal of DT technology here is to render fuel manufacturing compliance responsive to detected changes in product composition and quality by potentially implementing a DT of the process with on-line enrichment assessment capability. Currently, product compliance in nuclear fuel manufacturing relies on off-line, lab-based analysis and manual inspection. In nuclear fuel DT research, we should test the hypothesis that a control network can be conceived using input data from online DT methods to render the process responsive. Any variance in product quality (UO_2 quality, enrichment or pellet shape) can be tested and hopefully reduced by adjusting feedstocks, process operations, or by identifying and amending machine faults.

4.3. Big data and cloud computing

The infrastructure for handling and storing high-volume data has been progressing considerably in recent years. Numerous platforms are now readily accessible, providing comprehensive capabilities for processing big data projects

encompassing storage, centralised management, analysis, visualisation, accessibility, and security. Several survey articles delve into various facets of big data, covering not only state-of-the-art technology and platforms but also methods that inherently address the critical requirements of DT applications [Qi and Tao (2018); Kkarchenko (2018)].

In virtually any industrial setup, sensors attached to a manufacturing process generate a substantial volume of data. Recognising that such data can often be tainted with systematic or unsystematic noise, it is essential to pre-process it before applying any machine learning-based algorithms [Wanasinghe et al. (2020)]. The potential of edge and cloud computing platforms to manage DT-related data is on the horizon. Edge computing, for example, enables distributed processing at the DT network's edge, with aggregate processing accomplished in the cloud. However, aggregating data in the cloud may lead to increased response times, impacting the performance of fast-paced dynamic systems. However, for nuclear fuel operations, this might be less of an issue, as most of the chemical processes discussed earlier can operate potentially within the latencies provided by a modern DT network. Due to diverse requirements, different DT scenarios necessitate varying computing speeds and latencies. Cloud servers, with their capacity to process large amounts of data in seconds, offer robust DT services. Additionally, a cloud architecture can facilitate the organisation the management of numerous connected physical objects and parallel virtual models, along with the amalgamation and integration of real-time and historical data. This proves particularly beneficial for the nuclear industry, where the practice of retaining months or even years of historical data for security purposes is commonplace [Westinghouse 2 (2024)].

5. Challenges

5.1. Security and privacy issues

The aforementioned data storage systems require protection against cyber-attacks and must be well organised to ensure fast data access [Lee and Huh

(2019); Kkarchenko (2018); Yao et al. (2020)]. Implementation of user identification protocols is crucial to prevent unauthorised data access and modifications. Consequently, the handling of data in DT systems for the nuclear fuel industry is deemed critical, necessitating strict security and privacy protocols. The inclusion of Internet of Things (IoT) devices in DT introduces heightened security concerns for the underlying communication protocols. Although physical processes may not be threatened easily during these situations, attackers could potentially manipulate the virtual model or tamper with the data fed back by it. Moreover, the extensive collection of asset-related data must be stored securely to prevent data breaches from both internal and external threats [Tao (2019)].

In the realm of data analytics, several challenges need addressing: (1) the choice between using cloud or local software and data warehouses for analytics and data storage; (2) determining the strategy for executing machine learning models; and (3) deciding when to perform batch, semi-batch, or real-time data analysis [Wanasinghe et al. (2020)]. To comply with Nuclear Power Plant (NPP) safety design, evaluation, operator training, and emergency management, the chosen framework must offer insights into the current process state and predictions of future state transients [Alamaniotis (2023)]. In fuel production security, utilising a DT to manage security-critical substances such as ^{235}U offers inherent benefits. By ensuring the security of the DT itself, the parameters governing the operation of manufacturing machines can also be safeguarded. This relationship is akin to holding a key; without it, the replication of the process becomes unfeasible. Moreover, employing a DT could reduce the necessity for numerous individuals to possess precise knowledge of the system's configuration. Instead, the DT serves as a virtual, non-invasive entity, devoid of the vulnerabilities associated with human involvement.

