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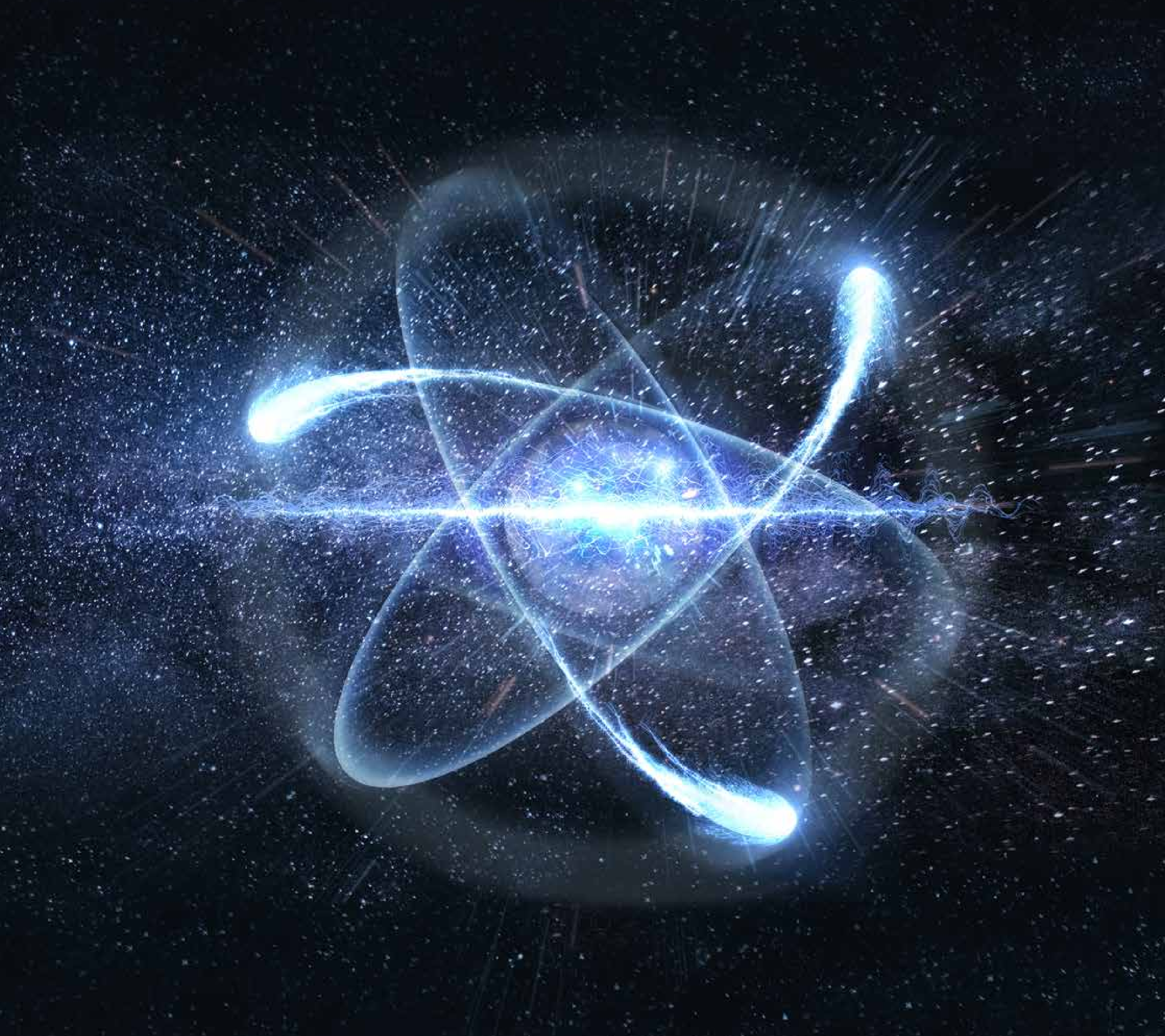

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The International Journal of Nuclear Safeguards and Non-Proliferation

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Editorial

Elena Stringa

Dear Readers,

It is with great pleasure that we present volume 66 of the 'ESARDA Bulletin - The International Journal of Nuclear Safeguards and Non-proliferation'. This volume contains five high quality and very interesting contributions on the following topics: implementation of safeguards, data analytics, techniques for non-destructive analysis (NDA) and support to safeguards by design. I wish you enjoy the reading.

I have an important news to share with you, but first please let me remind you that the ESARDA Bulletin is now a rolling publication. Articles can be submitted on a continuous basis and will be published online with their DOI as soon as they are ready, usually between 4 and 8 weeks after the submission. If you wish to publish your work in the ESARDA Bulletin, send your article at any time together with the paper submission form duly filled and signed to EC-ESARDA-BULLETIN@ec.europa.eu. If accepted, the article will be published as soon as the review process will be completed. Before submitting your work, please ensure that your paper fits the Bulletin scope and that its content presents some novelties: we do not accept work that has already been published in other journals or conference proceedings, unless new aspects of the work are introduced (e.g. new results and related discussion). You can find the publication policies in the ESARDA Bulletin website under documents and forms.

I would like to use this editorial to inform you that Volume 66 is the last one that I am publishing as journal editor. After almost 8 years it's time to pass the torch to a new editor-in-chief who can bring new ideas and new momentum to our magazine. So, for myself, this is the time to analyze what we have achieved in the last 8 years. I am very proud of the results: the quality of the published works is extremely good, as evidenced by the fact that our Journal has been included in the Scopus database. We have modernized the publication, making it a rolling publication, to speed up the time it takes to publish accepted papers, which is very important for authors working in the research field.

Of course, I did not carry out all the work alone; in fact, most of the credit goes to the authors who chose to publish their work in the Bulletin and to the reviewers who volunteered to review papers, providing authors with valuable and interesting comments that led to the publication of high-quality works: many thanks to the authors and reviewers. Excellent results were also achieved thanks to a great cooperation with the editors team, composed of Andrea De Luca, Guido Renda, and Simone Cagno: working with them has always been very pleasant and enriching thanks to the constructive discussions that allowed us to improve the publication process. In January 2025, in occasion of the next ESARDA Editorial Committee meeting, a new editor-in-chief and new members of the editors team will be appointed; I wish them a successful and smooth job, confident that they are inheriting a Journal in good health and with the potential to grow even more.

So it's time to say goodbye: despite the initial difficulties we had before being admitted to Scopus, I will keep good memories of this experience. Thank you all, colleagues, authors, reviewers, and readers, for your interest and support.

I wish you a peaceful Christmas with your loved ones and a happy new year full of success and love.

All the best,

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Small Quantities Protocol to Comprehensive Safeguards Agreement: Transition Challenges for Saudi Arabia to Embark on the Nuclear Energy Program

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Abstract:

As a non-nuclear weapon State, the Kingdom of Saudi Arabia (KSA) is a party to the Treaty on the Non-Proliferation of Nuclear Weapons (NPT). It has signed a bilateral comprehensive safeguards agreement (CSA), INFCIRC/746, with the International Atomic Energy Agency (IAEA). It is monitored through the original standard text of small quantities protocol (SQP) due to the country's limited nuclear material or activities. Despite significant developments in nuclear energy during the last few years, the KSA has not updated its operative SQP but recently decided to transition towards CSA. Nevertheless, IAEA discovered in 2005 that its ability to verify whether the SQP States continue to qualify for the agreement is undermined due, inter alia, to the suspension of submission of an initial report on all nuclear material subject to safeguards, provision of early design information of the facility and inspection activity are, therefore held in abeyance. The SQP will remain operational if the total quantity of nuclear material within the territory of KSA or under its jurisdiction does not exceed the amount specified in Article 36 of INFCIRC/746 or till the introduction of fuel in the low-power research reactor. A typical regional safeguards model for the Middle East, considered as a golden standard, is to conclude CSA with additional protocol (AP) without implementing the nuclear fuel cycle activities. It is likely that eventually, the KSA may follow suit with the region and conclude an AP to its CSA. However, KSA's ambitions to utilize domestic uranium resources to develop an indigenous nuclear fuel cycle pose additional safeguards obligations and implementation challenges for the country. As an SQP country, preparing for international legal obligations to show transparency in its nuclear energy program for the peaceful use of nuclear energy is a big challenge. This essay analyses the obligations associated with adopting the legal framework for verification and the corresponding challenges that will emerge in its implementation for KSA. The most important areas include the development of regulatory infrastructure, an effective State system of accounting for and control of nuclear material (SSAC), preparation of initial physical inventory listing, inspection regimes, human capacity building, and nuclear import/export control, to name a few.

Keywords: Nuclear Safeguards, Small Quantities Protocol, Saudi Arabia, Comprehensive Safeguards Agreement

1. Introduction

Nuclear safeguards for non-nuclear weapon States are vital technical measures to promote the peaceful use of nuclear energy by substantiating the exclusive use of nuclear material and activities for the benefit of humanity. The SQP to CSA [1], which the IAEA designed in the early seventies to incentivize novice non-nuclear weapon States with negligible nuclear materials and activity, proved a blessing in disguise for the signatory countries. Since SQP undercut IAEA's ability to monitor real-time transparency of nuclear materials and activities as most of the actions in Part II of INFCIRC/153 (Corr.) [2], are held in abeyance, and thus, currently, the original SQP has become a dilemma for the IAEA. Despite substantial international diplomacy to either rescind or amend SQP [3], numerous countries are still party to the original text of SQP, which emerges as a significant challenge for the Agency [3, 4].

The agreement between the KSA and the IAEA for the application of safeguards in connection with the Treaty on the NPT [5] was signed in Vienna on June 16, 2005 and entered into force on January 13, 2009 [6]. The safeguards agreement between KSA and the IAEA was documented in the INFCIRC/746. The SQP was appended to its CSA INFCIRC/746 pursuant to the treaty obligation of NPT. According to the SQP, most of the implementation provisions of PART II of the CSA have been held in abeyance due to presence of the small or no nuclear materials in the Kingdom [6]. However, Articles 32, 33, 38, 41, and 90 of part II of the agreement are operational regarding material in mining or ore processing activities (not subject to safeguards), import and export of pre-c(33)[1] and c(33)[2] nuclear materials, subsidiary arrangements detailing the scope of the agreement to fulfill its responsibilities, design information of existing and new facilities as early as possible before fuel loading, international transfer of nuclear materials in or out of Saudi Arabia and exchange of safeguards responsibility of the material respectively.

1 Reporting of exports/imports of any material containing U or Th (pre-33(c) material).

2 Nuclear material of a composition and purity suitable for fuel fabrication or isotopic enrichment (33(c)-material) subject to the other safeguards procedures.

 Ahmad, K. (2024, December). Small Quantities Protocol to Comprehensive Safeguards Agreement: Transition Challenges for Saudi Arabia to Embark on the Nuclear Energy Program, *ESARDA Bulletin - The International Journal of Nuclear Safeguards and Non-proliferation,* 66, 2-6. https://doi.org/10.3011/ESARDA.IJNSNP.2024.1

The KSA is moving ahead in its nuclear energy program as bids have been received to build large nuclear power reactors, and the introduction of nuclear fuel in the first nuclear research reactor which is currently being installed by INVAP of Argentina, is expected to be operational soon. The SQP will no longer be applicable as and when either nuclear fuel is loaded into the reactor or nuclear material exceeds the limit stated in Article 36 of INFCIRC/746 [6], which follows:

I. One kilogram in total of special fissionable material, which may consist of one or more of the following:

   a. Plutonium;

   b. Uranium with an enrichment of 0.2 (20%) and above, taken account of by multiplying its weight by its enrichment; and

   c. Uranium with an enrichment below 0.2 (20%) and above that of natural uranium, taken account of by multiplying its weight by five times the square of its enrichment;

IV. Ten metric tons in total of natural uranium and depleted uranium with an enrichment above 0.005 (0.5%);

V. Twenty metric tons of depleted uranium with an enrichment of 0.005 (0.5%) or below; and

VI. Twenty metric tons of thorium.

Whenever the amount of nuclear material exceeds the aforementioned limit, the safeguards procedures in Part II of INFCIRC/746 will no longer be held in abeyance. Consequently, a CSA will take into account for of all nuclear material in the country. The Kingdom has recently shown its intention to rescind the SQP and move on to the CSA [7], which will be in effect after fulfilling the official formalities with the IAEA. Since most of the States with SQP have minimal nuclear materials or any facility, they need more experience in establishing and maintaining the SSAC, reporting nuclear materials, facilitating inspection activities, etc. [8, 9]. Subsequently, the obligation under CSA will pose immense challenges to the implementation of the safeguards agreement in the Kingdom. Moreover, if KSA moves further towards accepting AP due to nuclear fuel cycle related ambitions [10], rigorous requirements would have to be fulfilled to demonstrate the confidence-building measures for the international community. Thus, a reasonable capacity in nuclear safeguards is required to support the transition from SQP to CSA and effectively implement CSA along AP (if applicable). This essay highlights some of the developments made by the KSA in fulfilling IAEA requirements and emerging challenges for the implementation of safeguards obligations under the respective legal framework. Some of the critical milestones yet to be achieved are the establishment of an effective SSAC, training of licensees/plant operators in reporting to State authority, capacity building of Nuclear and Radiological Regulatory Commission (NRRC) staff, and development of safeguards infrastructure of NRRC for licensees' verifications and the promulgation of regulations and its flexibility to adapt to the AP (if applicable).

2. Establishment of the national nuclear regulatory authority

The Kingdom's State nuclear law has been developed in consultation with the IAEA and enacted in connection with the international legal instruments [11]. The NRRC has been established to implement the Kingdom's international obligation under the safeguards agreement with the IAEA [12]. The NRRC is the competent authority designated by the Kingdom responsible for maintaining a SSAC as a regulator. Moreover, NRRC is responsible for the transmission of correct and complete reports, declarations, and other relevant information to the IAEA. NRRC has designed the technical regulations for the implementation of safeguards in the KSA. Some critical functions of NRRC are evaluating and issuing licenses for nuclear materials-related activities, facilitating IAEA inspection under CSA/SQP and/or AP, conducting inspections and audit activities of licensees, etc.

3. Legal framework

A robust national framework is vital for effective regulatory control for the safe, secure, and peaceful application of nuclear energy and ionizing radiations. The KSA is a party to NPT and has a safeguards agreement (INFCIRC/746) with the IAEA [6]. The government recently promulgated the Law of Nuclear and Radiological Control as a national legal framework through Royal Decree No. M/81 of 25/7/1439 AH (10/4/2018 AD) to fulfill the Kingdom's obligations invoked by signing safeguards agreements and other relevant treaties and conventions [13]. This demonstrates a firm commitment of KSA to the responsible use of nuclear materials and exhibits transparency of its nuclear activities within the international community.

According to the national legal framework [13], a license is required to carry out any activity related to nuclear materials unless an exemption from the NRRC is granted as per the rules described in Article V of the Law on Nuclear and Radiological Control. The licensee will be responsible for safety, security, and safeguards, and maintaining the account and operational records of nuclear and radioactive materials, and submitting periodic reports to the NRRC. As described in Article XIII of the law, the NRRC will adopt an accounting system to manage and monitor the inventory of nuclear materials. Moreover, the Commission is responsible for the verification of the implementation of the safeguards agreement and coordinating with the concerned agencies to facilitate the entry of the IAEA inspectors into the Kingdom. The Commission is also responsible for setting up an inspection program for activities and facilities and has powers to conduct periodic and unscheduled inspections to examine the appropriateness of procedures for nuclear safety, security, safeguards, etc., as per Article XX of the law.

It is essential to highlight that in some cases, the national legal framework would require some modification if AP is adopted. The national legal framework is believed to have the flexibility to cater to the obligations under CSA and AP (if applicable).

4. State system of accounting for and control of nuclear material

According to Article 7 of the IAEA safeguards agreement (INFCIRC/746), the KSA is required to set up and operate a SSAC. The NRRC is working on the development and management of the SSAC. The organization is solely responsible for controlling nuclear-related items such as nuclear material goods, technology, software, and/or nuclear-related information and non-nuclear dual-use items. In order to effectively implement the nuclear law, the regulation (NRRC-R-12) Nuclear Material Accountancy and Control regulation has been designed to define the responsibilities of the licensee and to establish the requirements for the application of the National System of Control of Nuclear Material and Nuclear Activities [14]. The main objective of this regulation is to implement the obligations under the CSA (INFCIRC/746) between the Kingdom and the International Atomic Energy Agency. The regulation provides the information and responsibilities for the licensees to carry out nuclear activities regarding accountancy and control of nuclear material and provisions of related information. It further describes the procedures for establishing and maintaining accounting for and control of nuclear material by the authorized person at the facility and location outside the facility (LOF) level. An effective SSAC will facilitate the NRRC and IAEA inspections to measure and verify nuclear material flow and physical inventory accurately.

Furthermore, the licensee has to provide the design information of the facility immediately after the decision is taken to construct the facility and will submit it to the NRRC and other relevant information about the LOF. The facility operator will submit a special report in the event of loss of nuclear material and breach or any damage of containment and surveillance equipment. Moreover, the operator of the facility is liable to submit an activity program regarding the domestic and international transfer, import, and export of nuclear material and ore containing uranium or thorium.

5. Responsibility of State under original SQP

The KSA is a party to SQP based on the original text of 1974 (GOV/INF/276/Annex II). Indeed, a very small quantity of nuclear materials well below the threshold limit is currently present across the Kingdom to maintain an SQP [15]. The possible existence of source material could be in the form of depleted uranium as shielding for medical and industrial radiographs and small laboratory-scale samples for education, training, and research purposes in national laboratories, universities, and oil drilling companies. Thus, the KSA is meeting the criteria to qualify for the SQP so far. The lab-scale nuclear materials are usually not under the license and should be disposed of at a safe and secure place. The obligations of the SQP based on the original text on KSA have remained operational if the quantities of nuclear material within the KSA territory or under its jurisdiction anywhere do not exceed the limits as stated in paragraph 37 of INFCIRC/153 (Corr.), or until nuclear fuel is introduced in a research reactor [8].

Furthermore, plans are underway to build the first nuclear power plant to generate electricity in the Kingdom. Under the current agreement with the IAEA, the KSA is required to report to the IAEA regarding the design information of the facilities, such as the research reactor, at least 180 days before nuclear fuel is loaded into it. In addition, KSA has to report to the IAEA any exports and imports of nuclear material (if applicable) and any material comprising uranium and thorium that has yet to be processed so finely qualifying for fuel fabrication or enriching isotopically. Moreover, the establishment of the operational SSAC, for which regulations have been formulated, and KSA is working actively to fulfill this obligation.

Upon rescission of the SQP and transition to CSA, the new responsibilities of KSA are to negotiate subsidiary arrangements if they have not been done before and make their best effort to achieve its entry into force as soon as possible within 90 days of CSA becoming effective. In addition, the KSA must provide the initial report on all nuclear material with a complete description of the material and the location information in the State within 30 days of the last day of the calendar month in which the CSA comes into force, and provision of information on nuclear material customarily used outside the facility (if available) with complete details. The KSA is responsible for providing the design information of the existing facility during the discussion of the subsidiary arrangements, such as the low-power research reactor. For new facilities, the time limit for the provision of design information to the IAEA should be specified in the subsidiary arrangements and should be provided as soon as possible before fuel is loaded. Finally, to facilitate access for IAEA inspectors, the KSA must provide IAEA access to locations and information necessary for the inspectors to conduct inspections, the most critical safeguards measure to verify the State obligations.

6. Developing human resources

Trained human resources with specialized skills and abilities are required for the NRRC's effective functioning, which poses a big challenge for an SQP country like the KSA. The staff must carry out various activities, ranging from regulatory development to inspections, and need multidisciplinary background and specialized training. The workforce has to be versed in communicating and explaining technical issues to administrations, diplomats, licensees, and IAEA inspectors.

In most cases, the possessors of nuclear materials in the country are unfamiliar with the international obligations about reporting of nuclear materials under the safeguards agreement. Therefore, the training of possessors of nuclear materials holders to maintain up-to-date records related to all nuclear materials in their custody and reporting to NRRC is essential. Moreover, this process is vital for annual reporting to the IAEA and verification by the NRRC and IAEA inspectors when it is required. In addition, capacity building is necessary in searching out various installations, industries, and R&D activities that are using nuclear materials subject to safeguards. Additionally, performing outreach to different entities that may come under the new national regulatory control regarding safeguards agreements has to be undertaken. In the case that the KSA signs AP, it is highlighted that the national legal framework may require modifications, and substantial efforts and capacity building are necessary by the NRRC to convey new regulations and responsibilities to the entities affected by the AP.

In consultation with the IAEA, the King Abdullah City for Atomic and Renewable Energy supports human capital development through academic programs in nuclear engineering. It is essential to highlight that the curriculum should be complemented by introducing nuclear safeguards courses to stimulate students' interest and establish a safeguards culture through education and training. In addition, specialized courses in safeguards to train the practitioners working in the field are also essential. For instance, the Kingdom's first low power research reactor (LPRR) will commence operation soon. It is of utmost importance to conduct training sessions for capacity building of the research reactor staff in nuclear safeguards before introducing fresh nuclear fuel in the reactor in handling all aspects of safeguards implementation-related activities with the IAEA and NRRC.