5.2. Condition responsiveness and control

Digital twinning offers an attractive outcome when implemented properly. Prognosis, or proper forecast of the remaining operational life, future condition,

or probability of reliable operation of equipment based on the acquired condition monitoring data, is needed. This feature has not been fully taken advantage of in real manufacturing settings in the context of DT [Grieves (2014)]. Prognosis can, for instance, improve the predictability of machinery failure rate and avoid unexpected corrective maintenance, hence becoming an intelligent predictive maintenance system. However, the automated data-collection, analysis and prediction of system state using DT is still not a mainstream practice in nuclear manufacturing. Nevertheless, DTs are becoming a valuable tool during the design process of complex nuclear reactors [Kochunas and Huan (2021); Bowman et al. (2022); Lin et al. (2021)].

With a suitable methodology (see Fig. 3), a DT for any of the nuclear fuel processes discussed earlier will include the processing of the sensors being used to measure the state of the machinery (flow rate, temperature, pressure and vibration), and these measures will be stored and analysed using physical-based (mathematical models) and data-driven (machine learning and/or neural networks on historical and current states) prognostics models. Within the context of the characteristics of the DTs, the techniques can apply metrology methods, physical-to-virtual data connections, when providing the state of the physical entity [Heng et al. (2009); Fernandez et al. (2017); Gong et al. (2022)]. The use of Model Predictive Control (MPC) along with DTs is a priority for the nuclear industry. Specifically, MPC research has thrived for control applications in chemical processes in the oil and gas industry. Therefore, it is viable to apply MPC in the nuclear fuel industry as well [Garc´ıa et al. (1989)], hence MPC and DTs can provide the means of controlling a process based on the proposed DT model. Physical processes are monitored and compared to their DT counterparts which are able to predict future states of the process, and optimise/adapt/control the process appropriately [Jones et al. (2020); Rasvan (2018); Dong et al. (2018); Zhu et al. (2022); Benitez-Read et al. (1992)].

Industrial applications requiring a robust automated means of control have been using MPC solutions for a long time. MPC is now used widely across engineering disciplines [Qin and Badgwell (2003)]. Every aspect of the MPC

implementation aims to achieve an ideal interaction with sensor-based DTs while delivering closed-loop control through the process and controller connections. Jones et al. (2020) compare the similarities between the DT and the Model-Based Predictive Control principles. MPC concepts such as sensor-to-controller and controller-to-actuator are analogous to the physical-to-virtual and virtual-to-physical interactions that are inherently necessary for DT implementations. Hence, a suitable integration of MPC and DT methods will help accomplish a closed loop approach for nuclear fuel manufacturing that achieves the benefits stated when the DT concept was first conceived [Grieves (2014)].

6. Conclusions

This article has presented a survey on recent research and technological development in the area of DT, focusing on how DT can be applied to the nuclear fuel manufacturing industry.

We have envisioned the deployment of DTs in the entire fuel manufacturing cycle. In particular, we provided key features and definitions of DTs and reviewed the key technologies for DT implementations. The proposed methodology is based on the following nine stages: (1) define the physical system of the manufacturing process; (2) determine the DT task or purpose (optimisation and/or control); (3) select a suitable modelling approach (physics-based, data-driven or, most likely, hybrid), particularly using chemical kinetics modelling due to the nature of the fuel manufacturing cycle; (4) collect appropriate quantity and quality of data; (5) rebuild the DT solution if the current design fails to produce the expected results; (6) establish the model parameters; (7) deploy the chosen model; (8) supervise the DT implementation within the application environment and (9) tune the parameters or configurations to optimise performance of the model.

We elaborated on the technical challenges in DT implementation and investigated potential approaches to address such issues. Finally, we showed promising application criteria, technology trends, and open research issues related to DT

for real nuclear fuel manufacturing industrial implementations. The challenges unique to the nuclear field will include the development of additional standards, determining how to best utilise the existing modelling and infrastructure, and the way to integrate technologies considering cloud security and privacy issues, while maintaining the desired condition responsiveness and control capabilities that are yet to become mainstream in the nuclear industry.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

The work reported in this paper has been undertaken as part of the project: Autonomous Inspection for Responsive and Sustainable Nuclear Fuel Manufacture (AIRS-NFM). This work was funded by the Engineering and Physical Sciences Research Council (EPSRC), Grant reference EP/V051059/1.

Appendix A. The Nuclear Fuel Cycle

Uranium is a naturally occurring heavy metallic element discovered in 1789. One of the uranium isotopes found in nature, ^{235}U is fissile, and has become the main fuel for nuclear reactors often in a relatively low-enriched form of uranium dioxide (UO_2). The atomic weight of uranium is 238.07 [Joyce (2018)], its atomic number is 92 and it is slightly radioactive [Kushner (1974)]. It is estimated that the concentration of uranium in the earth's crust is 2.8 parts per million. This means that uranium is as plentiful as lead and more plentiful than silver or mercury. Approximately 85% of the known uranium global reserves are located in 6 countries: Australia, Kazakhstan, Canada, Namibia, Niger and Russia [Piro and Lipkina (2020)].

A.1. Uranium ore concentrate production

Oxides, silicates, phosphates and vanadates are some uranium-bearing minerals that can be mined commercially for fissile material useful in nuclear power generation. Most of these ores contain 0.1% to 0.3% U_3O_8. Traditionally, there have been two techniques to mine uranium, open-pit and underground mines (deep mining). However, alternative techniques such as in-situ leach (ISL) mining have become more extensively used. The ISL technique uses a number of chemical solutions that are injected into underground deposits to dissolve the uranium [Piro and Lipkina (2020)].

The recovery of uranium is planned carefully to extract the fissile material from mined ore. The ore is transported to a recovery facility where it is milled and leached. During milling, the uranium bearing ore is crushed and then ground into a slurry. The purpose is to increase effectively the surface area to volume ratio of the material, which eases chemical leaching. Next, the slurry is leached in solution, in some cases, sulphuric acid is used as the leaching agent, but alkaline leaching can also be applied. Fig. A.5 shows this process. The leaching agent is required to remove the uranium and other constituents from the ore.

A subsequent stage in the process requires separation of liquids and solids. After solids have been separated from a solution, the resulting liquid solution must be purified. This is accomplished typically using ion exchange or solvent extraction yielding an enhanced concentration of uranium in solution. Next, the uranium nearing compounds are precipitated out of the concentration by the introduction of a neutralising agent such as ammonia, magnesia or caustic soda depending on the composition of the solution. The final product produced from this process is a triuranium octoxide (U_3O_8) which, after drying, produces a compound still containing some impurities. This compound is referred to as uranium ore concentrate (UOC) or "yellow cake". This product is shipped in drums to a conversion facility for further processing [IAEA (2009)].

A.2. UOC to UO_3

Concentrated HNO_3 at 95-100% is used to dissolve UOC. Oxidising dissolution occurs to ensure that all the uranium is dissolved. This process produces a slurry that contains approximately 40% uranium [IAEA (2009); Murchie and Reid (2020)]. A subsequent filtration stage removes impurities from the UOC such as nitrogen oxide gases. Depending on the concentration of the HNO_3, one of the following chemical reactions occur where the resulting uranyl nitride ($UO_2(NO_3)_2$) is the product of interest

$$U_3O_8 + 8NHO3 \rightarrow 3UO_2(NO_3)_2 + 2NO_2 + 4H_2O \quad (A.1)$$

or

$$3U_3O_8 + 20HNO_3 \rightarrow 9UO_2(NO_3)_2 + 2NO + 10H_2O \quad (A.2)$$

The uranyl nitride slurry is filtered through rotary filters. The resulting filtered liquor contains 35% w/v uranium. Subsequently, the uranyl nitrate solution is treated by using tributyl phosphate (TBP) extraction techniques.

$$UO_2^+ + 2NO_3^- + 2(TBP) \longleftrightarrow UO_2(NO_3)_2 \bullet 2(TBP) \quad (A.3)$$

The extracted compound is discharged onto a water flow at 60^{o}C where it is then precipitated to form a concentrate 110 w/v uranium. Finally, the precipitate must be calcined to produce UO_3 with a denitration process at about 300^{o}C to 350^{o}C which can be described as

$$2UO_2(NO_3) \rightarrow 2UO_3 + 4NO_2 + O_2 \tag{A.4}$$

or

$$UO_2(NO_3) + xH_2O \rightarrow IO_3 + NO_2 + NO + O_2 + xH_2O \tag{A.5}$$

The entire process is illustrated in Fig. A.6.