7. Conclusion and the way forward

The KSA has made significant progress in its nuclear power generation infrastructure to diversify its energy mix program. For instance, a national legal framework has been formulated, NRRC and Saudi Nuclear Energy Holding Company have been established, a research reactor facility in collaboration with Argentina has been built, and the government has received technical bids for two large nuclear reactors. As a non-nuclear weapon State, KSA is a party to NPT, efficiently fulfilling its obligation regarding the safeguards agreement of small quantities protocol appended to its CSA (INFCIRC/746). However, there may be a proliferation risk due to the exemption of most of the reporting and inspection obligations. Eventually, the Kingdom is gearing up for a full-scale civilian nuclear energy program, including a front-end nuclear fuel cycle. The government has finally decided to revoke its SQP and adopt the CSA. This will facilitate KSA to load the fuel in the low-power research reactor, undertake construction of new power plants, and perform other activities under the verification regime of the IAEA. Despite significant developments in nuclear infrastructure, enormous challenges still exist for KSA to fulfill the requirement of the IAEA through stricter checks on its nuclear activities. The development of a strong-trained manpower is a prerequisite to address and tackle such issues. The most crucial challenge for KSA in the transition from SQP to CSA lies with NRRC in developing and operating an effective SSAC and preparing it for the implementation of CSA to meet complete requirements of the agreement, including bringing into force the timing of subsidiary arrangements, training of NRRC and operating personnel in safeguards, collecting and inspecting the initial physical inventory listing information to be provided to the IAEA for all nuclear material subject to safeguards and preparing for the IAEA inspections for verification of information contained in the report. It is essential to highlight that KSA should work more closely with the regional States and IAEA to benefit from their experience and best practices for safeguards implementation effectively and efficiently.

8. Acknowledgements

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Early Inference of Nuclear Technology-Directed Research Activities of Authors from Scientific Publications

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Abstract:

Nuclear research articles can provide information about early nuclear proliferation indicators such as influential research entities and technology capability levels of a country, but detection of nuclear activities typically occurs after they have started. We investigate the extent to which nuclear research articles can be used to infer whether a research entity will acquire or develop a nuclear technology before it happens. Early detection of nuclear proliferation or technology development indicators from data is challenging due to partial observability, sparse and unlabeled information, and confounding signals from multiple concurrent activities. This paper presents the early detection problem as a sequential decision-making, goal inference problem, where the objective is to characterize and predict an individual's, organization's, or a country's intent (unobserved goal-directed behavior) towards developing a nuclear capability from partially observed sequences of their research publications, using inverse reinforcement learning and Bayesian goal inference methods. A computational framework is presented, and its application demonstrated using 29,196 Scopus records for a case study related to a civil nuclear capability. The case study results serve as a proof-of-concept demonstration for inference of technology-directed research activity of authors who publish in the nuclear domain. The inference method, combined with advanced computing, may be used to assess and monitor activities pertaining to early developmental stages of a nuclear technology or capability, which in turn can help to identify and prioritize activities with nuclear proliferation potential for further investigation.

Keywords: Nuclear, Reinforcement, Learning, Bayesian, Inference, AI

1. Introduction

The goal of nuclear proliferation detection is to deter state and non-state actors from pursuing the development and acquisition of nuclear weapons. Traditional methods for nuclear proliferation detection focus on detecting proliferation indicators such as chemical signatures and activities associated with the acquisition and production of special nuclear materials (Sheffield, 2020). Advanced data-driven methods are required to enable detection of proliferation indicators that are not only associated with special nuclear materials but also with the research, development and acquisition of specialized equipment, and technical expertise needed for building a nuclear weapon (Sheffield, 2020; Alexander et al., 2020). Such methods may also enable the detection of undeclared nuclear materials and activities from technical sources of information that are relevant for IAEA safeguards (Barletta et al., 2014; Carlson et al., 2006; Cojazzi et al., 2013; Ferguson and Norman, 2010; Pabian et al., 2014).

Recent advancements in computing, data science, and artificial intelligence / machine learning (AI/ML) technologies might offer opportunities for enhancing current data-driven detection methods to characterize and detect nuclear proliferation indicators at earlier stages of material production or nuclear weapon development (Sheffield, 2020). For example, scientific publications and networks (e.g., coauthorship, citation networks) have been analyzed using machine learning and natural language processing (NLP) techniques to identify early potential proliferation indicators such as influential entities in a research topic (Chatterjee et al., 2023), or the level of an entity's nuclear expertise and technology capability (Kas et al., 2012). Here, an entity can be a person, organization, city, state, or a country. Early detection of nuclear proliferation indicators from data is however challenging due to partial observability, sparse and unlabeled information, confounding signals from multiple concurrent activities, and difficulty in differentiating between peaceful and detrimental nuclear activities.

Nuclear research articles may provide valuable insights into an entity's intent (unobserved goal-directed behavior) to develop or acquire nuclear expertise and technology. Technical documents and publications contain information to characterize and detect potential early proliferation indicators such as influential researchers, author collaborative patterns, nuclear expertise levels, and technology capabilities (Chatterjee et al., 2023; Kas et al., 2012). Recently, Chatterjee et al. (2023) performed a case study with author collaboration networks that were constructed using text (titles, abstract) and metadata of 33,517 Scopus records of nuclear research articles published from 2000 to 2019. They applied topic modeling and topic-aware influence maximization algorithms to identify authors who are the most influential in diffusing information about a selected topic mixture through collaboration networks. They also analyzed the collaboration dynamics of the influential authors over time, such as their ability to maintain old and to start new collaborations. Information about author influence and their collaborative patterns or behavior may be used to assess advancements in technological capabilities and expertise by key players (at the individual, organization, city, state, or country level) in a nuclear research area. Kas et al. (2012) used author affiliation information from 20,000+ nuclear physics articles in arXiv to extract coauthorship networks and to identify key players (authors, countries) based on network centrality measures. They also used text mining tools to extract information about nuclear processes from full-text contents of the articles for assessing the nuclear expertise level of countries. These studies indicate that scientific publications are useful for identifying key players and for assessing their nuclear expertise and technological capability levels, which in turn can help with early proliferation detection.

Instead of assessing the nuclear expertise or technology capability levels of an entity, we take the problem of early detection a step further to predict whether a research entity will attain a nuclear expertise or technological capability by observing their temporal sequences of past activities. Drawing inspiration from the literature on inference of driver route behavior and destinations from partial trip trajectories (Krumm and Horvitz, 2006; Snoswell et al., 2020; Xue et al., 2015; Ziebart et al., 2008), we develop a novel computational framework based on topic modeling, inverse reinforcement learning (Adams et al., 2022; Arora and Doshi, 2021; Ng and Russell, 2000) and Bayesian goal inference methods to predict the technology-directed publication behavior (intent) of authors from partial trajectories of their publication sequences in time. To our knowledge, this work represents the first attempt at using research articles and reinforcement learning framework to formulate and solve a sequential decision-making problem for modeling and predicting author behavior towards developing a technology or performing a research activity in a nuclear technology area.

The remainder of this paper is organized as follows. First, we briefly describe the reinforcement learning (RL) and inverse RL frameworks, followed by the problem of Bayesian goal inference from partial trajectories (sequences) of state transitions. Next, we formulate the sequential decision-making problem for technology-directed goal inference and present a case study for the approach. We then describe the approach and present the results of the case study. Finally, we discuss the performance aspects of the method and future research directions for technology-directed goal activity inference.

2. Background

2.1. Reinforcement learning

In the basic RL framework, a goal-seeking and domain-aware agent interacts with an external environment by performing various actions and learning what actions to take at each step to achieve a goal (Sutton and Barto 2018). An action performed by the agent causes a change in the internal and external environment (state) of the agent, and the environment in turn responds to the change by giving the agent a reward/penalty for taking the action. The agent learns to choose actions in such a way to maximize the total rewards accumulated along a sequence of state (s)-action(a)-state(s') transitions that lead to the goal state from any starting state. For example, let's consider a simple RL problem with a 5 x 5 grid world environment, as shown in Fig. 1. Each grid cell can be considered a state and an agent can move from one state to a neighboring state by choosing one of four actions: *left*, *right*, *up*, *down*. Given a destination cell (goal state), the RL agent must learn to take the most optimal sequence of transitions from any starting cell location (starting state) to the destination cell. Fig. 1 shows one such sequence from state S_1 to state S_{25}.

When the agent is in a state s, it must decide which action a to choose and to which state s' it should move to. This decision-making process depends on a Monte Carlo probabilistic criterion that uses two types of information: a transition probability and a reward for the (s, a, s') transition. In most RL problems, the sequence of (s, a, s') transitions is modeled as a first order

Markov decision process (MDP). That is, to choose the next action and the next state in a first order MDP, the agent in state s, does not need to have information about the path that it took to state s. A MDP can be finite or infinite, deterministic or stochastic. A finite MDP has a finite number of states like the grid world example in Fig. 1, which has 25 states. An infinite MDP has infinite number of states, i.e. the state space is continuous.

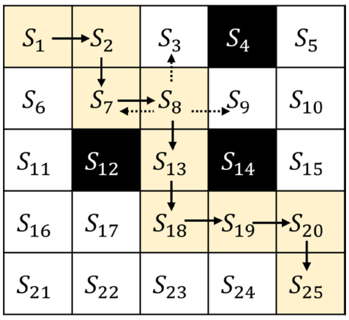

Figure 1. A 5 x 5 grid world environment with 25 states and 4 actions (left, right, up, down), illustrating a full sequence of state-action-state transitions (yellow-shaded cells) taken by a RL agent from state S_1 to goal state S_{25}. The dotted arrows from state S_8 indicate the actions that were not chosen by the agent along the path from S_1 to S_{25}. The black-shaded cells indicate inaccessible states.

To solve a finite MDP problem in the RL framework, we must specify five inputs: state space, action space, transition probabilities, reward functions, and a discount factor for calculating the discounted sum of rewards along a sequence. Thus, a finite MDP is typically denoted as a tuple (S, A, T, R, γ), where the state space, denoted as $S = \{S_i | i = 1, \dots, N\}$, is a finite set of N states; the action space, denoted as $A = \{A_j | j = 1, \dots, M\}$, is a finite set of M actions; T is the state-action-state transition probability matrix of size $N \times M \times N$, R is the reward function, and $\gamma \in (0,1)$ is the discount factor. Given these inputs, the RL agent computes a reward-based policy by which it determines an optimal sequence of state-action-state transitions from any starting state to the goal state. The policy is the probability of choosing an action a and the next state s', given the agent is in state s; which, in turn is a function of the state-action-state transition probabilities and the rewards. The optimal sequence is the sequence that would give the highest discounted sum of rewards from the starting state to the goal state. Various methods such as value iteration, policy iteration, Q-learning, Sarsa, have been developed to solve an RL problem (Sutton and Barto, 2018).

The reward function captures the goal-directed behavior of the agent. Reward functions must be designed specifically for the goal state of interest and in many cases have non-trivial structures. The reward along each transition is defined either independently or as functions (linear or non-linear) of state, state-action, and/or state-action-state features. The state-based reward, denoted as $R_1(s)$, is the reward for moving to state $s \in S$ from any state. The state-action reward, denoted as $R_2(s, a)$, is the reward for taking action $a \in A$ in state s. The state-action-state reward, denoted as $R_3(s, a, s')$, is the reward for moving to state $s' \in S$ from state s through action a. For example, let's consider a sequence, τ, of L state-action-state transitions, as ((s_1, a_1, s_2), (s_2, a_2, s_3), …, (s_t, a_t, s_{t+1}), …, $(s_L, \text{none}, \text{none})$), where s_1 is the starting state and s_L is the terminal (goal) state. The general formula for calculating the discounted sum of rewards for the sequence, $R(\tau)$, based on any combination of $R_1(s)$, $R_2(s, a)$, and $R_3(s, a, s')$ rewards, can be written as (Snoswell et al., 2020):

$$R(\tau) = \sum_{t=1}^{L} \gamma^{t-1} R_1(s_t) + \sum_{t=1}^{L-1} \gamma^{t-1} [R_2(s_t, a_t) + R_3(s_t, a_t, s_{t+1})]. \quad (1)$$

When γ is close to zero, the agent makes decisions by giving more importance to acquiring *immediate* rewards than *future* rewards. When γ is close to 1, the agent makes decisions by giving more importance to acquiring *future* rewards than *immediate* rewards.

A deterministic MDP is one where only one state is accessible when an action is performed, whereas in a stochastic MDP, two or more states may be accessible. The deterministic and stochastic MDP dynamics are modeled using the transition probability. If $T(i, j, k)$ represent the transition probability from state S_i to state S_k through action A_j, then by definition, $T(i, j, k) \in [0,1]$ and $\sum_{k=1}^{N} T(i, j, k) = 1$. For deterministic dynamics, $T(i, j, k) = 1$ for $k = k^*$, where $k^* \in \{1, \dots, N\}$ and $T(i, j, k) = 0$ for $k \neq k^*$. For example, the grid world environment in Fig. 1 is a finite MDP with 25 states and 4 actions: $S = \{S_i | i = 1, \dots, 25\}$ and $A = \{A_j | j = 1, \dots, 4\}$, where, we denote the actions, *left*, *right*, *up*, *down* as A_1, A_2, A_3, A_4, respectively In the grid world example (Fig. 1), when the agent in S_8 moves right, it can access only state S_9 if $T(8,2,9) = 1$ and $T(8,2,k) = 0$ for $k \neq 9$. For stochastic dynamics, $T(i, j, k) < 1 \ \forall \ k \in \{1, \dots, N\}$. For example, if $T(8,2,3) = 0.1$, $T(8,2,7) = 0.2$,

$T(8,2,9) = 0.6$, and $T(8,2,13) = 0.1$, the agent can move to any of the four neighboring states, S_3, S_7, S_9 or S_{13}, in a Monte Carlo step. For deterministic MDPs, the RL agent will follow the same optimal sequence or path from a starting state to the goal state. In a stochastic MDP, the agent is allowed to take sub-optimal paths to the goal state.

2.2. Inverse reinforcement learning

In the inverse RL (IRL) problem, one can observe a partial sequence of state-action-state transitions of an agent, not knowing the agent's intended goal state and the structure of the reward function. The objective of an IRL algorithm is therefore to compute the rewards for a selected goal state from historically observed expert trajectories (Adams et al., 2022; Arora and Doshi, 2021; Ng and Russell, 2000; Ramachandran and Amir, 2007), and then to use these rewards to infer the probability that a future agent will pursue the same goal state given its partially observed path. Therefore, the inputs to the IRL problem are the state space, action space, transition probabilities, and the goal-specified expert trajectories. An IRL algorithm computes the rewards by predicting and matching the state, state-action, or state-action-state feature expectations observed in the expert trajectories. If the reward function is known, the intended goal state can be inferred from a given partial trajectory using Bayesian formulations (Snoswell et al., 2020, Ziebart et al., 2008).

2.3. Bayesian goal inference from a partial trajectory of states

The problem of Bayesian goal inference is to predict the probability that an agent will reach a destination state in a MDP environment, given a partial trajectory of states. Given a partial path from state A to state B, denoted as $\tau_{A:B}$, the probability of reaching a goal state G is given by the Bayes formula:

$$P(G|\tau_{A:B}) = \frac{P(\tau_{A:B}|G) \cdot P(G)}{P(\tau_{A:B})} \propto \frac{P(B \to G)}{P(A \to G)} \cdot P(G|A), \qquad (2)$$

Here, $P(G|A)$ is the prior probability of reaching goal state G along all observed paths from A in the set of expert trajectories; $P(A \to G)$ and $P(B \to G)$ are the probabilities of reaching goal state G along all possible paths from states A and B, respectively.

Most approaches for route preference and driver destination prediction use historical trip trajectories and Bayes rule to compute the probability that a location is the destination while a trip is in progression (Krumm and Horvitz, 2006, Snoswell et al., 2020, Xue et al., 2015, Ziebart et al., 2008). The first step in all these approaches is to segment the trips and map them on a 2-dimensional grid representation of the geographical area where the trips were observed. These methods differ in the way the likelihood and prior probabilities are computed.

Ziebart et al. (2008) developed an IRL algorithm based on maximum entropy (MaxEnt) principles to model driver behavior for route preference and destination prediction. The inverse RL algorithm solves for the unknown rewards to match the observed feature expectations of states, state-action pairs, or state-action-state triples in the expert trajectories. The prior destination and probabilities of the likelihood function are then calculated based on the state-action-state transition probabilities and IRL rewards. Specifically, the probability from a state, e.g., state A, to a goal state G is computed using the product of transition probability and an exponential function of the reward along each state-action-state transition and summing the products over the transitions in all possible paths from state A to G. The prior probabilities are computed in the same way but only over all previously observed paths of drivers from state A to G.

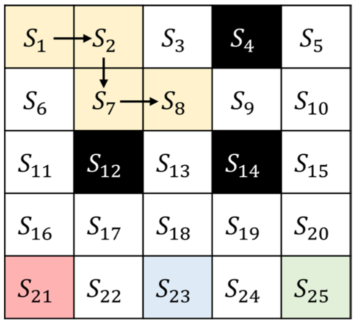

Figure 2. A 5 x 5 grid world environment illustrating a partial sequence of transitions (yellow-shaded cells) taken by a RL agent from state S_1 to state S_8 whose intended goal state must be determined from among three possible goal states, $\{S_{21}, S_{23}, S_{25}\}$, using IRL-based Bayesian formulation. Black-shaded cells indicate inaccessible states.

For example, consider the partial sequence of transitions taken by a RL agent from state S_1 to state S_8 in the 5 x 5 grid world environment, shown in Fig. 2. We want to determine which of the three goal states, S_{21}, S_{23}, and S_{24}, is the agent pursuing. To solve this in the IRL-Bayesian formulation, we need to compute the IRL reward functions and the corresponding reward-based policies π_i for each goal state, G_i, using expert trajectories that terminate at each goal state. The posterior probability is computed using the formula:

$$P_{\pi_i}(G_i|\tau_{A:B}) = \frac{P_{\pi_i}(\tau_{A:B}|G_i)P_{\pi_i}(G_i|A)}{\sum_j P_{\pi_j}(\tau_{A:B}|G_j)P_{\pi_i}(G_j|A)} \qquad (3)$$

where A and B correspond to states S_1 and S_8, respectively; G_i and $G_j \in \{S_{21}, S_{23}, S_{25}\}$. The most likely goal state is then the state with the maximum posterior probability.

In this work, we used the exact maximum entropy (ExactMaxEnt) IRL algorithm developed by Snoswell et al. (2020) to learn the rewards, instead of the original MaxEnt IRL algorithm developed by Ziebart et al. (2008) on which it was based on, because the ExactMaxEnt algorithm can be applied with variable length trajectories and various combinations of reward types ($R_1(s)$, $R_2(s, a)$, and $R_3(s, a, s')$). It also improves the reward learning by computing marginal probabilities exactly.

3. Problem formulation and computational approach

Here, we present the problem of predicting the destination of authors from partial trajectories of their state transitions in their research topic vector space. The problem is formulated starting with a set of research publications of authors working in a nuclear domain. We convert each author's sequence of publications in time into a sequence of state transitions on a rectangular grid that is defined by the research topic vector space of the publications. We then model the sequence of state transitions as a first-order Markov decision process (MDP) and use IRL to compute rewards that capture technology (goal state)-directed behavior of a group of authors. Finally, we develop and use a Bayesian formulation to compute the probability that a state in the topic space is the intended goal state, given a partial sequence of state transitions of an author.

3.1 Case study

To develop and test our approach, we selected papers based on a well-documented civil nuclear activity. In this work, we considered the construction of the Open Pool Australian Lightwater (OPAL) reactor in Australia (Olsen et al., 2008), as our case study application for the approach. The OPAL reactor is a 20-MW multi-purpose reactor, used for producing radioisotopes for cancer detection and treatment, and neutron beams for fundamental materials research (ansto.gov). It went critical in August 2006 and was officially opened in 2007. The goal inference problem is to infer the development of OPAL reactor activity from temporal sequences of publications of authors conducting nuclear research.

3.2. Approach

The computational approach involves the use of topic modeling, reward learning, and Bayesian inference methods to solve the problem of predicting technology-directed publication behavior of authors from partial trajectories of their publication sequences. The approach consists of the following ten steps:

Step 1. Find a paper or an initial set of papers associated with a technology or research activity. We call these papers the "coin" papers.

Step 2. Identify the authors of these coin papers and create a primary set of all papers written by these authors, which also includes the coin papers. We refer to these authors as the coin authors.

Step 3. Create a secondary set of papers published by co-authors of all the papers in the primary set.

Step 4. Combine the primary and secondary set of papers into one dataset.

Step 5. Extract the title, abstract, author information, and publication date of all the papers in the dataset.

Step 6. Perform topic modeling using the titles and abstracts of all the papers to define the research topic weight vector space.

Step 7. Construct a state-action-state transition graph to represent the state transitions of all author trajectories.

Step 8. Select the goal state associated with the technology of interest and the corresponding trajectory set for IRL reward learning.

Step 9. Compute state and state-action rewards based on the trajectory set, using the IRL algorithm.

Step 10. Calculate goal probability given a partial trajectory with a Bayesian formulation.

3.2.1. Creating the dataset (Steps 1 to 4)

The selection of the papers depends on the case study in hand. For our case study, we first identified a flagship publication associated with OPAL reactor development or application, by searching Scopus for papers with keywords “Opal” and “reactor”, found in the title, abstract, and/or keyword fields. Since the OPAL reactor went critical in August 2006, search results from 2004 through 2008 were considered. We considered a two-year time lag between the inception of a research activity and its publication. Hence a two-year buffer period for the search was applied after the year the OPAL reactor become operational. The chosen paper was written by Olsen et al. (2008). Here onwards, we shall call this flagship paper as the “coin” paper and the authors of this paper as coin authors (Step 1). The paper was written by nine authors, of whom five had Scopus ID's associated with a previous publication history.

After identifying the coin paper, we searched Scopus for papers written by the coin authors by their Scopus IDs (Step 2). Based on the search, we created a primary set of 278 coin-authored papers, including the coin paper. We then created a secondary set of papers that were written by all the non-coin authors of papers in the primary set, and this set contained 28,918 Scopus records (Step 3). Thus, a total of 29,196 Scopus records (spanning over the years from 1950 to 2008) were used to define the topic weight vector space of the OPAL MDP environment.

3.2.2. Defining the topic weight vector space (Steps 5 and 6)

We defined the topic weight vector space by first identifying an optimal number of K research topics to characterize the information extracted from the titles and abstracts of the 29,196 Scopus records. We used the Non-negative Matrix Factorization (NMF) algorithm, as implemented in the Scikit-learn Python package (Pedregosa et al., 2011), to obtain a list of topics and weights associated with the K topics for each paper.

To extract the features (relevant words) from the abstracts and titles, we used the *TfidfVectorizer* function provided by Scikit-learn Python package. English stop words, words that occurred only in one record, and words that occurred in over 95% of the records were removed during feature extraction. To fit the NMF model and to compute the weights of the K topics per record, we used the NMF function from *sklearn.decomposition*.

In addition to finding the optimal number of topics, we also determined the optimal combination of settings for three hyperparameters in the NMF analysis: *alpha*, *solver*, and *initialization*. This required running the NMF analyses for all possible hyperparameter combinations across a range of feature counts and number of components (topics) per feature count. The possible options for each hyperparameter were {‘0.02’, ‘0.1’, ‘0.5’} for *alpha*, {‘nndsvd’, ‘random,’ ‘nndsvda’} for *initialization*, and {‘cd’, ‘mu’} for *solver*. It is noted that the ‘mu’ solver does not use ‘nndsvd’ initialization. Therefore, a total of 15 combination of these hyperparameter values were explored. Due to the longer run times associated with the full paper set, we assumed the optimal hyperparameters for the primary set to be optimal or near optimal for the full paper set. Eight papers that were written in 2008 (about the same time as the coin paper) were omitted from the initial NMF training set to reduce the likelihood of papers with similar topics as that of the coin paper. Thus, the hyperparameter exploration was limited to 270 papers in the primary set. Specifically, for each feature count and hyperparameter combination, we ran the NMF analysis and calculated the residual errors for all number of components (topics) ranging from 1 to the number of features. Using the Kneedle algorithm (Satopaa et al., 2011) from the *kneed* python package, we then determined the optimal number of components, which corresponded to the point of maximum curvature (“knee”) in the error curve described by the residual error versus the number of components. For each hyperparameter combination, we then took the geometric mean of the optimal number of components across the sample features counts and compared these means to select the hyperparameter combination of *solver*, *initialization*, and *alpha* parameters that resulted in the lowest geometric mean value. The geometric mean value is the nth root of the product of number of component values across all sample feature counts per hyperparameter combination. The resulting hyperparameter values were ‘0.02’ for *alpha*, ‘cd’ for *solver*, and ‘random’ for *initialization*. To avoid model overfitting, we applied the NMF function with *Frobenius* norm minimization and regularization, where the *L1 to L2* ratio was set to 0, and *alpha*, the constant multiplying the regularization term was set to 0.02.

Keeping the above hyperparameter settings, we then examined a more limited range of feature counts (up to 140) for the full set of 29,196 papers and determined the optimal number of components (K topics) following the same steps above. Our analysis indicated that seven topics ($K = 7$) with a feature count of 50 was optimal. In all the NMF calculations, the maximum number of iterations was set to 20,000 and the stop condition tolerance was 0.0001.

3.2.3. Constructing the state-action-state transition graph (Step 7)

Based on the publication dates of all the 29,196 Scopus records, we created a temporal sequence of publications for each author, and then converted it to a sequence of state-action-state transitions, which were combined afterwards to form a state-action-state transition graph. The construction of a state-action-state transition graph involves defining the state space, action space, and state-action-state transition probabilities of the author topic grid MDP environment. The nodes and edges of the graph represent the states and actions of the author topic grid MDP, respectively. The transition probabilities were specified along each edge based on the number of authors who traversed the edge as per the data. The resulting state-action-state transition graph is a directed multi-edge graph, since more than one action (edge) is possible from one state to the other.

State space: We defined the states as the cells of a *K*-dimensional rectangular grid that represented the topic vector space of all the publications in the dataset. As described in the previous section, the topic weight vectors represent the topic vector space of the papers. Let $\boldsymbol{w} = (w_1, w_2, \cdots, w_K)$ denote a topic weight vector of a publication record in the K-dimensional topic vector space, such that $\sum_{i=1}^{K} w_i = 1$. We represent the topic vector space as a *K*-dimensional rectangular grid, where each axis represents the range of weight values from 0 to 1 for each research topic. The grid space may be discretized using uniform or non-uniform grid intervals. We used a partially uniform grid where each grid dimension is divided into m intervals, such that the width of the first and the last interval is half the width of the intermediate intervals whose widths were $1/(m-1)$. The half-width interval was used to separately group publications with topic weights close to zero and one. Each publication can be mapped to a cell on the topic grid based on their topic weight values. For example, Fig. 3 illustrates a map of 20 publications on a 2-dimensional topic grid ($K = 2$), characterized by topic vector weights w_1 and w_2. Each axis is divided into 5 intervals ($m = 5$), where the half-width interval is 1/8. This grid contains 25 grid cells (states), which can be numbered from 1 to 25 and these numbers are used to identify the states. The grid cell in which a publication is located is considered as the state (active research state) of an author of the publication. The number of grid cells (states) in the author topic MDP environment will depend on the choice of the grid cell spacing along each grid dimension. But not all grid cells will be occupied with a publication. For IRL reward learning, we considered only those grid cells with a minimum record occupancy of one to constitute the state space of the author topic grid MDP environment. Thus, the number of states in the state space is the number of grid cells with a minimum record occupancy of one. If N is the number of states, the state space of the MDP is represented as $S = \{S_i | i = 1,2, \dots, N\}$.

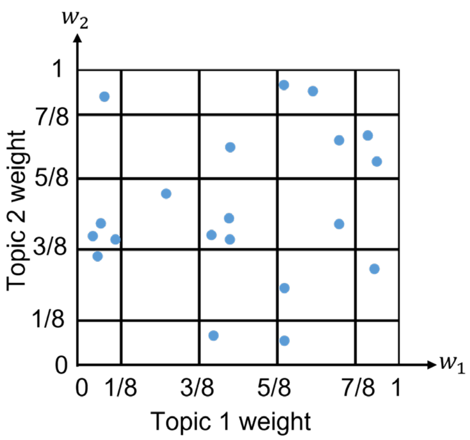

Figure 3. A 5 x 5 topic grid world environment illustrating the mapping of 20 research publications on a two-dimensional grid with 1/8 grid spacing for weight values near zero and one, and 2/8 spacing for the others.

Action space: We defined the actions as the difference in the number of years it took for authors to move from one state (grid cell) to another in the topic MDP grid environment. For example, if an author has a paper published in year t_1 and is in state S_1, and the author's next publication is in year t_2 and in state S_2, the action taken by the author to move from state S_1 to S_2 is calculated as $t = t_2 - t_1$. The graph will have a directed edge for the action t drawn from state S_1 to S_2. If the year difference was 0, we used the month and day information from the publication dates to determine the direction of the edge along each state transition. Actions that do not cause a change in the state of the author will result in self-loops, which are ignored in the state-action-state transition graph. If M is the number of states, the action space of the MDP is represented as $A = \{A_j | j = 1,2, \dots, M\}$.

Differences in state transitions between a standard grid world walk and the author topic grid world walk: In the RL framework, it is important to understand how the RL agent will move (walk) from one state to the other.

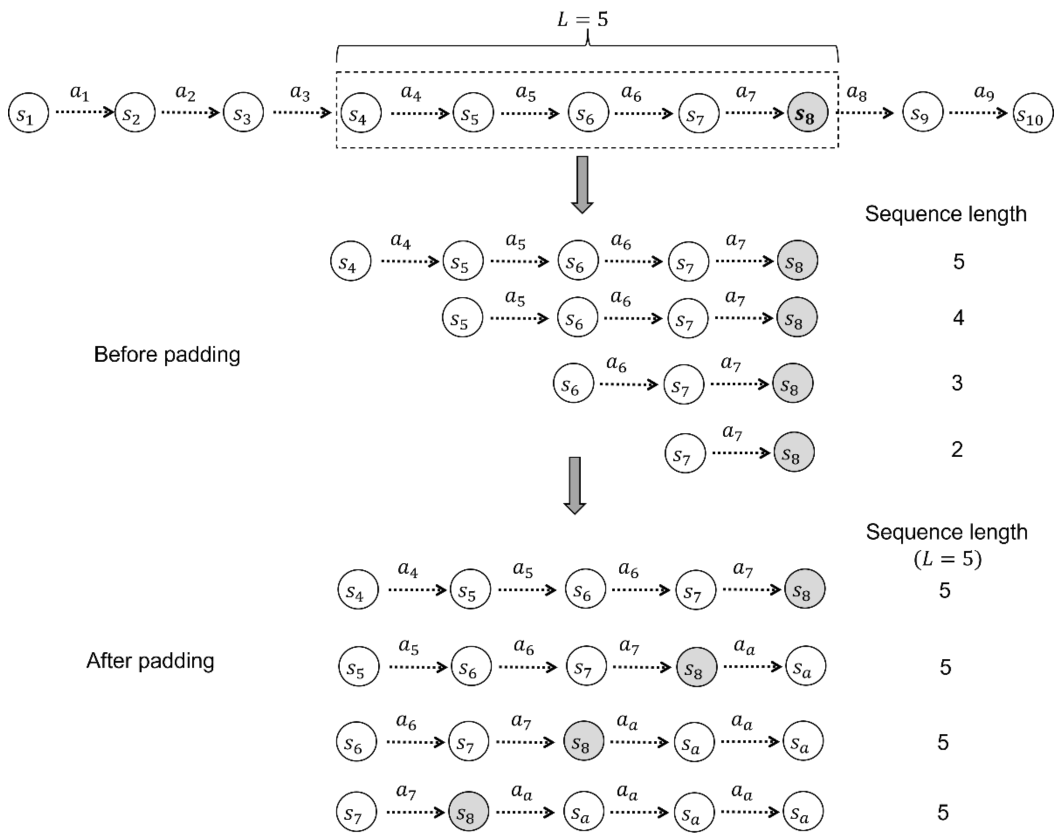

Figure 4. An illustration of how sub-trajectories of a specified length $L = 5$, with goal state s_8, are derived from an author trajectory with 10 states, before and after padding with auxiliary state s_a and action a_a.

Compared to a geo-spatially constrained grid world MDP walk, such as the 5 x 5 grid MDP walk shown in Fig. 1, the author MDP grid walk is not limited to adjacent state transitions in the topic grid space. There are no self-loops in the grid world walk because the agent needs to move out of a state to come back to that state. On the other hand, self-loops can exist in the author topic grid walk because an author can publish an article that falls in the same state as the previous one in time. In the grid world walk, an agent cannot jump over states in its path. In the author topic grid walk, authors can jump from one state to every other state. In the grid world walk, all the accessible states from each state are known. In the author topic grid walk, however, not all accessible states from each state are known because new state transitions can occur in the future, although they do not exist at the current point in time. Although, in theory, an RL agent can move from one state to every other state in the author topic grid walk, in our work, we limit the RL agent movements only to state transitions known from all the author trajectories in the dataset.

Transition probability: The transition probability, denoted as $T(s'|s,a)$, along each (s,a,s') edge was computed by dividing the number of authors who moved from state s to state s' through action a by the total number of authors who moved to all accessible states from s through a.

3.2.4. Trajectory set for IRL reward learning (Step 8)

The IRL reward learning begins by selecting a goal state, followed by a set of expert trajectories $\mathcal{T}$ that terminate at the goal state. In the author topic MDP grid space, authors can take different paths to a goal state, from different starting states. This will result in trajectories of unequal lengths in the set $\mathcal{T}$, where the length is defined as the number of states from a starting state to the goal state in a trajectory. Additionally, sub-trajectories can be realized as starting from states away from the goal state in varied number of steps, in an author trajectory. To form the trajectory set $\mathcal{T}$ for reward learning, we first select a sub-trajectory of a specified length L, which terminates at the goal state in each author trajectory. Each sub-trajectory and their subsequent ones are reduced in length by one, after removing the first state until the length is two. This process results in a set of trajectories of length varying from 2 to L. To illustrate this process, let's consider an author trajectory with 10 states as shown in Fig. 4, where s_8 is indicated as the goal state. If $L = 5$, then four sub-trajectories can be derived from this trajectory, as shown in Fig. 4. These trajectories vary in length from 2 to 5 states. Thus, the IRL training set used for the reward calculations will contain trajectories of variable lengths from 2 to L, which are obtained from all author trajectories that contain the goal state. To make the reward learning efficient, we make all the trajectories in the IRL training set to be of the same length, L, using the padding trick described by Snoswell et al. (2020). Specifically, we pad trajectories shorter than the longest trajectory, which is of length L in the set, with auxiliary state-action sequences, $\{(\cdot, a_a), (s_a, \cdot)\}$. An example of padding is shown in Fig. 4, where all the trajectories are of length 5 after padding. It should be noted that in our implementation of the IRL reward learning algorithm, we represented each sub-trajectory of length L as a sequence of state-action transitions as $((s_1, a_1), (s_2, a_2), \ldots, (s_t, a_t), \ldots, (s_L, a_a))$ where an author starts from state s_1 and ends at the terminal state s_L in $L - 1$ action steps. The transition (s_t, a_t) refers to the state $s_t \in S$ and action $a_t \in A$ at step t. The last action step, (s_L, a_a), is an added step for the transition from the terminal state s_L to the auxiliary state s_a through the auxiliary action a_a (not shown in Fig. 4). In this work, we set the L value to the length of the shortest coin author trajectory.

3.2.5. Reward learning (Step 9)

We used the ExactMaxEnt IRL algorithm (Snoswell et al., 2020) to compute the rewards of the author topic grid MDP and implemented it in Python. The algorithm can be used to compute three types of rewards: state rewards $R_1(s)$, state-action rewards $R_2(s, a)$, or state-action-state rewards $R_3(s, a, s')$. Each reward type is defined as a linear function of the respective state, state-action, or state-action-state feature vectors, with reward weight vectors $\boldsymbol{\theta_1}$, $\boldsymbol{\theta_2}$, and $\boldsymbol{\theta_3}$, respectively. The objective of the algorithm is then to fit the reward weights to match the discounted feature expectations in the set ($\mathcal{T}$) of observed trajectories that terminate at the goal state. For the author topic MDP, we used the state and state-action rewards to model the goal-directed behavior of the authors, and they were calculated as follows.

Let n_1 and n_2 represent the number of state and state-action features of the author topic MDP, respectively. The state reward function is written as $R_1(s) = \boldsymbol{\theta_1}^{\mathrm{T}} \boldsymbol{f_1}(s)$, where $\boldsymbol{f_1}(s)$ is the feature vector of state $s \in S$ of size $n_1 \times 1$, and $\boldsymbol{\theta_1}$ is the state reward weight vector of size $n_1 \times 1$. The state-action reward function is written as $R_2(s, a) = \boldsymbol{\theta_2}^{\mathrm{T}} \boldsymbol{f_2}(s, a)$, where $\boldsymbol{f_2}(s, a)$ is the feature vector of the state-action pair $(s, a) \in (S, A)$ of size $n_2 \times 1$, and $\boldsymbol{\theta_2}$ is the state-action reward weight vector of size $n_2 \times 1$.

The actual state and state-action features of the author topic MDP are not known, and such information may not be readily available, or may be difficult to obtain or learn from data. Therefore, we considered the rewards to be independent of these features by setting the state and state-action feature vectors as unit vectors of length $n_1 = N$ and $n_2 = NM$, respectively. For example, the state-feature vector for state S_i is specified as $\boldsymbol{f_1}(s = S_i) = (b_k)_{k=1}^{N}$ such that $b_k = 1$, if $k = i$ and $b_k = 0$, otherwise. Similarly, the state-action feature vector for all state-action pairs (S_i, A_j) is specified as $\boldsymbol{f_2}(s = S_i, a = A_j) = (c_k)_{k=1}^{MN}$ such that $c_k = 1$, if $k = (i-1)M + j$ and $c_k = 0$, otherwise. This makes the reward weights equivalent to the respective rewards. In our work, we fitted the reward weights (rewards) to predict and match the average state and state-action visitation frequencies in the set of expert trajectories, as described below.

If there are n_T trajectories in the expert trajectory set $\mathcal{T}$, and each trajectory τ_k is a sequence of L states, represented as $(s_{k,t}, a_{k,t})_{t=1}^{L}$, where $s_{k,t} \in S$ and $a_{k,t} \in A$, then the average state visitation frequency for each state in S is calculated as

$$\overline{\boldsymbol{f_1}} = \frac{1}{n_T} \sum_{k=1}^{n_T} \sum_{t=1}^{L} \boldsymbol{f_1}(s_{k,t}), \tag{4}$$

and the average state-action visitation frequency for each state-action pair in $\{(S_i, A_j) | S_i \in S, A_j \in A\}$ is calculated as

$$\overline{\boldsymbol{f_2}} = \frac{1}{n_T} \sum_{k=1}^{n_T} \sum_{t=1}^{L-1} \boldsymbol{f_2}(s_{k,t}, a_{k,t}). \tag{5}$$

In addition to the state and action spaces, S and A, we also include an auxiliary state space $\{S_a\}$ and an auxiliary action space $\{A_a\}$. The combined state and auxiliary state spaces is denoted as $S^* = S \cup \{S_a\} = \{S_j \,|\, j = 1, \ldots, N + 1\}$, where $S_{N+1} = S_a$. The combined action and auxiliary action spaces is denoted as $A^* = A \cup \{A_a\} = \{A_j \,|\, j = 1, \ldots, M + 1\}$, where $A_{M+1} = A_a$.

In the trajectories, the auxiliary state is treated as a self-absorbing state and is accessible from all states only through the auxiliary action. Thus, we set the transition probability for all state-action-state transitions involving the auxiliary state and action as follows:

$$T(s_a|s,a) = \begin{cases} 1, \forall s \in S, a = a_a \\ 0, \forall s \in S, a \neq a_a \\ 1, s = s_a, a = a_a \\ 0, s = s_a, a \in A \end{cases}. \quad (6)$$

To remove the effect of the auxiliary state and action on the rewards accumulated along a trajectory, we set $R_1(s_a) = 0$, $R_2(s_a, a_a) = 0$, and $R_2(s_a, a) = 0 \ \forall \ a \in A$.

$$\alpha_{t+1}(s') = \sum_{s \in S^*, a \in A^*} \alpha_t(s)\, T(s'|s,a) \exp\left(\gamma^t R_1(s')\right), \text{ for } 1 \le t < L, \quad (10)$$

$$\beta_1(s) = \exp\left(\gamma^{L-1} R_1(s)\right), \text{and} \quad (11)$$

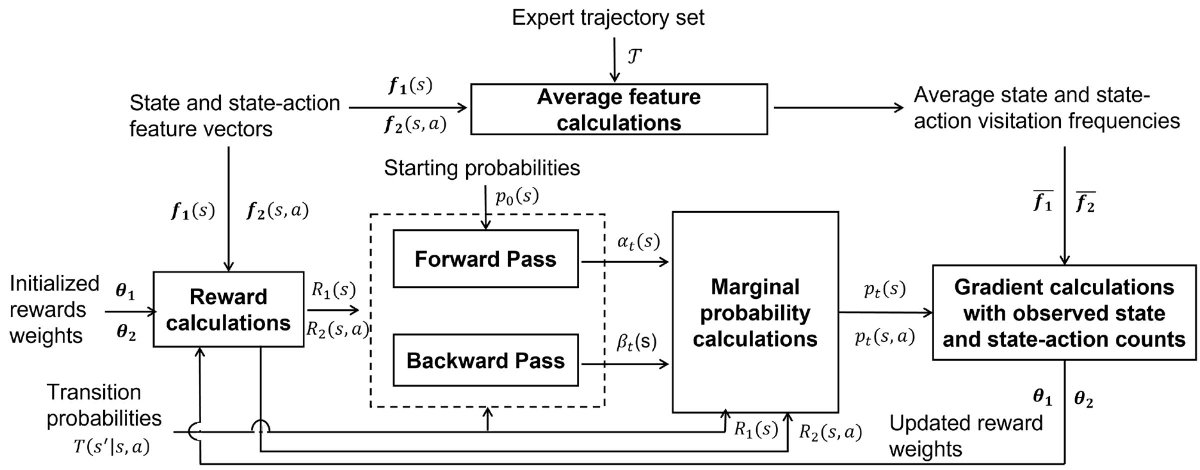

Figure 5. Steps of the reward learning process based on the ExactMaxEnt IRL for the author topic MDP.