A.3. UO_3 to UF_4

The conversion process consists of the hydration of UO_3 by adding dilute nitric acid and a wetting agent. This highly exothermic reaction forms a slurry that is dried in a kiln. This part of the process creates uranium trioxide hydrate as a free flowing powder. The hydrate is dehydrated by an endothermic dehydration process to remove as much H_2O as possible. The dehydrated UO_3 is reduced subsequently by hydrogen as a reducing agent [IAEA (2009); Murchie and Reid (2020)], hence

$$UO_3 + H_2 \rightarrow UO_2 + H_2O. \tag{A.6}$$

Finally, the UO_2 compound goes to a hydrofluorination stage in order to obtain metalling uranium. The UO_2 is reacted with hydrogen fluoride to produce UF_4 at 450^{o}C, hence

$$UO_2 + 4HF \rightarrow UF_4 + 2H_2O. \tag{A.7}$$

Fig. A.7 illustrates the UF_4 production process.

A.4. UF_6 Production

It is known that the cost of UF_6 production depends deeply on the cost to manufacture and handle fluorine and its precursor, hydrogen fluoride. Both substances are extremely difficult and dangerous substances to work within a manufacturing facility [Murchie and Reid (2020)]. Hydrogen fluoride (HF) is produced by the reaction of fluorspar (calcium difluoride) with sulphuric acid [DOE (1999)], hence

$$CaF_2 + H_2SO_4 \rightarrow 2HF + CaSO_4. \tag{A.8}$$

This reaction is endothermic and reactors are run typically at temperatures higher than 200^oC. HF is a transparent substance that dissolves in water to become hydrofluoric acid in aqueous form. This acid is highly corrosive and hazardous. Fluorine can be isolated by electrolysing molten salt $KF \bullet 2HF$, hence

$$KF \bullet 2HF = K^+ + HF_2^-. \tag{A.9}$$

Fluorine is the most reactive element in the periodic table as it reacts with all other elements except helium and neon. Reactions of fluorine are generally highly exothermic due to its reactivity. Therefore, the construction of a manufacturing plant to handle fluorine in a safe manner is usually expensive. The production of uranium hexaflouride (UF_6), requires uranium tetraflouride or green salt (UF_4) to be passed into a Monel reactor with elemental fluorine in a fluid bed using nitrogen for direct fluorination. This is a highly exothermic reaction at 450^oC. The resulting UF_6 is filtered and condensed into a liquid. The process is illustrated in Fig. A.8 and described in the following chemical reaction:

$$UF_4 + F_2 \rightarrow UF_6 \tag{A.10}$$

A.5. Uranium enrichment

Uranium enrichment methods have been demonstrated since the 1940s. These methods are based on a physical separation, hence they are not chemical reactions. Gaseous diffusion enrichment was the first commercially-available process. The system uses a diffuser or converter that has a number of diffusion barriers (i.e. membranes with perforated sub-micron holes). Gaseous UF_6 is pumped into the diffuser at a high pressure where molecules comprising ^{235}U tend to pass through the membrane to a lower pressure section of the converter. This diffused gaseous UF_6 in the low pressure stage contains a higher concentration of ^{235}U. This is processed in a subsequent stage where the process is repeated to achieve the required enrichment concentration [Murchie and Reid (2020)].

Gas centrifuge enrichment technology allows for the separation of gaseous UF_6 with a higher concentration of ^{235}U by employing long narrow rotary cylinders. The cylinders rotate at around 50 000rpm. The resulting centrifugal forces operate at thousands of times that of gravity, creating a density gradient in the gas mixture. ^{238}U molecules gather at the centre of the cylinder while the heavier ^{235}U move toward the outer wall. Both depleted and enriched uranium streams are withdrawn from the rotary cylinder via a fixed outlet at each end [USNRC (2012a)]. A general uranium enrichment process is shown in Fig. A.9.