To compute the rewards, we first initialized the reward weights with uniformly distributed random values and updated them until convergence. Fig. 5 shows the basic steps involved in a single iteration of the reward learning process based on the ExactMaxEnt IRL algorithm (Snoswell et al., 2020). The discount factor, $\gamma = 0.99$ in all the calculations. We define the frequency of times a state $s \in S$ occurred as the starting state in the expert trajectory set, as its starting probability, which is denoted as $p_0(s)$. We then use the forward-backward algorithm for a first-order MDP to efficiently compute the state marginal probability, $p_t(s)$, that an author will visit each state s at step t, and the state-action marginal probability, $p_t(s,a)$, that the author perform an action a at step t, from all observed starting states, respectively. The state marginal probability, $p_t(s)$, is calculated for $t = 1$ to $L - 1$ as,

$$p_t(s) = \frac{\alpha_t(s)}{Z} \sum_{a \in A^*, s' \in S^*} T(s'|s,a) e^{\gamma^{t-1} R_2(s,a)} \beta_{L-t}(s'), \quad (7)$$

and for $t = L$ as,

$$p_L(s) = \frac{\alpha_L(s)}{Z}, \quad (8)$$

where $\alpha_t(s)$ and $\beta_t(s)$ are the forward and backward message variables, defined as

$$\alpha_1(s) = p_0(s) \exp\left(R_1(s)\right) \quad (9)$$

$$\beta_{t+1}(s) = \sum_{s' \in S^*, a \in A^*} T(s'|s,a) \exp\left(\gamma^{L-t-1} R_1(s)\right) \beta_t(s'), \text{ for } 1 \le t < L. \quad (12)$$

The partition function, Z, is calculated as

$$Z = \sum_{t=1}^{L} \sum_{s \in S} \alpha_t(s). \quad (13)$$

The state-action marginal probability, $p_t(s,a)$ is calculated as

$$p_t(s,a) = \frac{\alpha_t(s)}{Z} \sum_{s' \in S^*} T(s'|s,a) \exp\left(\gamma^{t-1} R_2(s,a)\right) \beta_{L-t}(s'), \text{ for } t = 1 \text{ to } L - 1. \quad (14)$$

We update the state and state-action reward weights using a gradient descent approach based on the difference between the observed and IRL-predicted values for both the state as well as the state-action visitation frequencies, respectively. The state reward weight is updated as,

$$\boldsymbol{\theta_1} \coloneqq \boldsymbol{\theta_1} + \varepsilon_1 \boldsymbol{\nabla\theta_1}, \quad (15)$$

where ε_1 is the learning rate and the state reward gradient $\boldsymbol{\nabla\theta_1}$ is calculated as

$$\boldsymbol{\nabla\theta_1} = \overline{\boldsymbol{f_1}} - \sum_{s \in S} \boldsymbol{f_1}(s) \sum_{t=1}^{L} p_t(s). \quad (16)$$

The state-action reward weight is updated as,

$$\boldsymbol{\theta_2} \coloneqq \boldsymbol{\theta_2} + \varepsilon_2 \boldsymbol{\nabla\theta_2}, \quad (17)$$

where ε_2 is the learning rate and the state-action reward gradient $\boldsymbol{\nabla\theta_2}$ is calculated as

$$\boldsymbol{\nabla\theta_2} = \overline{\boldsymbol{f_2}} - \sum_{s\in S, a\in A} \boldsymbol{f_2}(s,a) \sum_{t=1}^{L-1} p_t(s,a). \quad (18)$$

The reward learning steps (Fig. 5) were repeated 3000 times with learning rates equal to 0.05 for both ε_1 and ε_2. These settings were needed to obtain converged results. We assessed the convergence of the IRL simulations based on the root mean squared values of the reward gradients and the strength of correlation between the observed and predicted values of both the state and state-action visitation frequencies. The lower the reward gradients and the higher the correlation, the better the convergence.

3.2.6. Goal probability calculation (Step 10)

Goal probability calculations were performed to infer which state out a selected set of possible goal states, an author is most likely to publish in, given a partial trajectory of their observed state transitions in the author topic MDP grid space. We have developed a Bayesian formulation for computing the goal probabilities, like how the driver destination probabilities are calculated from partial trip trajectories (Ziebart et al., 2008). In the case of driver destination prediction, it is assumed that the driver's intent towards a destination occurs at the start of the trip. In the case of author trajectories, which are based on their sequences of publications in time, it cannot be known at what point (in time) along the trajectory, the author begins to have an intent to publish in a particular goal state. Therefore, in our Bayesian formulation, we considered the publication intent to begin at the previous state of each step along the trajectory, and computed the goal probability as follows.

Let's consider a set of N_g goal states, denoted as $G = \{G_i | i = 1\colon N_g\}$, where $G \subset S$. One of the goal states is the coin state, which is the state where the coin paper is located. The objective of the goal inference is to determine which of the N_g goal states is an author pursuing, given the observed steps (or states) of a partial trajectory. In other words, which reward policy (behavior) is the author following? Let π_i denote the RL agent's reward policy based on the rewards calculated for each goal state $G_i \in G$.

Let's consider a partial trajectory of t state transitions, $(s_{k-1}, s_k)_{k=1}^{t}$. For each step s_{k-1} to s_k in the partial trajectory and for each reward policy π_i, we calculate the posterior probability of reaching each state $S_j \in S$ of the MDP in $L-1$ steps, using the formula,

$$P_{\pi_i}(S_j | s_{k-1} \to s_k) = \frac{P_{\pi_i}(s_{k-1} \to s_k | S_j) P_{\pi_i}(S_j | s_{k-1})}{\sum_j P_{\pi_i}(s_{k-1} \to s_k | S_j) P_{\pi_i}(S_j | s_{k-1})}. \quad (19)$$

Here, the likelihood,

$$P_{\pi_i}(s_{k-1} \to s_k | S_j) = \frac{P_{\pi_i}(s_k \to S_j)}{P_{\pi_i}(s_{k-1} \to S_j)}, \quad (20)$$

is the probability that the agent with policy π_i will move from state s_{k-1} to state s_k, if the agent's intended (desired) goal state is S_j. $P_{\pi_i}(S_j | s_{k-1})$ is the prior probability based on all paths of length $\leq L$ observed in the expert trajectory set from state s_{k-1} to S_j. This is computed with a starting probability of 1 for the state s_{k-1}. $P_{\pi_i}(s_{k-1} \to S_j)$ and $P_{\pi_i}(s_k \to S_j)$ are the total path probabilities of reaching the state S_j within 1 to $L-1$ steps through all possible paths in the author topic MDP from s_{k-1} and s_k, respectively. The total path probabilities to the S_j state from each state of the partial trajectory were computed using the forward pass algorithm, where the starting probability of each state s_k was set as

$$p_0(s_k) = \begin{cases} 1, & \text{if } k = 1 \\ P_{\pi_i}(s_{k-1} \to s_k), & \text{if } k > 1 \end{cases}. \quad (21)$$

To infer the reward policy (or the associated goal state) of an author along each step s_{k-1} to s_k of the author's partial trajectory, we compute the probability of reaching each of the N_g goal states, $G_i \in G$, in $L-1$ steps using the reward policy π_i, as,

$$P_{\pi_i}(G_i | s_{k-1} \to s_k) = \frac{P_{\pi_i}(s_{k-1} \to s_k | G_i) P_{\pi_i}(G_i | s_{k-1})}{\sum_j P_{\pi_j}(s_{k-1} \to s_k | G_j) P_{\pi_i}(G_j | s_{k-1})}, \quad (22)$$

where, the likelihood is calculated using Eq. (20), and $P_{\pi_i}(G_i | s_{k-1})$ is the prior probability based on all paths of length $\leq L$ observed in the expert trajectory set from state s_{k-1} to G_i.

Finally, the goal probability of reaching the goal state G_i by the agent with policy π_i based on observing t state transitions is given by the normalized cumulative sum of the probabilities $P_{\pi_i}(G_i | s_{k-1} \to s_k)$ from each step (s_{k-1}, s_k), where $k = 1,2,\dots,t$, and is written as,

$$P_{\pi_i}(G_i | (s_{k-1}, s_k)_{k=1}^{t}) = \frac{\sum_1^t P_{\pi_i}(G_i | s_{k-1} \to s_k)}{\sum_j \sum_1^t P_{\pi_j}(G_j | s_{k-1} \to s_k)}. \quad (23)$$

4. Results

We present the topic modeling, IRL and goal inference results for the OPAL case study application to demonstrate technology-directed goal inference of author behavior in the nuclear research topic MDP grid environment. For demonstrating the inference problem, we selected four goal states; one of them is the coin state where the OPAL coin paper is located.

- *Crystal structure and diffraction* (Topic 4),
- *Surface reaction-based analysis of materials* (Topic 5),
- *Properties of compounds* (Topic 6), and
- *Electron orbitals as the basis for crystal properties* (Topic 7).

Based on the topic weight distribution, a paper may cover multiple topics with varying weights, and one topic may be highly weighted than all

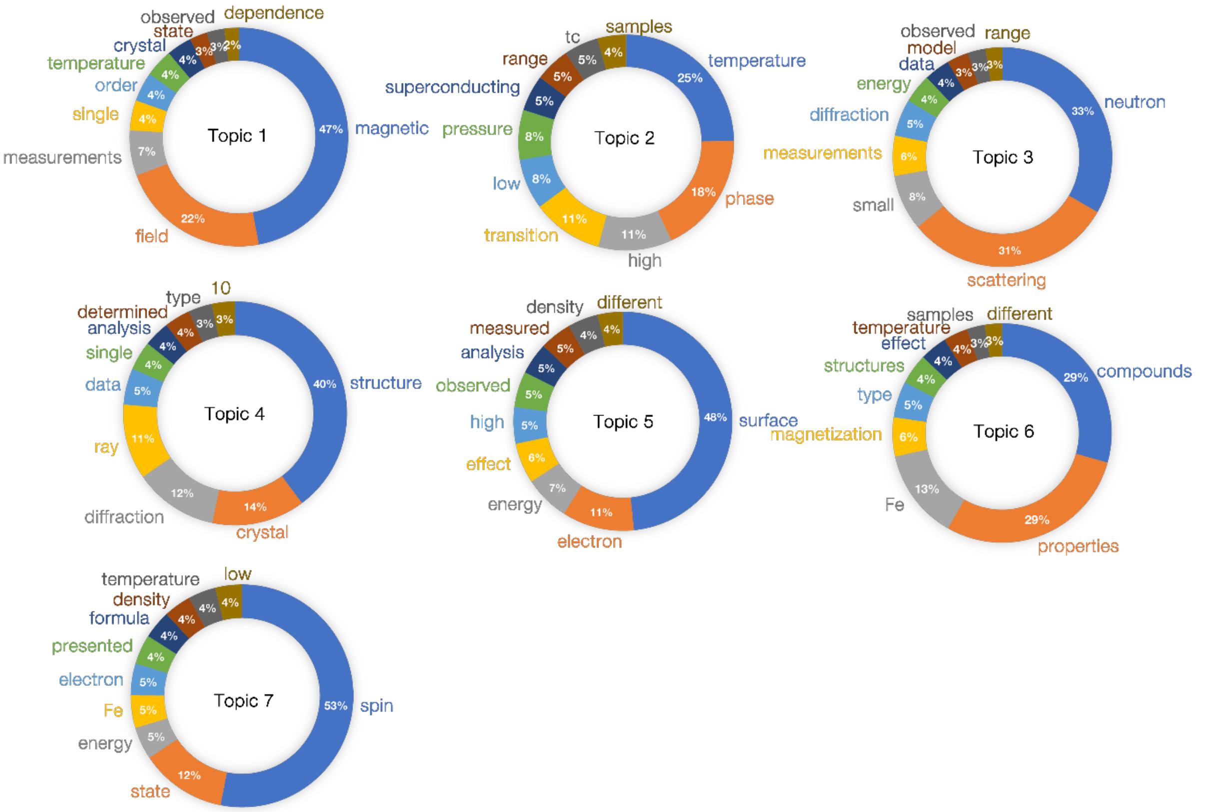

Figure 6. Normalized weight distribution of top ten keywords in each of the seven topics used for characterizing the topic vector space of 29,196 Scopus records.

4.1 Topic modeling

Based on NMF topic modeling, we defined the topic vector space of the 29,196 Scopus records in the OPAL case study application with seven topics. Fig. 6 presents the seven topics with normalized weight contributions of the top ten distinct keywords per topic, where the topics are numbered from 1 to 7. The keywords are distinct enough to provide a unique meaning to each topic. All the topics indicate some measurement study or analysis related to nuclear research. Based on these keywords, we interpret the topics as:

- *Magnetic field effects* (Topic 1),
- *Temperature-based phase transition* (Topic 2),
- *Small angle neutron scattering measurements and models* (Topic 3),

others. For example, the coin paper has two topics, Topics 1 and 3, with weights 0.27 and 0.73, respectively. The abstract of the coin paper mentions the use of OPAL cold neutron source for small angle neutron scattering experiments (Topic 3) and the use of horizontal field HTS magnet (Topic 1) in its cold neutron instruments. Approximately 22.24% of the records have a dominant topic weight greater than 0.7 (6494 out of 29196 records). Specifically for topics 1 to 7, this number was 577, 1818, 999, 1214, 845, 622, and 419, respectively.

4.2 OPAL state-action-state transition graph

We discretized the seven-dimensional topic vector space by dividing each dimension into six intervals with 0.1 width for the first and last intervals, and 0.2 for the intermediate intervals. Mapping the topic weights of the records on to the grid resulted in 1,276 grid cells with occupancies ranging from 1 to 942 records, as shown in Fig. 7. About 75.6% of the grid cells (i.e., 965 out of 1,276) contained less than 26 records each, which accounted for 51.3% of the total records (i.e., 6,265 out of 12,196). The highest number of 942 records, which accounted for 3.2% of the total records, was found in the state with the lowest range of weight values across all seven topics in the topic grid space.

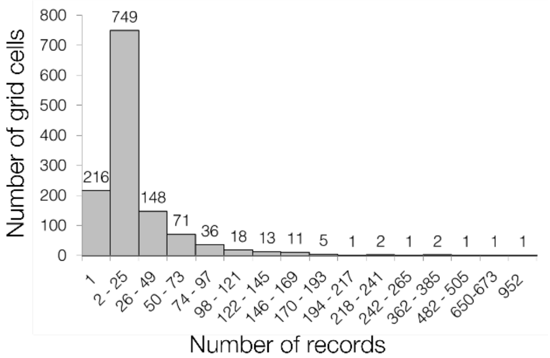

Figure 7. Frequency distribution of the number of grid cells occupied according to the number of records

The occupied grid cells were selected as the states for the author topic MDP. Our action definition resulted in 15 actions, where the maximum year difference observed between two sequential publications was 15 and the minimum was 0. A year difference of 13 was not observed in the data. The data contained 403 author publication sequences, out of which 402 were represented as state-action-state trajectories using the 1,276 states and 15 actions. The states were numbered from 1 to 1276 for identification. One author trajectory was ignored because it had only one state transition with a self-loop. The frequency of transitions in the 402 trajectories were used to compute the transition probabilities. The state-action transitions present in the author trajectories formed the OPAL state-action-state transition graph with 1276 nodes (states) and a maximum of 15 incoming/outgoing edges (actions) per node. Thus, the author topic MDP was represented as a stochastic MDP with 1,276 states, 15 actions, transitional probabilities, and a discount factor $\gamma = 0.99$. We note that the author trajectories are of different lengths and within a trajectory, an author can re-visit a state two or more times. For example, the length (number of states) of the five coin author trajectories were 17, 37, 58, 80, and 98. Fig. 8 shows the state transitions of one coin author based on their whole publication sequence, starting from their initial publication to the coin publication.

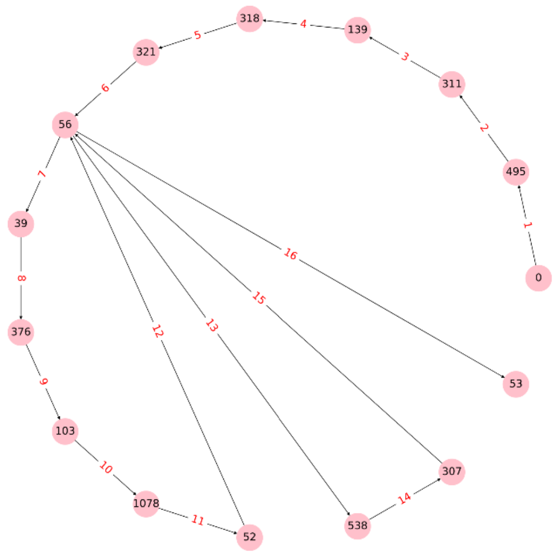

Figure 8. State transitions of a coin author based on their whole publication sequence in the dataset. The author begins in state 0 and ends in coin state 53 through 16 steps. The number along each arrow represents the step number.

4.3 IRL-based Bayesian goal inference

We computed the state and state-action rewards for four sets of author trajectories. These trajectories terminate at one of four different goal states, with one of the states being the coin state. We identify the four goal states by numbers, as 53, 132, 145, and 212, and denote the corresponding trajectory sets as $\mathcal{T}_{53}$, $\mathcal{T}_{132}$, $\mathcal{T}_{145}$, and $\mathcal{T}_{212}$, respectively. Goal state 53 is the coin state. Goal states 132, 145, and 212 were arbitrarily picked while ensuring their corresponding trajectory sets do not contain the coin state. The length of all the trajectories used in the IRL training set was set to $L = 17$, based on the length of the shortest coin-author trajectory. The coin state trajectory set $\mathcal{T}_{53}$ contained 45 author trajectories, out of which six were of the five coin authors. There were six instead of five coin-authored trajectories in the set because one coin author, whose full trajectory had 98 states, had visited the coin state twice and they were coincidentally 17 steps apart, resulting in two trajectories of length ≤ 17 for this author. For the IRL reward calculations, we excluded the six coin-author trajectories from $\mathcal{T}_{53}$ and used them as a test set for external validation. Thus, the number of $\mathcal{T}_{53}$ trajectories used for the reward learning was 39. The sets $\mathcal{T}_{132}$, $\mathcal{T}_{145}$, and $\mathcal{T}_{212}$ contained 14 trajectories, and all of them were used for reward learning.

The IRL simulations converged with root mean squared values below 0.003 for the reward gradients. The linear correlation coefficients between the observed and predicted values of both the state as well as state-action visitation frequencies were approximately 0.99 for all four trajectory sets, which provided further validation for convergence after 3000 reward updates. Each IRL simulation took about 17 hours to complete on a Windows laptop with 32 GB RAM and 20 2.4-GHz processors.

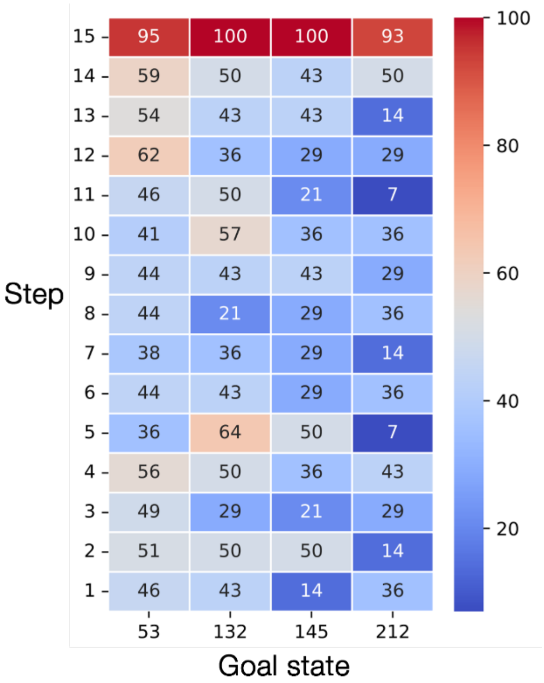

Figure 9. Percentage frequency of times (trajectories) each goal state (53, 132, 145, and 212) was ranked first at each step by their respective reward policy-based posterior probabilities. The last step, step 16, is not shown because the authors have already reached their goal state.

After learning the reward policies of the authors for the four goal states, we performed three types of validation for goal inference, on the trajectories that were used for learning the reward policies (the training sets). First, we evaluated whether the posterior probabilities that are computed based on each trajectory set's actual goal state reward policy (Eq. (19)) can be used to infer the goal state of the trajectories in the set. Specifically, we determined if the reward policy captures the correct goal-directed behavior of the authors by resulting in higher posterior probability values for the actual goal state than that for the other 1,275 states. In the second validation, we performed goal inference with all four reward policies on each trajectory set to determine if the posterior probabilities are lower for the reward policies that are not of the actual goal state. In the third validation, we computed the goal probabilities using Eq. (23), to determine if they are higher for the reward policy associated with the actual goal state of each trajectory set.

To further evaluate the performance of the learned reward policy for inferring the goal-directed behavior of coin authors, we performed a fourth validation by testing the goal inference on the six coin-author trajectories and comparing the goal probabilities based on each reward policy. These tests provided an external validation for the reward policies by testing on trajectories that are not in the training sets.

4.3.1. Goal inference via ranking all the MDP states by their posterior probabilities in each training trajectory set using the set's goal state reward policy

Using the reward policy learned from each trajectory set, we computed the posterior probability of reaching each of the 1,276 OPAL MDP states at every step of a trajectory in the set (using Eq. (19)). We then ranked the states in descending order of their posterior probability values. The state with the highest rank, i.e., the state with the maximum posterior probability, was considered the most probable goal state. After identifying the highest ranked state in the first 15 steps of each trajectory, we computed the frequency of times (percentage of trajectories) each state was ranked first in every step. Fig. 9 shows the frequency values of the goal states 53, 132, 145, and 212, when they ranked first at each step in their respective trajectory sets. In most steps, the frequency was the highest for the actual goal state of each trajectory set (although not fully at 100%), signifying that the reward policies are able to capture the correct goal-directed behavior of the authors in their respective training sets. For example, with reward policy π_{53}, the state 53 was inferred to be the most probable goal state at step 4 in 56% of the trajectories ($\mathcal{T}_{53}$) (i.e., approximately 22 out of 39 trajectories). For the set $\mathcal{T}_{212}$, at steps 5 and 11, the goal state was correctly inferred for only one out of the 14 trajectories in the set. In this case, the inferred goal state varied across all the 14 trajectories. For each set of trajectories, the rankings indicate that other states can be inferred as the goal state besides the actual goal state, but at lower frequencies. In total, there were 173, 56, 87, and 96 states inferred at least once as the goal state in the trajectory sets $\mathcal{T}_{53}$, $\mathcal{T}_{132}$, $\mathcal{T}_{145}$, and $\mathcal{T}_{212}$, respectively. It can also be seen that the frequencies are nearly 100% in the step before the trajectories terminate at their respective actual goal states.

Although the actual goal states were not ranked first all the time (i.e., in all steps) in their respective trajectory sets using the goal state's reward policy, they ranked among the top 5 states, in at least 90% of the steps per trajectory, as shown in Fig. 10. The rankings varied from 1 to 13 for state 53, 1 to 12 for states 132 and 145, and 1 to 10 for state 212. From these results, we can generally expect that the posterior probabilities, computed using the actual goal state's reward policy (Eq. (19)), will rank the goal state among the top 5 (out of the 1,276) states in at least 90% of the steps observed (on average per trajectory) in the training sets. This is the best ranking and frequency profile that can be achieved if an author were to follow the correct reward policy in a goal inference test.