A.6. UO_2 Production

A commercial process for producing UO_2 called Integrated Dry Route (IDR) was developed in the United Kingdom in 1969 [IAEA (2009)]. The IDR process has the benefit of avoiding the use of liquids. In this process, UF_6 in solid form is evaporated to a gas by adding heat to the shipping container inside a vaporisation chamber. The heat is added by circulation of steam or electric heat through the chamber. The evaporated UF_6 is sent to a hydrolysis reactor where it is mixed with superheated steam [USNRC (2012b)]. The UF_6 reacts with the steam instantaneously and forms uranyl fluoride (UO_2F_2) powder and HF gas [Richards et al. (2020), Wang and Pitzer (2001)]. This is a highly exothermic reaction described as

$$UF_6 + 2H_2O \rightarrow UO_2F_2 + 4HF. \quad \text{(A.11)}$$

When the UF_6 reacts with the superheated steam, the reaction takes place at approximately 260 ^oC. The uranyl fluoride (UO_2F_2) falls to the bottom of the chamber and is moved to a slightly slanted rotating cylindrical kiln. The uranyl fluoride is converted subsequently into nuclear-grade UO_2 powder by means of a counterflow of superheated stream and hydrogen. The mechanism of the reaction at approximately 600 ^oC proceeds through separate pyrohydrolysis and reduction steps. Therefore

$$UO_2F_2 + H_2O \rightarrow UO_3 + 2HF, \quad \text{(A.12)}$$

and

$$UO_3 + H_2 \rightarrow UO_2 + H_2O. \quad \text{(A.13)}$$

The overall process is endothermic. There is a temperature profile along the rotating kiln [Murchie and Reid (2020); IAEA (2009)] that is controlled to meet the required powder characteristics such as particle size, specific surface area, O/U ratio and bulk density. The IDR is not the only process available to produce UO_2 powder. Nevertheless, it is the most inexpensive and commonly applied. Another common method is the precipitation of ammonium uranyl carbonate (AUC) where the resulting produced UO_2 powder has a good flow-ability so that it can be compacted without a subsequent granulation step [Murchie and Reid (2020)]. The UO_2 dry conversion process is shown in Fig. A.10.

A.7. Fuel Assembly

When UO_2 powder has been produced using the IDR method, it is first blended at a low pressure and then granulated with a number of additives for lubrication and pore forming. This process provides green pellets with high stability [USNRC (2012b)]. The aforementioned additives also provide a preferential path for diffusion and help to improve sintering, as they introduce vacancies in the UO_2 crystal structure.

The UO_2 is sent to a pelleting press where it is pressurised into cylindrical pellets. The shape of the pellets are determined during this process, usually including chamfers on the edges or dishes at the top. These shapes are used to improve the mechanical stability of the pellet during operation. After pressing, the pellets are sintered in a reduced atmosphere at 1700 ^{o}C [Ohai (2002)] in order to form a coherent bonded mass without melting. Grinding is necessary for correction of slight uneven thermal deformations during the sintering process [USNRC (2012b)]. After an inspection process, the pellets are inserted into fuel clad tubes to constitute fuel pins that are later pressurised and sealed by Tungsten Inert Gas (TIG) welding. The pins are sent to an annealing furnace to eliminate any unresolved stresses associated to the welding process. A gamma scanner is used to corroborate if the pellets are distributed evenly within the pins. After cleaning the pins, the next step is the mechanical loading of UO_2 pins into rods or assemblies [Kang et al. (2008)]. Fig. A.11 shows the overall fuel assembly process.