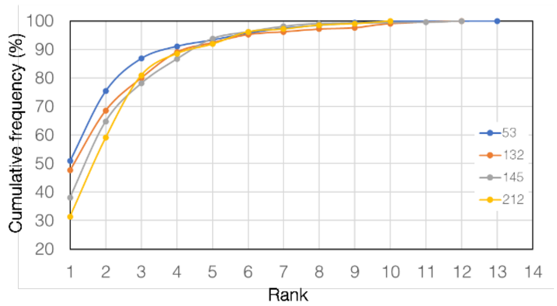

Figure 10. Cumulative frequency of inferred goal rankings for the states 53, 132, 145, and 212 based on their respective reward policy in trajectory sets $\mathcal{T}_{53}$(a), $\mathcal{T}_{132}$ (b), $\mathcal{T}_{145}$ (c), and $\mathcal{T}_{212}$ (d).

4.3.2. Goal inference via ranking the MDP states by their posterior probabilities in each training trajectory set using the reward policies of all goal states

The above goal inference tests were performed on each trajectory set using the reward policy learned for that set. That is, the goal state associated with the reward policy and with the trajectory set used for inference test are both the same. If the goal inference was performed with a reward policy other than that associated with the actual goal state of a trajectory set, then we should expect the ranking for the goal state associated with the reward policy to be lower. To verify this, we computed the posterior probabilities based on all four reward policies on all trajectory sets and determined the rankings (and their frequencies) for the goal state of each reward policy. As seen in Figs. 11 (a-d), the frequency of rankings among the top 1 to 10 states are generally 30 to 40 % lower for all goal states inferred with reward policies different from that of the actual goal state. A few exceptions are noted in Fig. 11(c) and (d), where the percentage of times state 53 ranked first was higher by 7.6% and 9% in trajectories whose actual goal states were 145 and 212, respectively. Overall, the ranking results in Fig. 11 verify that only the reward policy for the actual goal state captures the correct behavior of authors in each trajectory set. For example, as shown in Fig. 11(a), state 53 ranked among the

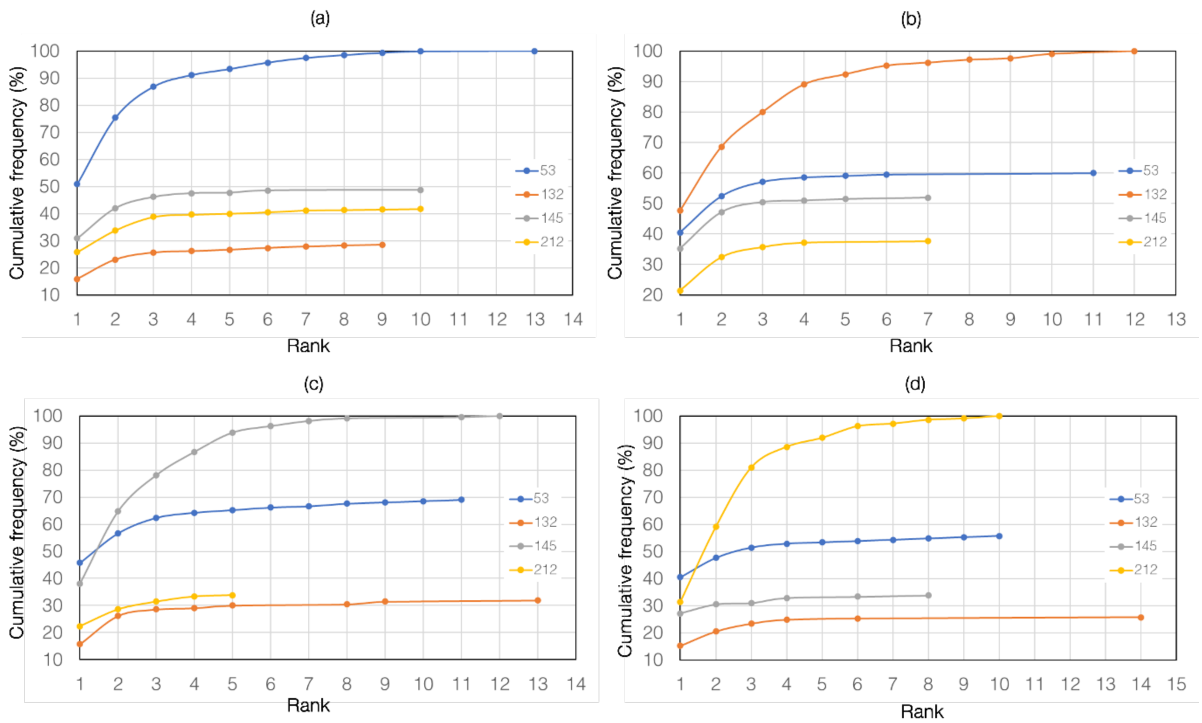

Figure 11. Cumulative frequency (%) of inferred goal rankings for the states 53, 132, 145, and 212 in trajectory sets $\mathcal{T}_{53}$(a), $\mathcal{T}_{132}$ (b), $\mathcal{T}_{145}$ (c), and $\mathcal{T}_{212}$ (d), respectively. For each trajectory set, ranking was done by comparing the posterior probabilities of all states computed based on the reward policy learned for the trajectory set's goal state.

top 10 states 100% of the time (steps per trajectory). State 132 ranked among the top 10 states in less than 30% of the time. States 145 and 212 ranked among the top 10 in less than 49% and 42% of the time, respectively. States 132, 145, and 212 ranked 394th, 367th, and 634th, respectively at other times (not shown). Thus the ranking results in Fig. 11 (a) verify that only the reward policy for goal state 53 predicts the correct behavior of authors in the trajectory set $\mathcal{T}_{53}$. Similar goal ranking results can be observed for the other trajectory sets, as shown in Figs. 11 (b-d).

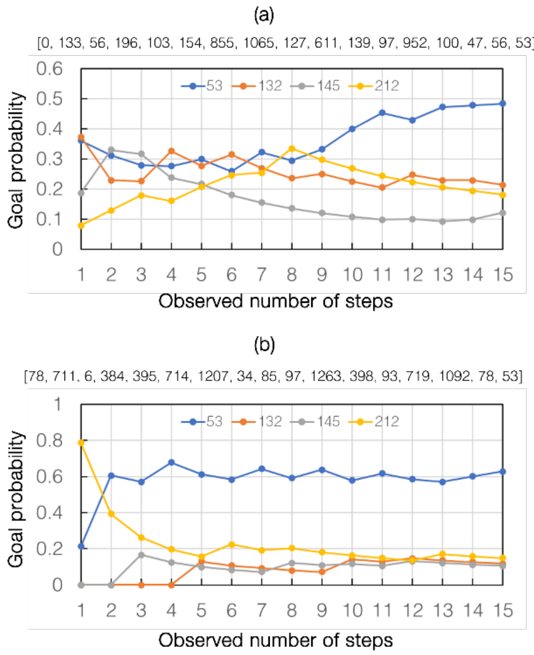

Figure 12. Goal probabilities of each state (53, 132, 145, and 212) as more number of steps (state transitions) are observed along two author trajectories that terminate at state 53 ((a) and (b)). Goal inference for each state was based on its respective reward policy. The sequence of states in the two trajectories are listed above each figure.

4.3.3. Goal inference via ranking the four goal states in each training trajectory set by their respective reward policy-based goal probabilities

To further validate the learned reward policies for goal inference, we determined which one out of the four states is the preferred goal state as an author progresses along a trajectory, by ranking the four states in decreasing values of their reward policy-based goal probabilities (calculated using Eq. (23)). For sake of illustration, we show in Fig. 12, the goal probabilities of two author trajectories that terminate at goal state 53. For the first author (Fig. 12(a)), state 53 is the most probable goal state after observing the first 9 state transitions (steps) of the trajectory. In the first 8 states of the trajectory, it is not clear which of the four goal states, the author is pursuing. For the second author (Fig. 12(b)) we can see that the author is pursuing state 53 after two state transitions.

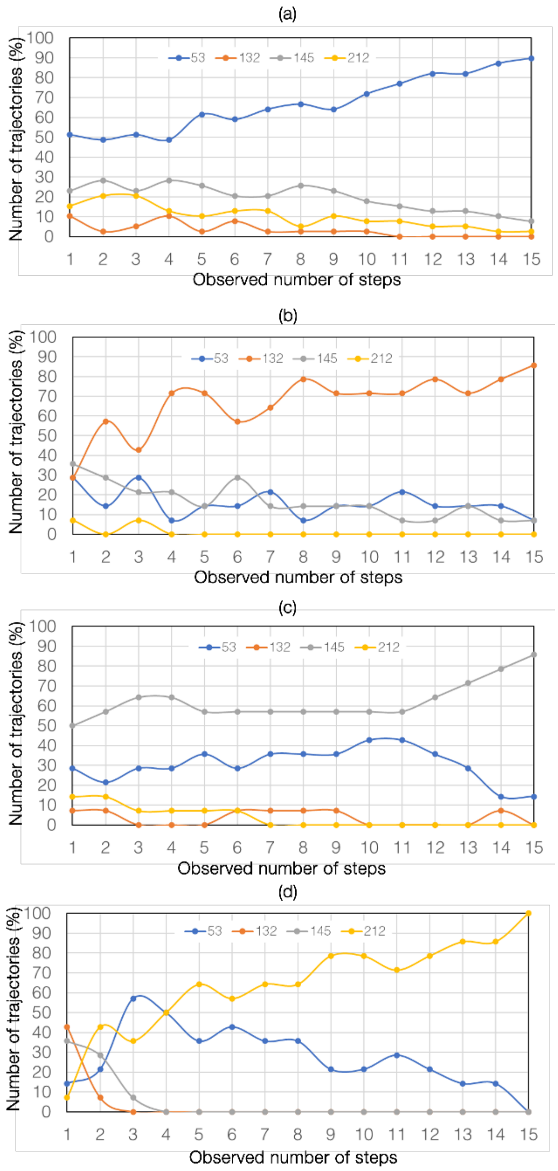

Figure 13. Percentage number of trajectories in sets $\mathcal{T}_{53}$ (a), $\mathcal{T}_{132}$ (b), $\mathcal{T}_{145}$ (c), and $\mathcal{T}_{212}$ (d), in which each state (53, 132, 145, and 212) was inferred as the goal state, based on the respective state's reward policy

Based on their respective reward-based goal probabilities, we ranked the four states in all trajectories of each set and counted how many times each state ranked first as the goal state, as more state transitions (steps) are observed along each trajectory. The results for each trajectory set are plotted in Figs. 13 (a-d). We can see in Figs. 13(a) and 13(c) that the actual goal states, 53 and 145, were inferred in at least 50% of the trajectories in their respective trajectory sets ($\mathcal{T}_{53}$ and $\mathcal{T}_{145}$), as the observed number of steps varied from 1 to 15. State 132 was inferred as the goal state in the first step of only 30% of the trajectories in set $\mathcal{T}_{132}$ (Fig. 13(b)), but this percentage rose above 50 after 4 steps. In the case of trajectories in set $\mathcal{T}_{212}$, the state 212 is the inferred goal state in at least 50% of the trajectories after 5 steps of observation. This number rose to 100% when the author was one step away from the goal state. There were only a small percentage of trajectories (about 10 to 15 %) in $\mathcal{T}_{53}$, $\mathcal{T}_{132}$, and $\mathcal{T}_{145}$, where the goal state could not be inferred. While the inference may be delayed in some cases, these results indicate that early inference of the actual goal state is possible, and the goal-directed behavior can be inferred using the reward policy-based goal probabilities of the four goal states.

their respective reward policy-based goal probabilities

We performed the goal inference test on the six coin-author trajectories that were not included in set $\mathcal{T}_{53}$. This test will determine how well the IRL-Bayesian goal inference approach will perform in inferring the coin state as the goal state out of the four states, 53, 132, 145, and 212. Using Eq. (23), we computed the probability of reaching each of the four states based on the number of steps observed in each coin-author trajectory. Figs. 14 (a-f) show the most likely goal state as more steps are observed along each of the six coin-author trajectories. As seen in Fig. 14, for some trajectories we can predict the coin state as the most likely goal state very early on in the author's observed trajectory. For example,

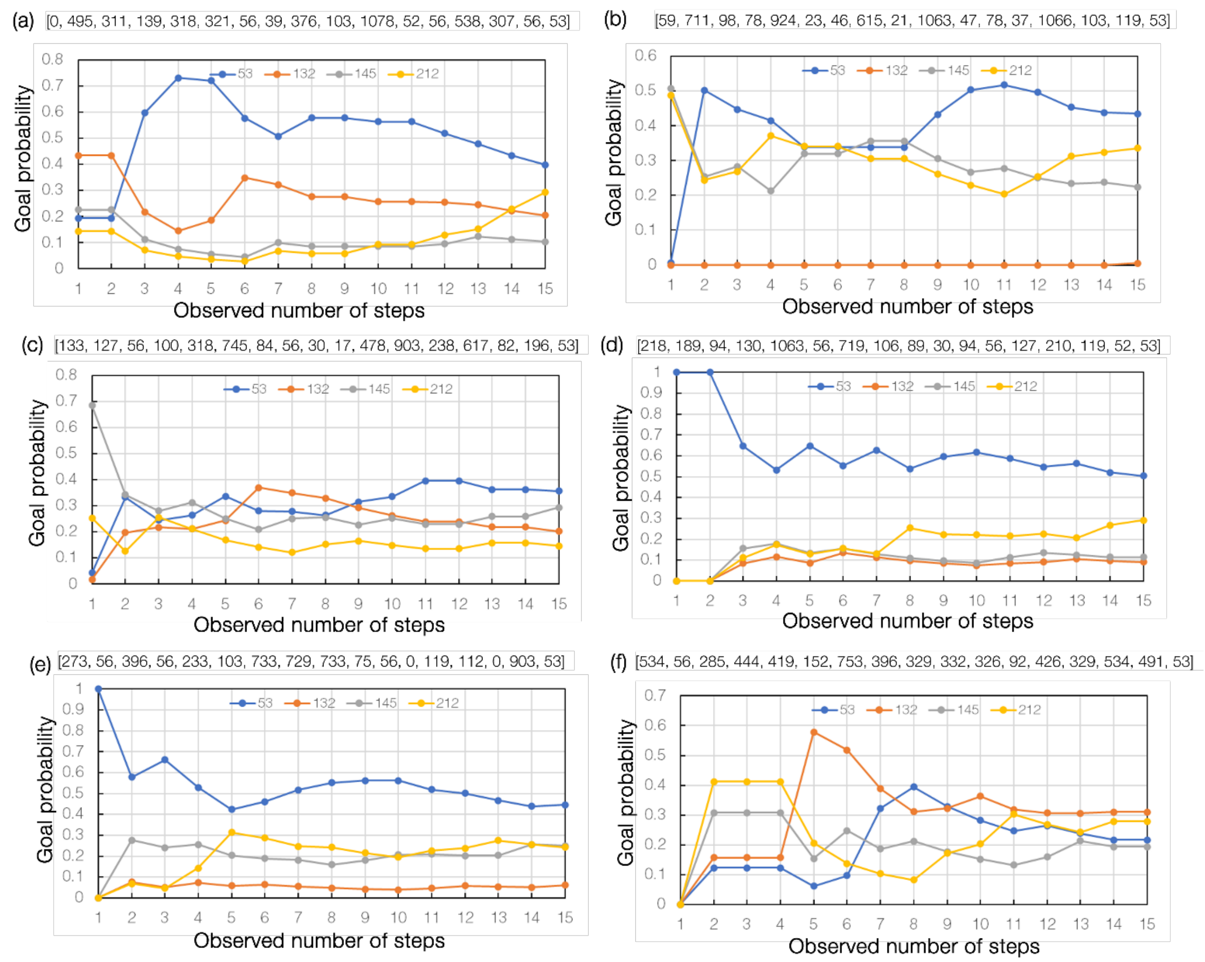

Figure 14. Goal probabilities of each state (53, 132, 145, and 212) as more number of steps (state transitions) are observed along the six coin-author trajectories that terminate at state 53 (a-f). Goal inference for each state was based on its respective reward policy. The sequence of states in the six trajectories are listed above each figure.

4.3.4. Goal inference via ranking the four goal states in previously unseen trajectories using

consider the trajectories in Figs. 14(a), 14(d), and 14(e). For the trajectory in Fig. 14(a), state 132 would be predicted as the goal state after observing the first two state transitions. However, after three state transitions, we can see the coin state as the most likely goal state for the remaining length of the trajectory. For the author trajectories in Figs. 14(d) and 14(e), the goal probability of the coin state is the highest over the whole length of each trajectory, and therefore, is the most likely goal state. For the trajectory in Fig. 14(f), however, the coin state could not be inferred as the goal state. In other two trajectories (Fig. 14(b) and Fig. 14(c)), the inference for the coin state is delayed by 9 steps, but it is still 6 steps away from reaching the coin state. For the trajectory in Fig. 14(b), it is not clear what the goal state is after observing 5 to 8 steps of the trajectory. But after observing 9 to 15 steps, we can see that the coin state is the predicted goal state.

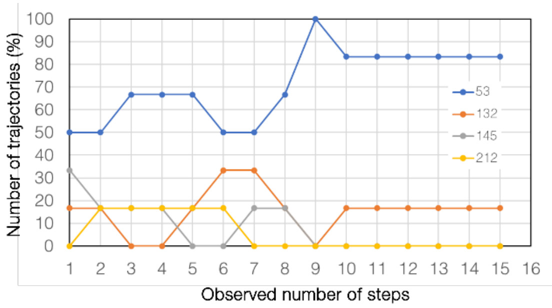

Figure 15. Percentage number of trajectories in the six coin-author trajectory set, where each state (53, 132, 145, and 212) was inferred as the goal state, based on the respective state's reward policy.

To quantify the accuracy of the IRL-based Bayesian goal inference approach, we counted the number of trajectories where the coin state is predicted as the goal state, as more steps are observed along each trajectory. As shown in Fig. 15, the coin state is correctly inferred as goal state in at least 50% of the trajectories (3 out of 6) after 1 to 8 steps of observation, and in 83% (5 out of 6) of the trajectories after 10 steps of observation. These results signify that with our IRL-based Bayesian formulation of goal probabilities, it is possible to infer whether an author is pursuing the coin state after observing a fraction of the author's trajectory before the state is reached.

5. Discussion

The results for the OPAL case study provide a proof-of-concept demonstration of the IRL-based Bayesian goal inference method to detect research activities of authors before they reach their goal state in a nuclear technology area. The case study focuses on a technology area related to the cold neutron source of the OPAL reactor, which may not directly relate to the building of the reactor, but indirectly points to its existence and operational use. The method used for the OPAL case study is, however, applicable to proliferation potential nuclear technologies, given the relevant datasets. Further research that goes beyond the scope of this paper is necessary to test the validity of the method for various technology use cases, assumptions, and variations in the method. In the following paragraphs, we discuss the different aspects of the method that can affect its performance and provide potential research directions to advance the method for applications in early detection of nuclear research activities.

The results and the performance of the IRL-based Bayesian inference method can vary depending on 1) how the topic weight vector space is defined, 2) which research articles are used in the dataset, 3) what grid spacing is used to discretize the topic weight vector space, 4) how the states and actions are defined for modeling the authors sequential decision-making process to publish in the coin state, 5) how much overlap in the state transitions exist among trajectories in a training set, and 6) how the reward function is defined. Future work may be directed towards understanding the effects of these factors.

In this work, we used NMF-based topic modeling to define the topic weight vector space of all the publications in the dataset. Other topic modeling approaches may be utilized, for example, Latent Dirichlet Association (LDA) method and classification algorithms based on large language models (LLMs) that are specifically trained on nuclear research articles. We trained the NMF topic model using the abstracts and titles of 29,196 Scopus records associated with the case study. These records comprised of a primary set of papers written by authors of the coin paper and a secondary set written by non-coin co-authors of the primary paper set. Instead of training the NMF model on the whole set, one could also train the NMF model using only the primary set and then compute the topic weights for the papers in the secondary set. This NMF fitting method can be used to confine the topic space to the primary set, which we have found to reduce the noise-to-signal ratio by resulting in a fewer number of author trajectories terminating in the coin state for IRL training. To avoid any bias due to the primary set, we considered to model the topics using the whole set.

In the case study, we used a single flagship publication of OPAL to define the coin state. The method can be extended to multiple coin states if there are multiple publications associated with the technology of interest. For the case with multiple coin states, the expert trajectory set used for IRL training will include trajectories terminating in any of the coin states.

For the IRL framework, we defined the states based on the location of the publications in the discretized topic weight vector space and actions based on the year difference between two consecutive publications in an author's publication sequence. There is no prescribed way to define actions for the author topic MDP. Future work may explore other ways of defining the actions and analyze grid discretization effects on the goal inference. Reducing the grid spacing will increase the number of grid cells (states) and lower the grid occupancy. This can reduce the overlap between author trajectories and create better separation of author behaviors, which in turn may improve the performance of the inference method. Higher resolution grids will increase the size of the MDP problem and will require high performance computing resources to perform the reward learning and inference calculations.

In the OPAL case study, we computed the state and state-action rewards independent of the state and state-action features, respectively. If these features are known and are readily available, then the performance of the inference method may be improved by representing the rewards as a function of these features. The current lack of knowledge of these features can limit the accuracy of the goal inference.

When applying the IRL-based Bayesian inference approach to infer whether an author will pursue the coin state, we must first convert the author's partially observed publication sequence into a sequence of state-action-state transitions in the topic MDP environment. This is done first by computing the topic weight vectors of all the author's publications using the trained NMF model and mapping them to states in the topic weight vector space. There could be states and actions in the author's sequence, that are not part of the topic MDP environment if they were not previously observed. Therefore, we must expand the state and action spaces of the MDP to include previously unobserved states and actions, and then re-compute the transition probabilities based on all the state-action-state transitions observed in the author's partially observed sequence, and subsequently re-learn the rewards for the respective goal states, including the coin state. This will also update the transition probabilities of previously observed state-action-state transitions, and possibly the rewards of previously observed states and state-action pairs. If all the states and actions in the author sequence already exist in the MDP, we could choose not to update the transition probabilities and rewards. But as more data becomes available, it would be necessary to update the transition probabilities and re-train the rewards even if no new states need to be included in the MDP's state space. In the OPAL case study, we included the transitions of the test trajectory set when computing the transition probabilities.

Although we can incorporate previously unvisited states in the MDP before doing the inference, the prior goal probabilities given these states (are observed) will be zero, since these states were not present in any of the expert trajectory sets used for IRL training. The zero observed priors will result in zero goal probabilities for all tested goal states. When no observed goal priors exist for a new state, one could perform an inference with a uniform prior or impute a prior value based on proximity of the new state to previously visited states. The imputation method is like the open-world assumption used by Krumm and Horvitz (2006) for driver destination prediction when a driver can visit locations (grid cells) that have not been visited before. For our application, one may use grid interpolation methods to impute the prior goal probability value for a previously unvisited state based on those of previously visited states that are within some L1 or L2 norm distance from the unvisited state in the topic grid. Alternatively, one may consider replacing the new state in the author trajectory with the closest of the previously visited states in the topic grid based on L1 or L2 norm distance. Further research is necessary to test the validity and accuracy of using uniform and imputed goal priors when there are previously unvisited states in an author's trajectory that is tested for goal inference.

In the OPAL case study, we evaluated the performance of the method using trajectories that terminated at four different goal states (including the coin state). We evaluated how well the IRL-based reward policies captured the correct goal-directed behavior of authors in two ways: 1) by comparing the frequency of rankings based on the posterior probabilities of all states, computed using the reward policy for each goal state (see Fig. 11), and 2) by comparing the goal probabilities of reaching each of the four goal states given an observed fraction of the steps in a test trajectory (see Figs. 12 to 14). Based on the posterior probabilities that were computed using the reward policy for a goal state, we found that the actual goal state would be the inferred goal state among the top 5 states 90% of the steps in a trajectory of the training set. With a different reward policy, the frequency of rankings would drop by 30 to 50%. This suggested that the reward policies capture the correct goal state behavior of authors. Based on the goal probability calculations, we found that the inference of the actual goal state can be early while in some cases delayed or unobservable. In practice, even though the actual goal state could be inferred five or six steps before it is reached, there is an uncertainty in finding the exact time of the event's occurrence due to the inherent time lag between the inception of a research activity and its publication date. This uncertainty will have to be quantified based on additional technology use cases and larger validation tests.

In this work, the length of the shortest coin-author trajectory was used as the maximum length of the trajectories ($L = 17$) in the IRL training set. But the trained model can be applied for making inferences on trajectories of length smaller or greater than L. In future studies, it will be instructive to look at how different values of L for the training trajectory set might affect the inference results. It is noted that the IRL-based Bayesian inference method is suited for inferring the goal state before an author reaches the goal state, even after one or two steps of observation. This is useful when inference must be made for cases where the observed sequence is short due to delays in publication reviews or due to fewer number of publications as in small (covert) projects compared to large public research programs.

Future work may be directed towards understanding what factors of the author trajectories limit the performance of the IRL-based Bayesian goal inference. For example, inference can be limited by high overlap in the state transitions between author trajectories, and by the fact that authors can re-visit a state multiple times or can access any state from a given state.

6. Conclusion

We have developed an IRL-based Bayesian goal inference method to predict whether an author would pursue a research activity (goal state) in a nuclear technology area, given partial observations of their state transitions in a research topic weight vector space. Our case study results surrounding a civil nuclear activity suggest that it is possible to infer whether an author would publish on a technology-directed research activity before it has occurred. This work represents the first attempt at using nuclear research articles for early detection of technology-directed research activities of authors. We have discussed various research directions to build upon this work and to improve the performance of the inference method. The present work provides a foundational framework for early detection of technology-directed activities from scientific and technical sources of information, where the early detection problem is formulated as a sequential, decision-making problem. The IRL-based Bayesian goal inference method, combined with advanced computing, may be used to assess and monitor activities pertaining to early developmental stages of a nuclear technology or capability, which in turn can help to identify and prioritize activities with nuclear proliferation potential for further investigation.

Acknowledgments

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The Impact of ^{234}U α-emission Induced Radiolysis on UF_6 Storage Composition for Non-destructive Verification via Passive Neutron Counting

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Abstract:

The mass of ^{235}U present in storage cylinders containing low enriched uranium (LEU) in the form of uranium hexafluoride (UF_6) may be verified nondestructively using a combination of gamma-ray based enrichment meter and passive neutron counting techniques. A hypothetical concern is that the (α,n) production rate in aged bulk UF_6 might differ from that of fresh material if the chemical composition changes over time, the thought being that this could be initiated by the self-induced radiation field, the process known as radiolysis. To support the physics-based interpretation of the observations Croft et al. measured, in 2020, for the specific ^{234}U-driven (α,n)-yield in UF_6, this work reviews available literature to quantify the possible impact of radiolysis on (α,n) production rate. Building on the review, a radiochemical yield value, G = 0.5 molecules of F_2 per 100 eV is selected, to calculate the impact of UF_5 production – via radiolysis – on the (α,n)-yield. Calculations demonstrate a negligible impact on bulk UF_6 concentration and respective neutron yield.

Keywords: UF_6 radiolysis, UF_6 verification, non-destructive assay, nuclear safeguards.

1. Introduction

Uranium hexafluoride, UF_6, is a prerequisite for ^{235}U enrichment; given the risk of UF_6 being 'lost', its monitoring is an international priority for non-proliferation security [1][2]. Extensive information on the properties of UF_6, and especially about its safe handling, conversion, enrichment, and fuel fabrication, can be found in Strunk and Thornton [3]. Long term stability is of concern because UF_6 is a dynamic substance even when thermal processes can be ignored, since chemical reactions can be induced by ionising radiation – the process known as radiolysis [4]. Consequently, one can expect a slow and spontaneous dissociation or decomposition of highly enriched UF_6 in storage due to the self-irradiation by ^{234}U α-particles [5]. It is well known that for the actinides, energy deposition is dominated by α-tracks [6]. There is also a suggestion that in bulk UF_6, α-particles are considerably more effective for a given amount of energy deposited at breaking chemical bonds [4] than other forms of ionising radiation (e.g. x-, γ- and β-rays). This is reflected in the radiation chemical yield. The radiation chemical yield, *G*, denotes the number of molecules produced, *M*, per 100 eV energy absorbed. Lind [7] defines *G* as the multiplication of ratio between ion-pair production energy of a molecule, *W*, per 100 eV, and molecules per number of ions, *N*. Binks [8] allows this to be simplified, finding a *W* in the region of 35 eV typical for low-pressure gases in the presence of $\gamma, \beta, \& \, \alpha$ radiation:

$$G = \frac{100eV}{W} \cdot \frac{M}{N} \cong 3 \cdot \frac{M}{N} \tag{1}$$

Fundamental considerations suggest a G ≅ 1.5 molecules of fluorine, F_2, produced per 100 eV of absorbed ionising radiation. Trowbridge et al. [9] – in their Table 2 on p.19 – which in turn refers to Saraceno [10] – and being one of the few published reports on radiolysis in UF_6 it has been widely adopted – summarise fluoride radiolysis of uranium fluorides and Molten Salt Reactor Experiment (MSRE) salts. They reinforce the fundamental assumption, presenting the radiation chemical yield, *G,* value as 1.5 molecules of F_2, for α-radiation in solid UF_6. The corresponding value quoted for x- (soft, *X*=0.13 MR/hr]) and γ-radiation (^{60}Co γ's, *X*=0.73 MR/hr) [11] – which liberate fast electrons that cause most of the associated ionisation – is considerably lower, ranging between 0.005 – 0.045$\pm$0.02 for various MSR salts – itself further referencing Haubenriech and Engel [12]. Both G values (α and x, γ) likely have large uncertainties given the sparse semi-theoretical and experimental data on which they are based and the difficulties associated in performing the experiments on uranium. Which in turn has a low specific activity and hence low rate of gas production (and in these studies pressure due to gas production was being used as the direct observable, rather than, say, optical spectroscopy [13]). The effect of

Byrne, S., Favalli, A., and Croft, S. (2024, December). The Impact of ^{234}U α-emission Induced Radiolysis on UF_6 Storage Composition for Non-destructive Verification via Passive Neutron Counting, *ESARDA Bulletin - The International Journal of Nuclear Safeguards and Non-proliferation,* 66, 28-34. https://doi.org/10.3011/ESARDA.IJNSNP.2024.3

recombination – F_2 reforming UF_6 after disassociating – is deemed negligible by Trowbridge et al. [9], at ambient temperature. However, models of recombination rate [14] find recombination cancelling out dissociation at temperatures in the region 343.15 – 393.15°K. The relationship between recombination and temperature is governed by chemical thermodynamics. The most stable state is expected when the Gibbs free energy, ΔG, is at its minimum. This occurs in the gas phase and at elevated temperatures thereby promoting recombination. In the solid phase ΔG is large due to low disorder and so recombination is not expected to be thermodynamically favourable. However, it is important to comment on localised amorphization of the solid matrix, as a result of α-induced defects; amorphous solids having high disorder, potentially influencing recombination. While unexplored for UF_6 storage, literature from mixed-oxide (MOX) fuels may present insight into this phenomenon [15,16]. Gibbs energy at constant pressure-temperature (P-T) is a function of enthalpy, ΔH, temperature, and entropy, S – temperature dependence of ΔG is determined from fundamental principles (the 2nd law of thermodynamics).

Present interest is motivated by a desire to quantify whether the rate of radiolysis is high enough to affect the (α,n) production rate observed for the range of items (enrichment and age) measured by Croft et al. [17]. However, it is unclear what uncertainty to assign the *G* values presented by Saraceno [10] and in turn on any conclusions made by assuming Sareceno's recommended G-values. In order to bound the quality of the data, a review of the available information has been undertaken.

2. Review

The G value proposed by Saraceno [10] is an upper bound, assuming no reverse reformation or back reaction, long-term dynamic-equilibrium that may be established in a sealed system; and that every ion-pair formed results in decomposition of one UF_6 molecule. The number of ion pairs, *i.p,* per α-particle assumed by Saraceno was 0.137×10^6 per ^{234}U α-particle. This value was taken from Bernhardt et al. [18] for UF_6 gas based on ionisation data measured by Steidlitz et al. [19]. Steidlitz et al. studied 13 gases, including a range of fluorocarbons, for which the average ion pair production energy, *W*, was within approximately 10 % of 30 eV/*i.p.* in all cases, this is comparable with Binks' assumption from fundamentals which was supported *W* in the region of 35 eV/*i.p.* They also confirmed additivity scaling rules for both range and ionisation – to be further discussed later.

Bernhardt et al. studied UF_6 radiolysis using radon (^{222}Rn) as the α-source – their findings are tabulated in table 2 of Trowbridge et al. [9]. The chemical reaction is reversible dependent on the radiation-field, this is evident via empirical plots utilising radioactive decay equations and pressure - the chemical reaction is as follows:

$$2 \cdot UF_6 \overset{\alpha}{\rightleftarrows} 2 \cdot UF_x + (6-x) \cdot F_2 \qquad (2)$$

The solid product was designated as UF_x because it could be either uranium tetra or pentafluoride, UF_4 or UF_5 respectively, but could not be identified owing to the small amounts generated. The present report is primarily concerned with loss of F(α,n)-targets in the bulk medium; thus, assume $x = 5$ consistent with the characterisation of solid uranium fluorides in UF_6-storage cylinder heels, and ignore the back reaction (discussed later). On this basis, equation 2 becomes:

$$2 \cdot UF_6 \xrightarrow{\alpha} 2 \cdot UF_5 + F_2 \qquad (3)$$

Across a series of 9 experiments (with no additional dilutant gases present) Bernhardt et al. obtained G values ranging from 0.24 to 0.70; the mean value being (0.45±0.05), where the uncertainty is the statistical standard error only. In a second series of measurements with nitrogen added a wide range of results was again obtained with extracted G values extending to approximately 2.8. In addition to the random scatter, Bernhardt et al. cautions that systematic bias, such as other unidentified dissociation mechanisms, which are difficult to quantify, may also be present in one or both types of experiment.

Dmitrievskii and Migachev [20] were primarily concerned with the decomposition of UF_6 under fission fragment irradiation, for its utilisation as a nuclear fuel. Therefore, UF_6 decomposition was measured in mole produced per kW unit of power – finding a G value = (0.8±0.1) for fission fragments. They also reference Migachev and Senchenkov's study [21] of UF_6 dissociation by fast electrons, concluding the importance of electrons to be negligible in comparison, the estimate being G = 0.011 for electrons. Further remarking, fast electrons aid the fluorination of dissociation products (UF_4 and UF_5) in the presence of free fluorine. The impact of fast electrons on UF_6 decomposition further negated as they aid the rate of the back reaction, reinforcing this reports choice to focus on revision of α induced radiolysis.

Trowbridge et al. [9] reviewed experimental radiolysis data reported in the literature with an emphasis on experimental molten salt reactor fuel. Some unconvincing arguments are made to justify that G-values for x-, γ-, and fast electron radiation is much less than for α-radiation; although, this does not matter for this discussion because α-radiation dominates the energy deposition. The relevant experimental data considered is mainly from the K-25 group at Oak Ridge Gaseous Diffusion Plant reported prior to the report by Bernhardt et al [18]. Again, they find a large variation in G-values, roughly spanning the range from 0.085 to 0.43, with a mean G ≈ 0.5 molecules of F_2 per 100 eV in the case of UF_6 gas subject to ^{220}Rn. The estimated value of Saraceno [10], of 1.5 molecules of F_2 per 100 eV, its origin discussed earlier, is also included in Bernhardt et al's review.

Recycled spent nuclear fuel (SNF, closed nuclear fuel cycle) also utilises UF_6 production, storage, etc; with the contribution of both concentrated ^{232}U and ^{234}U, the samples are highly active. Literature analysing the radiochemical yield, *G* value, of UF_6 from recycled fuel was also considered to gain insight into the influence of radiolysis under highly active conditions. Belov et al. [22] provides a recent study, neglecting UF_4 production and simulating UF_5 + $1/2F_2$ concentrations, that concludes the concentration of UF_5 developed is 10^7 times smaller than UF_6. The study used *G* values obtained from Bernhardt et al., and Dmitrievskii and Migachev – both of which have been considered already – and modelled a very active example with mass fractions: $2.36 \cdot 10^{-5}$, 0.681, 20, 6.54 and balance for $^{232, 234, 235, 236, 238}U$ respectively.

Yakovlev et al. [23] provides a modern study of low enriched (LE)UF_6 stored for up to 12 years. Gas pressure increases of 4.5% per year were measured within the fixed volume containers. Further, noting negligible (3 orders of magnitude difference) contribution from hydrolysis – it can be reasonably assumed that only radiolysis contributes. The study uses tetravalent uranium (IV) content as the gauge for radiolysis (assuming UF_5 production via UF_6 radiolysis and dissociation of UF_5) a reaction highly subject to conditions [24] via the equation:

$$2 \cdot UF_5 \underset{low\ T.}{\overset{high\ T.}{\rightleftarrows}} UF_6 + UF_4 \qquad (4)$$

Analysing the formation enthalpies, $\Delta_f H^0$, of uranium tetra, penta and hexafluoride, allows for the kinetics of the dissociation to be determined under the storage conditions. Table 1 presents formation enthalpies. However, it is crucial to note, UF_5 exists in two allotropic forms – β and α, of which β-UF_5 is more stable regarding dissociation into UF_4 and UF_6 [25].

UF_x	Phase	$\Delta_f H^0$ (298.15 [K°]) / $kJ \cdot mol^{-1}$
UF_4	cr (s)	-1914.2±4.2
UF_5	α (s)	-2075.3±5.9
	β (s)	-2083.2±4.2
UF_6	cr (s)	-2197.7±1.8

Table 1: Formation enthalpies of UF_x [x = 4,5,6] with phase information, relevant for UF_5.

For storage containers at Oak Ridge, at a working pressure = 100 psi ≅ 6.9 bar [26], application of Gay-Lussac's law (fixed volume) shows that, at ambient temperature, β-UF_5 is stable for pressures < 9.2bar – and so it can be concluded that β-UF_5 exists in storage conditions. This is reinforced in MSRE experiments [10]. Finally, using formation enthalpies of table 1, reaction enthalpy ($\Delta_r H^0$) dictates that UF_5 (reactant) is thermodynamically more stable in ambient temperature conditions, via equation 5:

$$\Delta_r H^0 = \Delta_f H_p^0 - \Delta_f H_r^0 = +54.5 \pm 10.2 \qquad (5)$$

Given the scant experimental data and concerns over both the precision and accuracy of the direct experimental data one can readily appreciate why Saraceno's estimate of G is included as a legitimate, technically defensible, and conservative choice. However, the overall situation is clearly unacceptable from a scientific perspective since in principle it is feasible to determine the quantity with far better precision and accuracy than is exhibited across the current technical literature.

3. Impact of Radiolysis on Molecular Composition

Adopting Saraceno's logic, if $0.137 \cdot 10^6$ ion pairs are formed per ^{234}U α-particle and each ionisation results in one molecule of UF_6 being dissociated into $UF_5 + {}^1/_2 F_2$. Given the mean α-particle energy emitted by ^{234}U is 4.75926×10^6 eV [27], then the average energy needed per UF_6 dissociation is 4.75926/0.137=34.74 eV, or 69.48 eV per molecule of F_2 produced. The corresponding G-value would therefore be estimated to be 100/69.48=1.44 (notionally rounded to 1.5) molecules of F_2 per 100 eV. The assumption that every ($UF_6^+ + e^-$) ion pair results in a permanent dissociation of a UF_6 molecule means that this estimate is an upper limit for G. Indeed, collectively the available experimental data supports a lower value. On this basis, a G-value of 0.5 molecules of F_2 per 100 eV seems more reasonable than Saraceno's widely adopted value of 1.5 – albeit with a relative uncertainty (68% confidence interval) of not less than 20%. Also, fluorine that stays trapped in the (solid) UF_6 matrix and does not emerge into the head space, remains as a potential α-particle target and is therefore not fully 'lost' from the bulk matrix from the perspective of self-induced (α,n)-production.

In terms of UF_5 – rather than F_2 – production, the choice of G-value (=0.5) equates to one molecule of UF_5 produced per 100 eV of α-energy deposited. For the purpose of the present study, assuming that the effect of radiolysis is to reduce the (α,n) production rate in the bulk medium, because instead of stopping in pure UF_6, emergent α-particles are stopped in a mixture of UF_6 and UF_5. Let f be the fraction of UF_6 molecules dissociated into UF_5, neglecting the dissociation of UF_5, and assuming all of the F_2 gas escapes, then the (α,n) yield of an aged item can be approximated by the linear sum of (α,n) yields from the two chemical forms present according to equation 6:

$$Y \approx (1-f) \cdot Y_{UF_6} + f \cdot Y_{UF_5} \tag{6}$$

The estimation of f proceeds as follows. It is well known from the field of nuclear calorimetry [5] that for actinide materials which decay by α-emission (e.g., the U, Pu isotopes and ^{241}Am) the majority of energy deposited in the material is due to the kinetic energy of the α-particles with recoil of the daughter nucleus being a small fraction. The range is short so α-particles are likely to stop within the material, the escape of γ- and internal conversion electron energy is minor. Spontaneous fission is usually negligible because the very low branching ratio more than off-sets the relatively high (about 200 MeV) energy release per event. With this in mind, for the present purposes of f(α,n) sensitivity analysis, the total radiation deposited per decay may be taken to a high degree of approximation to be equal to the Q-value of the reaction without need to consider the fine details of the decay scheme; that is, non α-particle radiation does not need to be treated differently.

The strongest effect is expected for highly enriched uranium (HEU), the ^{234}U α-emission rate dominates – neglecting ^{235}U and ^{238}U α-emission due to the disparity in $t_{1/2}$. For ^{234}U the specific α-activity, A, is $2.302 \cdot 10^8$ Bq·g^{-1} with a mean α-particle energy, E_α, of $4.7594 \cdot 10^6$ eV [27]. In one year (= 365.25 d), 1 g of ^{234}U will therefore dissociate (assuming constant rate) $3.458 \cdot 10^{20}$ molecules of UF_6 – see equation 7, where ζ is molecules of UF_5 produced per eV α-energy deposited (=0.01).

$$A \cdot E_\alpha \cdot t \cdot \zeta \sim 3.458 \cdot 10^{20} \tag{7}$$

Suppose a starting sample of HEU (typical of concentrations seen in Croft et al. [17]) pure UF_6 with a nominal isotopic composition of 1.2, 93 and 5.8 wt.% ^{234}U, ^{235}U and ^{238}U respectively, such U molar mass is 235.2064 g·mol^{-1}. Then, 1 g of ^{234}U corresponds to 83.33 g of U, and $2.13355 \cdot 10^{23}$ molecules of U. There is one U atom per UF_6 molecule, such the fraction, f, of UF_6 molecules dissociated is approximated by equation 8:

$$f \sim \frac{3.458 \cdot 10^{20}}{2.1355 \cdot 10^{23}} \sim 0.00162 \tag{8}$$

To first order (which is all that is justified given knowledge of the radiation chemical yield, *G,* value) this estimate can be scaled for other isotopic compositions and sample ages. The example chosen has purposefully illustrated the calculation to the extreme – most radiolytically active condition plausible. For recycled material ^{232}U also needs to be considered; even at the ppb level ^{232}U could contribute significantly to the *G* value because of its high specific activity (short half-life) relative to other present uranium isotopes. Additionally, it has roughly half a dozen α-particles in its decay chain. The calculation of the fraction, f in such cases requires a more careful temporal treatment to account for the decay chain kinetics.