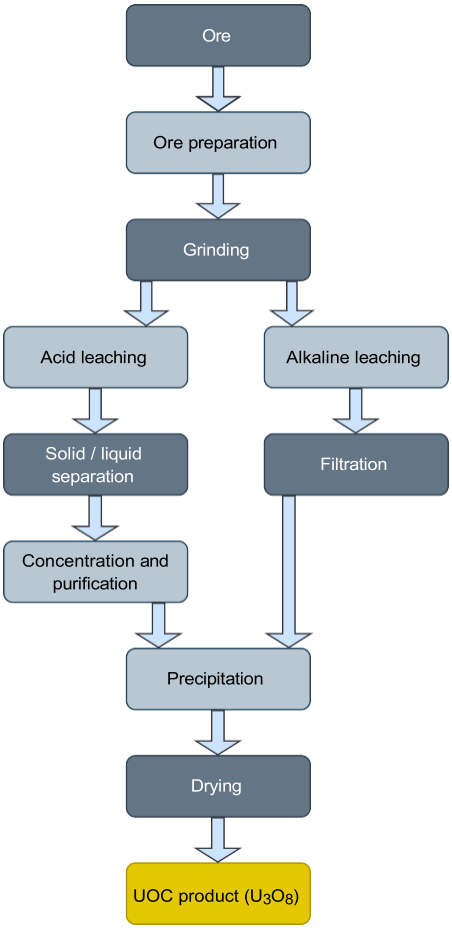

Figure A.5: A generic schematic of the leaching process. Adapted from Piro and Lipkina (2020).

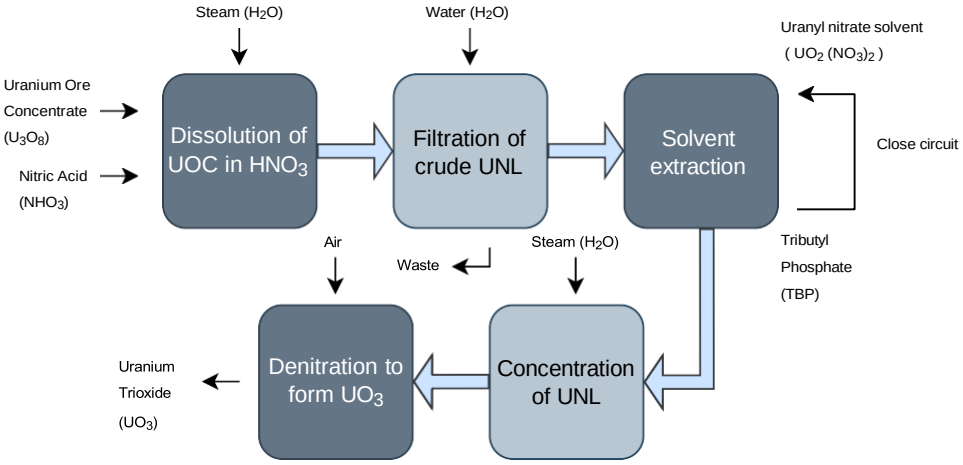

Figure A.6: UOC to UO_3 conversion process. Adapted from Alfaro et al. (2015).

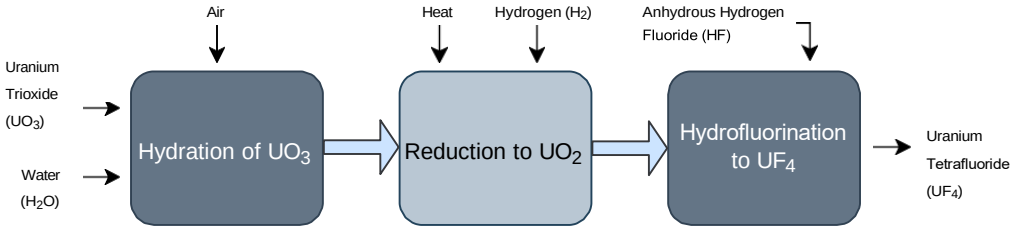

Figure A.7: UF_4 production from UO_3 by hydrofluorination. Adapted from Alfaro et al. (2015).