From the earlier result (equation 6):

$$\frac{Y}{Y_{UF_6}} \approx (1-f) + f \cdot \frac{Y_{UF_5}}{Y_{UF_6}} \tag{9}$$

Inserting $f \sim 0.00162$ for the illustrative example and adopting $Y_{UF_5}/Y_{UF_6} \sim 0.927$ (from simple scaling rules [28][29]), this specific case $Y/Y_{UF_6} \sim (0.99988 \pm 0.00008)$ where the 1-σ uncertainty estimated by propagation of variance assumes a 20% and 5% relative standard deviation in the values of f and Y_{UF_5}/Y_{UF_6} respectively. Repeating the calculation for 2, 3, 4, and 5-year-old source material by manipulating the value of f, finds the fractional reduction in (α,n) production – see Table 2.

The choice of HEU was the extreme case (highest ^{234}U decay rate), and the samples studied by Croft et al. [17] are not very old from the date of the last liquid transfer. Therefore, the computed results demonstrate that the effect of radiolysis on composition is rather modest, and quite small compared to other sources of experimental uncertainty in (α,n) yield data from UF_6.

Age/ (y = 365.25d)	Y/Y_{UF_6}
1	0.99988 ± 0.00008
2	0.99976 ± 0.00016
3	0.99964 ± 0.00024
4	0.99952 ± 0.00032
5	0.99940 ± 0.00040

Table 2: Indicative fractional reduction in (α,n) production rate from a HEU sample with age based on the illustrative example discussed in text.

Utilising the preceding methodology developed to analyse the fractional reduction in (α,n) production rate, the allowable upper limits of the variables *G* and ^{234}U wt%, that would exceed defensible uncertainty [(1-σ) < 2%] stated by Croft et al. [17] can be determined analytically. The fraction of UF_6 dissociated into UF_5, f, is a function of the isotopic composition and ^{234}U- α-emission; suppose, a starting sample of nominal composition *'x',* 93, and *'z'* wt% ^{234}U, ^{235}U and ^{238}U respectively. The greatest dissociation will occur at z = 0 and serves as the upper limit of the notional extreme radiolysis scenario; at x = 7wt% – such z = 0wt% – f~0.00944, Y/Y_{UF_6} ~ 0.99931 and 0.99655 for 1- and 5-years storage respectively. Finally, the value of f required to exceed uncertainty is solved, making f subject with 0.98 < Y/Y_{UF_6}:

$$f < \frac{Y/Y_{UF_6} - 1}{Y_{UF_5}/Y_{UF_6} - 1} < \sim 0.274 \qquad (10)$$

The upper limits of a *G* value required to cause considerable uncertainty (using f = 0.274) is analysed by returning to the initial HEU starting sample composition – as mentioned earlier. Where *G* is required to compute the molecules of UF_6 dissociated – via equation 7 – its upper limits are found equal to 5.85127·10^{22}. The accompanying *G* required to provide so many dissociations in a single year is *G* > ~169 (= 338 molecules of F_2 per 100eV), or for 10 years storage a *G* > ~16.9. Both these values are entirely unreasonable to attribute to the production rate of UF_5 from UF_6 following the review of the available literature, from which it is clear *G* does not exceed 100 times less than this upper limit.

Extending the analysis to other hypothetical extreme cases (e.g. 7wt% ^{234}U in a pure UF_6, and *G* values many time that supported by experiment) simply reaffirms the conclusion that the impact of radiolysis on composition leading to a change in probability that an α-particle will undergo an (α,n) reaction in stored UF_6 is not significant.

Finally, for completeness, re-addressing the influence of concentrated ^{232}U in the reprocessing of SNF. The preceding methodology – see equation 7 – can be adopted for ^{232}U, taking E_α = 5.414·10^6 eV and $t_{1/2}$ = 68.9 years [27]; such, the specific α-activity is, A = 8.274·10^{11} Bq·g^{-1}. In one year (= 365.25 d), 1 g of ^{232}U will therefore dissociate (assuming constant rate) 1.414 · 10^{24} molecules of UF_6. The resulting dissociation is ~ 4 orders of magnitude greater than ^{234}U per gram of material. Neglecting $^{234,235,238}U$ dissociations, and taking a pure ^{235}U sample, for simplicity, other than the ^{232}U concentration. Beginning with a measured concentration of ^{232}U, equal to 1.4·10^{-6} g/ g ^{235}U – taken from pressurised water reactor (PWR) fuel with burnup between 15 - 60 MWd/ kg U [30]. Increasing ^{232}U concentration by an order of magnitude, calculations of the fractional reduction in (α,n) production rate over a 1-year timespan are presented in Table 3.

^{232}U g / ^{235}U g	U per g ^{232}U /kg	Y/Y_{UF_6}
1.4·10^{-6}	714	0.9999±0.00004
10^{-5}	100	0.9996±0.00002
10^{-4}	10	0.996±0.0002
10^{-3}	1	0.9598±0.00005

Table 3: Indicative fractional reduction in (α,n) production rate for a sample with increasing orders of magnitude for ^{232}U vs ^{235}U composition over a timespan of 1 year.

Ultimately, these calculations – table 3 – provide a preliminary understanding of self-induced radiolysis in UF_6 for recycled material – concentrated ^{232}U in the sample. Calculations conclude, that at realistic concentrations of ^{232}U, fractional reduction in (α,n) production rate is negligible. Further, finding that an increase in ^{232}U concentration to 1 g per kg U is required to observe radiolysis capable of exceeding uncertainty in passive neutron counting of UF_6. This increase is 3 orders of magnitude greater than the measured ^{232}U concentration in SNF. Thus, significant influence from ^{232}U radiolysis on composition of UF_6 in recycled material can be assumed to be negligible.

4. Conclusions

Recently attention has been focused on generating high quality (α,n) yield data from UF_6 to support the interpretation of verification measurements for international nuclear safeguards. An imagined concern was whether radiolysis can alter the chemical composition and affect the neutron production rate. Following a review of the available literature, the chemical yield, *G,* value adopted in this study was 0.5; such, one molecule of UF_5 produced per 100 eV of α-energy deposited – with a roughly estimated uncertainty of 20% at 68 % confidence. Using this value estimates of the (α,n) yield reduction in HEU as a function of age have been made – where the theoretical example is the most radiolytically active. Calculations display that the impact of radiolysis is not significant in the recent measurements performed to obtain high quality integral UF_6(α,n) nuclear data by passive neutron counting of UF_6 samples. Further calculations verify the conclusion using a hypothetical scenario of an unrealistically ^{234}U rich sample and error in current *G* values – both of which reinforce a negligible effect on composition resulting from radiolysis in realistic scenarios. Finally, this study analysed self-induced radiolysis of recycled material, with concentrated ^{232}U. Finding that for real SNF, ^{232}U self-induced radiolysis had negligible influence – requiring an increase of 3 orders of magnitude (equivalent to 1 g ^{232}U per kg U) to influence chemical composition above levels of uncertainty in (α,n) yield data.

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Declarations – Conflicts of Interest

On behalf of all authors, the corresponding author states there is no conflict of interest.

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Approach to Prioritizing Safeguardability Evaluation Parameters Using the Delphi Method and Analytic Hierarchy Process

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Abstract:

Newer nuclear facilities, such as small modular reactors and dry storage facilities for spent nuclear fuel, are expected to be constructed in the Republic of Korea. The safeguards by design (SBD) approach has been introduced to integrate nuclear safeguards and safety provisions in the earlier stages of nuclear facility design, enabling more effective implementation of safeguards in new nuclear facilities. Thus, the Korea Institute of Nuclear Non-Proliferation and Control has conducted extensive research on establishing domestic nuclear regulations to consider SBD in a new nuclear facility. This study analyzed the parameters used to evaluate the safeguardability of new nuclear facilities. First, we identified, analyzed, and compiled existing studies on the safeguardability evaluation of new nuclear facilities. Subsequently, among the compiled parameters, those applicable to regulations were identified using the Delphi method, where we surveyed a panel of experts to arrive at a consensus. We applied the Delphi method twice to determine the evaluation parameters, identifying the validity, reliability, and convergence of expert opinions. Further, the analytic hierarchy process (AHP) was used to prioritize the safeguardability evaluation parameters. From the AHP results, the experts deemed 'the use of nuclear materials verification equipment (NDA, DA) (0.123)' to be the most important parameter. Our findings can be used to develop a facility safeguardability analysis program that evaluates SBD for new nuclear facilities in the Republic of Korea.

Keywords: Nuclear safeguards, Safeguards by design, Delphi method, Analytic hierarchy process, Safeguardability evaluation parameters

1. Introduction

Nuclear facilities must implement appropriate safeguard measures because nuclear materials and related technologies can be used to produce nuclear weapons. The Nuclear Non-Proliferation Treaty (NPT) was adopted in response to international concerns about nuclear non-proliferation, and efforts to prevent nuclear proliferation continue through the International Atomic Energy Agency (IAEA). The IAEA applies safeguard measures to prevent the diversion and misuse of nuclear materials in nuclear facilities. These measures are customized to meet the specific needs of each facility. While changing the design of nuclear facilities can be costly and time-consuming, implementing safeguard measures from the design stage to ensure their effectiveness and efficiency is crucial. Safeguards by design (SBD) refers to the continuous review of the application of safeguard measures from the decision stage of introducing nuclear facilities to

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the conceptual design, preliminary design, design, and construction stages.

The IAEA promotes SBD when designing or constructing a new nuclear facility to apply the safeguards effectively and efficiently [1]. Research conducted in the early 2000s and led by the IAEA, the International Project on Innovative Nuclear Reactors and Fuel Cycles (INPRO), and Gen IV Forum's PR/PP WG, an expert group for proliferation resistance (PR) and physical protection (PP) of next-generation reactors, showed that SBD is the surest and most effective means of improving the proliferation resistance (PR) of future nuclear facilities [2,3,4]. In 2010, the Idaho National Laboratory in the United States developed practical measures to promote SBD as part of the Next Generation Safeguards Initiative (NGSI) Program of the US Department of Energy/National Nuclear Security Administration (DOE/NNSA) [5]. Bari Johnson proposed the Facility Safeguardability Analysis (FSA) process, which includes a toolkit for comparing existing nuclear facilities with safeguards in place to new facilities and suggesting safeguard approaches for the latter [6]. Additionally, various SBD methodologies have been applied to new nuclear facilities, such as spent fuel, dry storage, and pyroprocessing facilities [7,8].

Moreover, newer nuclear facilities are expected to be built in the Republic of Korea (ROK). The storage pools for spent nuclear fuel from light-water reactor nuclear power plants in the ROK have recently reached near saturation. Accordingly, considerable progress has been made toward constructing temporary dry storage facilities for spent nuclear fuel on nuclear facility sites in the ROK. Furthermore, several studies have been conducted in the ROK to develop various small modular reactors (SMRs), which are quite different from traditional nuclear facilities. In such situations, it is essential to collaborate closely with the designer, operator, national nuclear regulator, and the IAEA when designing or constructing new nuclear facilities.

Establishing a legal basis and evaluating the safeguardability of nuclear facilities are necessary when considering SBD. Having a legal basis for applying safeguard measures to new nuclear facilities from the design phase is highly efficient and effective. Additionally, evaluating the sufficiency of safeguard measures during the design and construction phases of new nuclear facilities is necessary.

However, previous studies have relied heavily on subjective evaluations by experts, with few proposing quantitative evaluation methodologies. This study examines existing safeguardability evaluation methodologies and the safeguard requirements and SBD guidelines of the IAEA. The study summarizes various safeguardability evaluation parameters and uses the Delphi technique and the analytic hierarchy process (AHP) to quantitatively convert the qualitative opinions of various experts.

2. Safeguardability evaluation parameters

First, it is important to note that safeguardability evaluation parameters refer to factors that can be used to assess how effectively and efficiently the design of a nuclear facility can be safeguarded by the IAEA. Several previous studies have proposed methods for evaluating the safeguardability parameters of nuclear facilities. This study aims to identify the key safeguardability parameters suggested by these earlier studies. This section provides a literature review of research related to safeguardability to compile a list of common safeguardability evaluation parameters that can be applied to new nuclear facilities.

2.1 Proliferation resistance evaluation methods

Proliferation resistance (PR) is defined as the characteristic of a nuclear energy system that impedes the diversion of nuclear material, undeclared production of nuclear material, or misuse of sensitive technology by states to acquire nuclear weapons. Various PR evaluation studies, such as Proliferation Resistance and Physical Protection (PR&PP) by the Generation IV International Forum (GIF), Technological Opportunities to Increase the Proliferation Resistance of Global Civilian Nuclear Power Systems (TOPS), and the International Project on Nuclear Reactors and Fuel Cycles (INPRO), have been conducted. In the early 2000s, the GIF PR&PP working group, led by the United States, began a study to improve nuclear PR. This was identified as a crucial factor in determining options for the next generation of nuclear systems. It has been confirmed that once the decision to deploy a nuclear system has been made, the only practical way to improve PR is to consider safeguards for the facility from the design stage. The methodology for assessing the proliferation resistance of the GIF PR&PP working group is a self-assessment conducted by the nuclear facility designer. The assessment is based on six scales: technical difficulty of proliferation, cost of proliferation, time to proliferation, type of nuclear material, probability of detection, and effectiveness of detection resources [2]. Safeguardability is a concept that replaces detection probability and detection resource efficiency in the GIF evaluation scale. This change aims to improve the qualitative assessment of safeguard effectiveness. The GIF PR&PP working group proposed 21 safeguardability evaluation parameters comprising three safeguards: design information verification, nuclear material accounting, and containment/surveillance. This study focuses on these 21 safeguardability evaluation parameters [3].

In 1999, the US DOE Nuclear Energy Research Advisory Committee (NERAC) formed a task force team on TOPS for technical research to increase the PR of nuclear power systems. This was aimed at quantitatively evaluating the PR of nuclear facilities by dividing them into physical, technical, and institutional barriers [9]. INPRO is a joint international project initiated by the IAEA in 2000 to develop guidelines to support future nuclear systems to meet the demand for sustainable energy in the 21st century. INPRO developed an evaluation methodology for nuclear power systems on a global, regional, and national basis for economics, industrial infrastructure, waste management, PR, PP, environment, and safety. Furthermore, they developed a set of requirements comprising a hierarchical structure of basic principles (BP), user requirements (UR), and criteria (CR) for each domain for evaluation [1].

We classified parameters related to (1) system safeguard design and (2) safeguardability evaluation and summary to derive the safeguardability evaluation parameters among the PR evaluation parameters of TOPS, GIF PR&PP, and INPRO.

2.2 IAEA safeguardability evaluation parameters

Safeguardability means the ease of applying and inspecting IAEA safeguards. The safeguards for achieving the safeguard goals of the IAEA include "nuclear material accounting" and "containment and surveillance." Therefore, to evaluate the safeguardability, we can evaluate and derive the applicability of the IAEA safeguard measures to determine whether the nuclear facility is designed to apply the technology and equipment of the IAEA for Nuclear Material Accounting (NMA) and Containment and Surveillance (C/S). The ease of IAEA inspection can be derived by evaluating the ease of safeguard application, whether the requirements for implementing the safeguards according to the safeguards agreement between the IAEA and the state are met, and whether ad-hoc, regular, and special inspections and Design Information Verification (DIV) inspections are executed effectively and efficiently [1]. Additionally, the IAEA offers overall guidance on safeguards during design and construction and facility-specific guidelines on design-based safeguards. The guidelines mainly aim to provide designers with recommendations that can be used during the design and construction phases. The guidance for each type includes an analysis of representative diversion/misuse scenarios and general design guidance for safeguard measures. These measures include containment, surveillance, monitoring, design information verification, material inventory verification, and metering. Safeguard-related considerations for designing specific points and critical points are also included. Best practices and implications based on experience with safeguards applied at similar facilities should also be considered [10].

This study focuses on the safeguard measures proposed in the guidance to derive the safeguardability evaluation parameters. The safeguardability evaluation parameters are a set of safeguard tools designed to prevent the diversion and misuse of nuclear materials in nuclear facilities during the design stage.

2.3 JRC safeguardability evaluation parameters

The safeguardability evaluation methodology developed as part of PR research is general-purpose owing to its inherent characteristics. Therefore, follow-up studies have been conducted in the United States and Europe as part of SBD research to cope with these problems. The Joint Research Centre (JRC) of the European Commission has proposed more safeguardability evaluation parameters (41 parameters total) than those proposed by the GIF to reflect the safeguard measures according to the strengthened safeguards, such as additional protocols. Furthermore, because all the evaluation parameters cannot be evaluated owing to the lack of available information at the beginning of the design phase of a nuclear facility, they proposed an evaluation methodology by classifying the design phase into three stages: (1) the design stage related to the basic inherent parameters; (2) the design stage related to safeguard installation equipment; and (3) the design stage related to the efficiency and effectiveness of safeguards [11]. Notably, the parameters identified in the JRC study are not limited to one safeguard measure but are included in multiple steps. This study leveraged the 41 safeguardability evaluation parameters of the JRC study.

2.4 KINAC safeguardability evaluation parameters

Lastly, KINAC has developed a safeguardability evaluation methodology to evaluate four safeguards (design information, NMA, verification, and C/S) over the three phases as part of the "development of evaluation methodology on future nuclear systems' proliferation resistance and physical protection" project, a nuclear safety research project initiated in 2013. The main features are (1) the safeguardability evaluation parameters were derived for the four safeguard measures, respectively, by improving the safeguardability evaluation parameters (comprising three safeguards—DIV, NMA, and C/S) proposed by the GIF, and (2) the factors that should be considered to improve the efficiency and effectiveness of executing safeguards were summarized separately by combining with the research results of JRC [12]. Therefore, the safeguard method by KINAC measures the evaluation parameters of 19 factors selected for analysis in this study.

3. Prioritizing safeguardability evaluation parameters

This study first used the Delphi technique to review the validity of the safeguardability evaluation parameters collected based on the results of previous studies summarized in Sector 2. Then, the AHP was used to determine the weights of the safeguardability evaluation parameters determined to be valid based on the Delphi survey. Alternatively, the AHP prioritized the safeguardability evaluation parameters. The Delphi method and AHP are often used in tandem in the decision-making processes. If the Delphi method evaluates the significance of each item by assigning fixed scores, the AHP can evaluate the relative importance of the derived items. In other words, the Delphi method can converge the opinions and judgments of experts to derive valid evaluation parameters, and the AHP provides a structured method for assigning weights to these parameters to further enhance the validity of the analysis [13,14,15,16,17]. The flow chart is shown in **Fig. 1**.

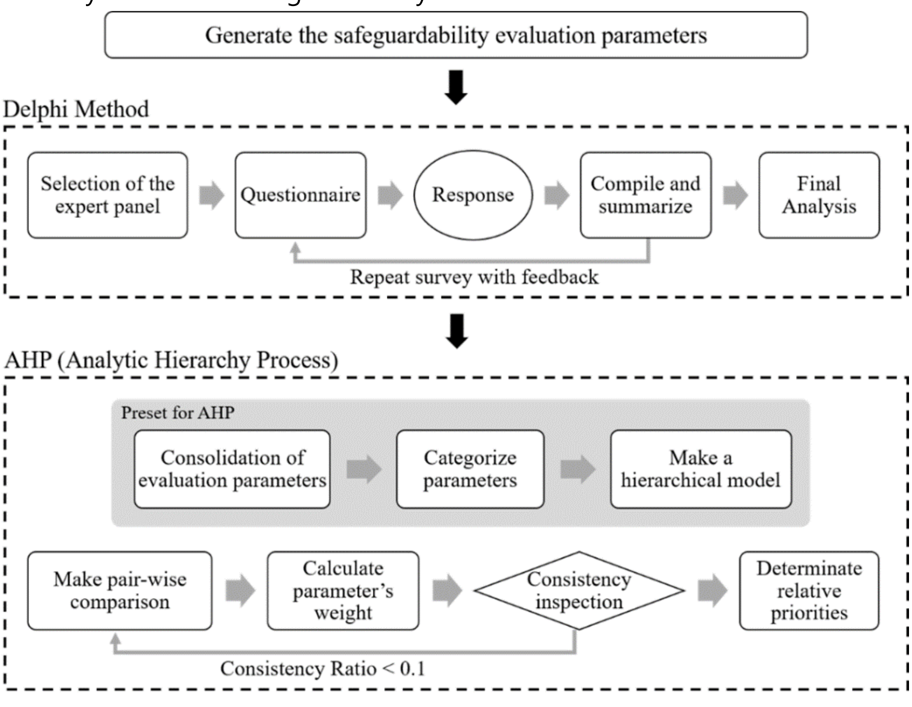

Figure 1. Flowchart of this study.

3.1 Delphi method

The Delphi method is an effective technique that can be used to make decisions through the consensus of expert opinions from a broader perspective by collecting various perspectives of relevant experts when decision-making based on objectified, accurate information is challenging [18]. Therefore, the Delphi technique is logically based on the principle of quantitative objectivity, which states that “the opinion of two persons is more accurate than that of one person,” and the principle of democratic decision-making, which states that “the judgment of the majority is more accurate than that of the minority” when there is no accurate information regarding the problem to be estimated. The Delphi technique reaches a consensus through repeated surveys of experts. Because the responses of each expert in each survey are anonymously disclosed to all other experts in the following survey round, one can revise, supplement, and then present their opinion based on other opinions. Narrowing down opinions through repeated feedback is the major characteristic of the Delphi technique. The main advantage of the Delphi technique is that experts who are difficult to gather in one place can participate simultaneously, the quality and reliability of information can be improved through the participation of experts, and opinions can be expressed freely with the guarantee of anonymity. Another advantage of the Delphi technique is that it can check and judge results roughly during the survey process. Given the limited number of previous studies that focus on prioritizing safeguardability evaluation parameters, we concluded that the Delphi technique, which leverages the knowledge of various experts, could be applied effectively [2, 3, 4, 5, 8]

Because the Delphi technique is aimed at deriving good results by relying on subjective and intuitive judgments based on confidence in the knowledge of experts, the selection and composition of the expert panel group are significant. This study targeted about 37 experts on safeguards in the ROK, including 16 safeguards inspectors at KINAC and 13 researchers with experience in safeguards. They also included five operators with safeguards experience at nuclear facilities, such as nuclear power plants in the ROK, and three university professors with research experience in safeguards. Before conducting the Delphi survey, a summary of previous studies on safeguardability evaluation, as outlined in Section 2, was provided to the experts to ensure a clear understanding of the prioritization of safeguardability evaluation parameters.