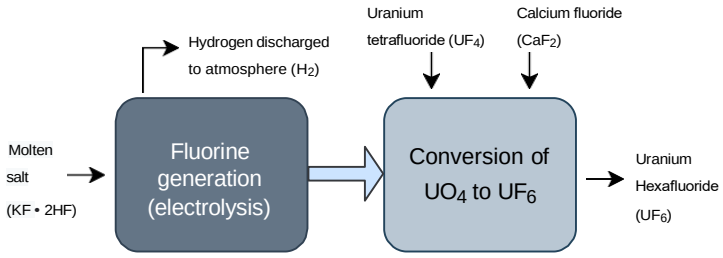

Figure A.8: UF6 production from UF4 by fluidisation method based on Springfields Fuels Ltd [Westinghouse 1 (2024)]

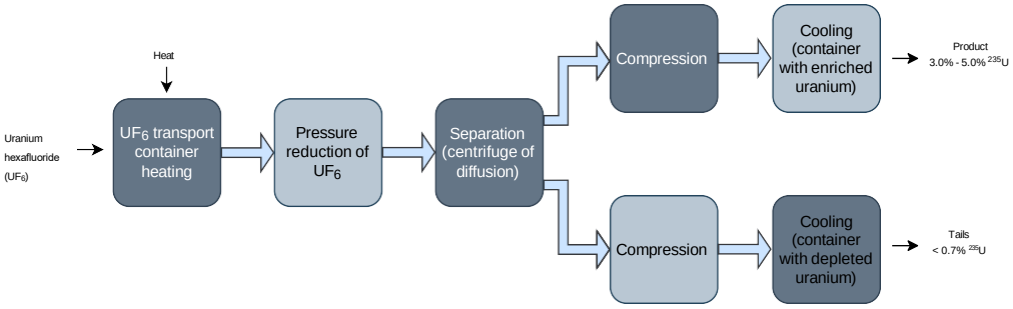

Figure A.9: Block flow diagram for an enrichment process. Adapted from Murchie and Reid (2020).

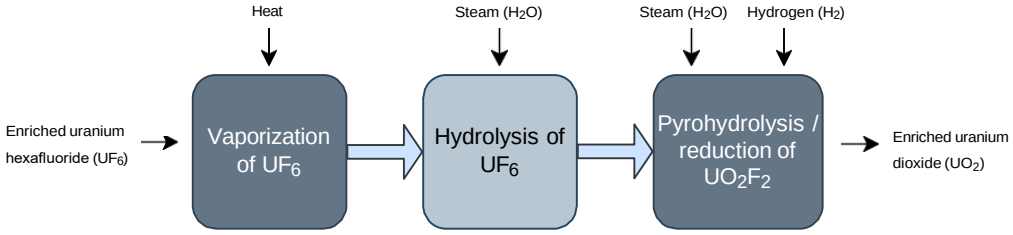

Figure A.10: Conversion of UF_6 to UO_2 using the IDR process. Adapted from Murchie and Reid (2020).

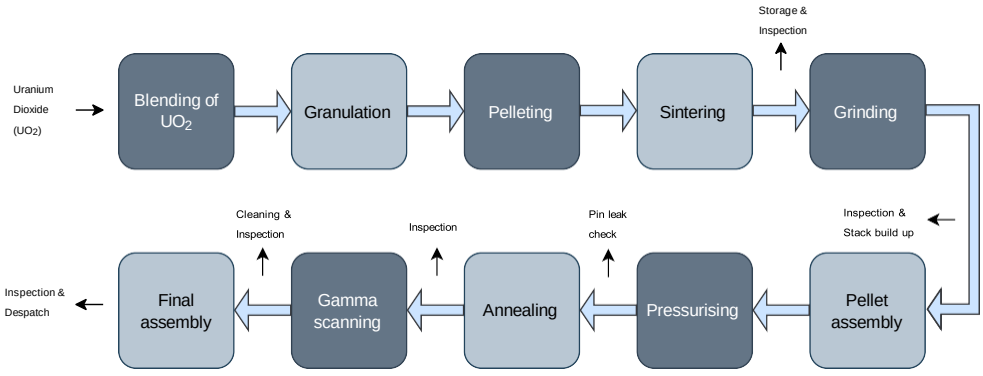

Figure A.11: Fuel assembly fabrication based on a process at Springfields Fuels Ltd [Westinghouse 2 (2024)].