The parameters identified in previous studies were organized into 34 parameters, eliminating duplicates and combining similar parameters into one. Thirty-seven experts were then asked whether the parameters were appropriate for evaluating safeguardability. In the first round of the Delphi survey, the previous research cases on safeguardability evaluation parameters were shared to improve understanding before answering the questionnaire. The questionnaire was designed to evaluate the validity of 34 safeguardability evaluation parameters across three categories, as compiled through previous research. Participants were instructed to rate each factor on a five-point Likert scale, with 'very valid (5)' indicating appropriateness for evaluating safeguardability and 'very invalid (1)' indicating inappropriateness. Additional parameters could be added if deemed necessary by an expert.

From the opinions freely written by experts in the first round regarding the safeguardability evaluation parameters, we found suggestions that the meaning of each evaluation parameter should be clarified. These individual opinions of experts were reflected in the second Delphi questionnaire. In other words, we revised the sentences of three items to clarify the meaning of the safeguardability evaluation parameters and added five items. We asked about the validity of the revised 39 safeguardability evaluation parameters and presented all responses from the expert group in the first survey to compare with the second round of responses. The validity of the evaluation parameters was reassessed in the second round by the experts, using the results of the first round as a reference. The expert opinions were aggregated through two Delphi surveys conducted in August and September 2022, with the participation of 37 selected experts. The questionnaires were distributed and retrieved via email.

3.2 Delphi method results

The first and second Delphi survey results for the safeguardability evaluation parameters are as follows: **Table 1** shows the evaluation results of the experts on the validity of the evaluation parameters, including the mean value (M) and standard deviation (SD) of the expert answers on a 5-point scale. After the experts reviewed the validity of the safeguardability evaluation parameters, the standard deviation of each evaluation parameter generally decreased during the two rounds of the Delphi survey. Further, the coefficient of variation (CV) was checked to determine whether the expert opinions were increasingly consistent owing to the survey. The CV is a measure of how much the responses differ in the repeated survey process [19, 20], and it is calculated by dividing the standard deviation by the mean:

$$\mathrm{CV} = \frac{standard\ deviation\ (SD)}{mean\ value\ (M)} \tag{1}$$

Further, if the CV is less than or equal to 0.5, it can be inferred that additional surveys are not necessary [21]. In other words, the CV of the first and second surveys showed that the stability was less than or equal to 0.5, and thus, no additional surveys were necessary. The expert evaluations of the validity of each evaluation parameter were narrowed down to reach a consensus.

We calculated the content validity ratio (CVR) to assess the consensus of the experts in the second-round Delphi survey results [22]. Here, CVR refers to the quantification of the consensus of experts and is calculated using the following equation:

$$\mathrm{CVR} = \frac{n_e - \frac{N}{2}}{\frac{N}{2}} \tag{2}$$

where n_e is the number of experts who responded that it is valid, and in the 5-point Likert scale used in this Delphi survey, it refers to the number of respondents who answered "valid (4)" and "very valid (5)." Here, N denotes the total number of experts who participated in the Delphi survey. Lawshe and Ayre suggested the minimum value of CVR according to the total number of panelists, and if there are 30 or more panelists, the minimum CVR value is 0.33 [22]. The Delphi panel in this study involved 37 people, and it can be determined that the content is valid if the CVR is greater than or equal to 0.33. **Table 1** shows the expert evaluation results and CVR for each evaluation parameter.

Table 1. Delphi method results of the safeguardability evaluation parameters . Questions numbered 6, 7, and 33 include superscripts "a" or "b." Those marked with superscript "a" are from the first round, while those marked with superscript "b" are from the second round. Additionally, five evaluation parameters—24, 25, 37, 38, and 39—were added based on the feedback from experts in the first round.

(M: mean, SD: standard deviation, CV: coefficient of variation, CVR: content validity ratio)

Category	Safeguardability evaluation parameters		First round			Second round			
			M	SD	CV	M	SD	CV	CVR
Design information verification	1.	Is the design information completed in accordance with the IAEA DIQ format?	4.46	0.69	0.15	4.86	0.46	0.09	**0.91**
	2.	Can inspectors access essential equipment during the operation of the nuclear facility for visual verification?	3.85	1.06	0.28	3.95	0.56	0.14	**0.64**
	3.	Can inspectors access the nuclear facility during the construction process for visual verification?	3.77	1.01	0.27	4.09	0.67	0.16	**0.64**
	4.	Can inspectors access the nuclear facility to confirm the change in design information during the life of the facility?	4.27	0.86	0.20	4.32	0.55	0.13	**0.91**
	5.	Are the radioactivity levels at the access point and the route of the inspector minimized during design information verification?	3.85	1.03	0.27	3.91	0.67	0.17	**0.45**
	6.	Is there any equipment or information that restricts access to inspectors due to security reasons? [a)] Is there any equipment or information that restricts access to inspectors for safety or security reasons? [b)]	3.92	0.92	0.23	4.00	0.67	0.17	**0.55**
	7.	Can inspectors use 3D scanners for design information verification at the nuclear facility? [a)] Can inspectors use the latest technology such as 3D scanners for design information verification at the nuclear facility? [b)]	3.08	1.14	0.37	3.23	0.85	0.26	**- 0.36**
	8.	Are documents such as layout and drawings of a nuclear facility managed accurately and systematically?	4.31	0.77	0.18	4.36	0.64	0.15	**0.82**
	9.	Are the initial, final DIQ, and major changes in the design information submitted in a timely manner?	4.42	0.69	0.16	4.73	0.54	0.11	**0.91**
Nuclear materials accountancy	10.	Can non-destructive analysis (NDA) equipment from the IAEA be installed in a nuclear material storage facility for verification? (space for installing, power cable, and evaluation of the safety impact of the nuclear facility)	4.27	0.94	0.22	4.68	0.55	0.12	**0.91**

	11.	Can inspectors access nuclear materials to confirm NDA verification? (appropriate space, lighting, access path, and radioactivity levels)	4.38	0.79	0.18	4.55	0.66	0.15	**0.82**
	12.	Is it possible to install sampling equipment for destructive analysis (DA) in the nuclear material process or storage at the nuclear facility? (sampling port, sampling equipment space for installation, power supply, and evaluation of the safety impact of the nuclear facility)	4.08	1.00	0.25	4.41	0.78	0.18	**0.82**
	13.	Is the independence of the sampling equipment for safeguard measures achieved in the nuclear material process? (exclusive sampling port for inspection, system for transferring inspection samples, and storage facilities for inspection samples)	3.92	1.07	0.27	4.09	0.60	0.15	**0.73**
	14.	Is the accessibility of inspectors secured for sampling verification? (appropriate space, lighting, access path, and radioactivity levels)	4.27	0.76	0.18	4.18	0.72	0.17	**0.64**
	15.	Is there sufficient space to store NDA and DA safeguards equipment at the facility? (possibly for installing seals or monitoring equipment)	3.96	0.94	0.24	4.18	0.65	0.16	**0.73**
	16.	Does the nuclear material storage facility have sufficient space and lighting for inspectors to count items?	4.38	0.62	0.14	4.45	0.66	0.15	**0.82**
	17.	If nuclear materials are stored in two or more layers, can inspectors apply safeguard measures to verify the bottom layer or install seals?	4.23	0.64	0.15	4.23	0.67	0.16	**0.73**
	18.	Is there a tag or label attached to the nuclear material for item identification?	4.38	0.68	0.16	4.68	0.63	0.13	**0.82**
	19.	Is there an index attached to the nuclear material storage facility to easily locate the items?	4.04	0.76	0.19	4.36	0.64	0.15	**0.82**
	20.	Are the tags or labels for identifying nuclear materials designed to prevent easy removal or alteration and to maintain readability over a long storage period?	4.19	1.04	0.25	4.64	0.57	0.12	**0.91**
	21.	Can assembled nuclear material items be dismantled or reconstructed in the nuclear facility?	3.65	1.04	0.28	4.23	0.67	0.16	**0.73**
	22.	Does the nuclear facility periodically calibrate nuclear material measuring instruments and manage the uncertainty of measuring instruments?	4.38	0.96	0.22	4.73	0.62	0.13	**0.82**

	23.	What is the annual throughput of nuclear material in a nuclear facility?	4.04	0.85	0.21	3.91	0.85	0.22	**0.36**
	24.	What is the heat generation rate of the nuclear materials?				2.82	0.89	0.32	- **0.55**
	25.	What is the radiation dose rate of the nuclear materials?				3.18	0.94	0.30	- **0.18**
	26.	Can real-time nuclear material measurement and accounting systems be established?	3.62	1.08	0.30	3.82	0.83	0.22	**0.27**
Containment and surveillance	27.	Is it possible to install a containment device? (including seals to protect the device against damage and power supply)	4.65	0.48	0.10	4.77	0.52	0.11	**0.91**
	28.	Is there an independent or auxiliary power supply, such as an uninterruptible power supply (UPS), for the containment device?	3.73	1.13	0.30	3.95	0.82	0.21	**0.45**
	29.	Can inspectors access the containment and surveillance equipment for installation and verification? (access path of inspectors for attachment or detachment of seals and radioactivity levels)	4.46	0.57	0.13	4.68	0.70	0.15	**0.91**
	30.	Is the containment structure (such as walls) designed to have no path (hole) through which nuclear materials can pass?	4.42	0.84	0.19	4.64	0.77	0.17	**0.82**
	31.	Can inspectors verify the integrity of the containment structure (such as walls) of the nuclear material storage facility?	4.38	0.68	0.16	4.00	0.67	0.17	**0.55**
	32.	Can the installation of sealing cables be facilitated in the containment structures (such as walls) of the nuclear material storage facility?	4.08	0.87	0.21	3.95	0.56	0.14	**0.64**
	33.	Dose the containment structure (such as walls) is not designed to be drilled after construction? [a)]	3.73	1.13	0.30	4.50	0.66	0.15	**0.82**
		Can the containment structure (such as walls) be drilled after construction? [b)]							
	34.	Are the nuclear material movement paths and frequencies standardized to facilitate containment and surveillance?	4.23	0.75	0.18	4.36	0.71	0.16	**0.73**
	35.	Can surveillance equipment be installed? (including surveillance equipment to protect the device against damage, visibility obstruction, power supply, and lighting)	4.58	0.49	0.11	4.77	0.52	0.11	**0.91**
	36.	Is there an independent or auxiliary power supply, such as an uninterruptible power supply (UPS) dedicated to surveillance equipment?	3.92	1.03	0.26	4.09	0.79	0.19	**0.64**
	37.	Is surveillance equipment installation, such as power or communication cables and lighting, considered in the design?				4.18	0.83	0.20	**0.64**

	38.	Can containment and surveillance equipment be connected online for verification in real time?				3.91	0.95	0.24	**0.45**
	39.	Can an independent network be established to transmit safeguard information?				4.05	1.02	0.25	**0.64**

3.3 Analytic hierarchy process (AHP)

The AHP is an analytical method that creates a hierarchy when there are many evaluation standards or goals in the decision-making process. It decomposes the main factors and sub-factors forming the main factors and performs a pair-wise comparison to prioritize the parameters [23]. This method first hierarchically classifies various properties and then allows different experts to individually prioritize each property. Various parameters can be systematically prioritized using the AHP, and the weights can be extracted using the ratio scales.

The AHP helps determine the relative priorities among the lower-level parameters by comparing them one-by-one. Humans can identify relationships between observed objects; they can compare these objects using a certain standard by pairing similar objects together; and they can determine their preferences among the factors comprising the pair. The most significant advantage of the AHP is that it mimics this human behavior to calculate the weights of the parameters through pair-wise comparison in situations requiring complex decision-making. Calculating the priorities by considering different evaluation parameters simultaneously is not feasible. However, comparing these evaluation parameters in a 1:1 manner is simpler and can be conducted to establish a comparison matrix by utilizing the results of the pair-wise comparison.

However, a pair-wise comparison becomes difficult when excessive quantities of evaluation parameters exist in each structure. For example, when performing a pair-wise comparison of 14 safeguardability evaluation parameters, 91 ((14 × 13) ÷ 2) questions are generated. Thus, the consolidation of the existing evaluation parameters is necessary.

In the previous section, we conducted two rounds of Delphi surveys with experts to evaluate the validity of the safeguardability evaluation parameters. Throughout this process, the parameters were continuously revised and refined based on expert feedback. After the second Delphi survey, the CVR was calculated. With a CVR threshold set at 0.33, the results indicated that 35 out of 39 safeguardability evaluation parameters were deemed valid by the experts [22].

Among these 35 parameters, we consolidated those with common factors before proceeding with the AHP analysis. For example, the two safeguardability evaluation parameters ['can non-destructive analysis (NDA) equipment from the IAEA be installed in a nuclear material storage facility for verification?' and 'is it possible to install sampling equipment for destructive analysis (DA) in the nuclear material process or storage at the nuclear facility?'] were consolidated into one parameter ('use of nuclear material verification equipment') because both parameters evaluated the verification of destructive and non-destructive equipment for nuclear facilities.

Through this process, the 'Design Information Verification,' 'Nuclear Materials Accountancy,' and 'Containment and Surveillance' categories contained six, seven, and six evaluation parameters, respectively. The hierarchical structure of the evaluation parameters for the AHP is shown in **Figure. 2**.

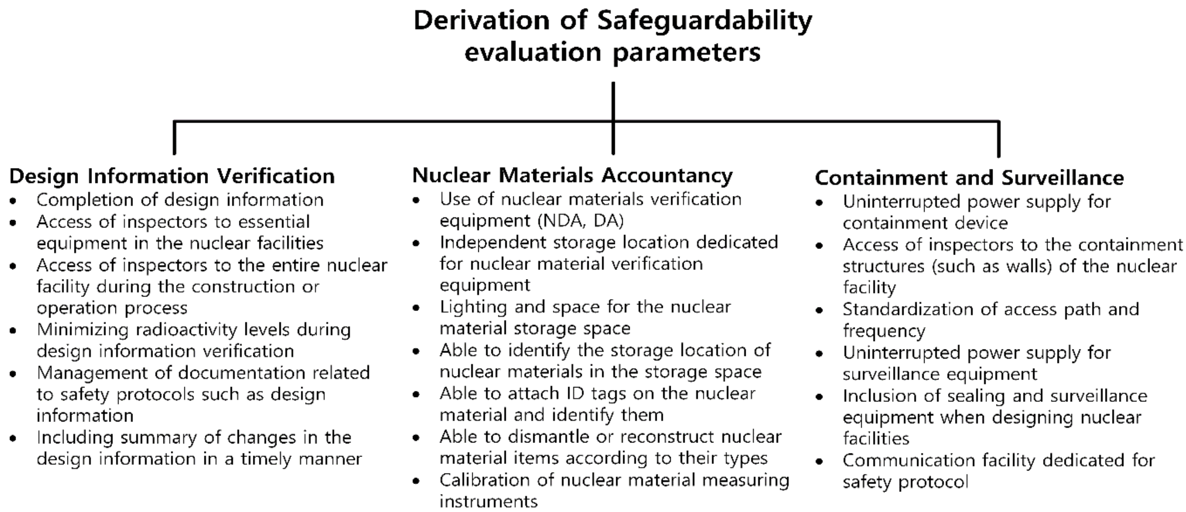

Figure 2. AHP hierarchical structure model for establishing the priorities of safeguardability evaluation parameters.

Based on the AHP hierarchical structure model, 37 safeguard experts who had participated in the Delphi-method survey were asked to evaluate the relative priorities of each evaluation parameter. The response percentage was 49% (18 responses). The experts first verified the lower-level evaluation parameters under the three upper-level categories ('Design Information Verification,' 'Nuclear Materials Accountancy,' and 'Containment and Surveillance') and assessed the relative priorities of the upper-level category. They then estimated the relative priorities of the lower-level safeguardability evaluation parameters for each upper-level category.

Ensuring that expert responses align with the AHP results is crucial for the accuracy of the evaluation. If inconsistencies were found in the responses, the experts were asked to review and adjust their answers. The Inconsistency Index measures how consistently the pairwise comparisons reflect the relative importance of different criteria, with lower values indicating more consistent judgments. The Random Index serves as a baseline for comparison, indicating the expected inconsistency in a random matrix. By comparing the Inconsistency Index to the Random Index, the Consistency Ratio is calculated. A Consistency Ratio of 0.1 or less is considered acceptable. If the Consistency Ratio exceeded 0.1, experts were asked to reassess their AHP evaluations. Only responses with a Consistency Ratio below 0.1 were accepted [24].

3.4 AHP results

In the AHP methodology, experts were asked to assess the relative importance of three primary categories, ensuring that the sum of their weights equals 1. Let C_i represent the primary categories, with the relative importance of each primary category denoted as $w(C_i)$, such that $\sum_{i=1}^{n} w(C_i) = 1$. Additionally, experts evaluated the relative importance of sub-categories S_{ij} under each primary category C_i, where the sum of the weights of the sub-categories under each category also equals 1, represented as $\sum_{j=1}^{m_i} w(S_{ij}) = 1$. The overall relative importance of each sub-category was then calculated by multiplying the relative importance of the primary category C_i by the relative importance of the corresponding sub-category S_{ij}, expressed as $w_{\text{total}}(S_{ij}) = w(C_i) \times w(S_{ij})$ [24].

Table 2 shows the detailed relative importance of the safeguardability evaluation parameters. First, the experts judged the upper-level category 'Nuclear Materials Accountancy (0.48)' to be more important than the 'Design Information Verification (0.25)' and 'Containment and Surveillance (0.27)' by a factor of 2.

Further, the significance of the lower-level parameters was investigated to determine the importance of the upper-level categories, and thus, the relative importance and priorities of all 19 safeguardability evaluation parameters were determined holistically. From the AHP results, the experts deemed the 'use of nuclear materials verification equipment (NDA, DA) (0.123)' as the most important parameter. Other parameters, such as being 'able to attach ID tags to the nuclear material and identify them (0.094),' 'calibration of nuclear material measuring instruments (0.078),' and 'inclusion of sealing and surveillance equipment when designing nuclear facilities (0.067),' were determined to be important as well. These parameters were necessary tasks for the IAEA inspector to verify the materials in the nuclear facilities. In comparison, parameters such as 'uninterrupted power supply for the containment device (0.033),' 'uninterrupted power supply for surveillance equipment (0.031),' 'independent storage location dedicated for nuclear material verification equipment (0.028),' and 'minimizing radioactivity levels during design information verification (0.015)' were not found to directly affect the activities of the inspector in the nuclear facilities.

Although the IAEA inspection can be performed efficiently and effectively if the 'uninterrupted power supply' and 'storage space location for nuclear materials' have been prepared beforehand for the nuclear facility, the absence of these parameters does not necessarily disturb the IAEA inspection process. Thus, among the safeguardability evaluation parameters, the experts determined that the parameters describing the tasks necessary for the IAEA inspection were more essential.

Table 2. AHP results of the safeguardability evaluation parameters

Higher elements (Weight of Category)	Sub elements (Weight of parameters)	Weight (Product of Weight of Category and Weight of parameters)	Rank
Design Information Verification (0.25)	Completion of design information (0.21)	0.053	8
	Access of inspectors to essential equipment in the nuclear facilities (0.23)	0.058	7
	Access of inspectors to the entire nuclear facility during the construction or operation process (0.21)	0.051	10
	Minimizing radioactivity levels during design information verification (0.06)	0.015	19
	Management of documentation related to safety protocols such as design information (0.14)	0.035	14
	Including summary of changes in the design information in a timely manner (0.15)	0.037	13
Nuclear materials accountancy (0.48)	Use of nuclear materials verification equipment (NDA, DA) (0.25)	0.123	1
	Independent storage location dedicated for nuclear material verification equipment (0.06)	0.028	18
	Lighting and space for the nuclear material storage space (0.13)	0.061	6
	Able to identify the storage location of nuclear materials in the storage space (0.13)	0.062	5
	Able to attach ID tags on the nuclear material and identify them (0.19)	0.094	2
	Able to dismantle or reconstruct nuclear material items according to their types (0.08)	0.038	12
	Calibration of nuclear material measuring instruments (0.16)	0.078	3
Containment and Surveillance (0.27)	Uninterrupted power supply for containment device (0.12)	0.033	16
	Access of inspectors to the containment structures (such as walls) of the nuclear facility (0.19)	0.05	11
	Standardization of access path and frequency (0.19)	0.051	9
	Uninterrupted power supply for surveillance equipment (0.12)	0.031	17
	Inclusion of sealing and surveillance equipment when designing nuclear facilities (0.25)	0.067	4
	Communication facility dedicated for safety protocol (0.13)	0.035	15

4. Conclusion

This study aims to derive safeguardability evaluation parameters for new nuclear power facilities. We reviewed previous studies related to PR and safeguards, and we extracted and compiled safeguardability evaluation parameters based on the review to derive the safeguardability evaluation parameters, classified into three categories: DIV, NMA, and C/S. In total, 39 evaluation parameters were compiled.

We conducted two rounds of the Delphi survey with a group of 37 experts to assess the validity of the safeguardability evaluation parameters. In the process, we continuously revised and supplemented the content of the safeguardability evaluation parameters by reflecting expert opinions. Through the opinion-gathering process, we calculated the CVR based on the results of the second Delphi survey. With the Delphi survey of 37 people, we can infer that the experts acknowledge the validity of the parameter when the CVR is greater than or equal to 0.33. The findings revealed that 35 out of the 39 safeguardability evaluation parameters had a CVR value of 0.33 or higher. In other words, 37 safeguard experts in the ROK confirmed 35 safeguardability evaluation parameters for new nuclear facilities.

The relative importance of each evaluation parameter was determined using the AHP. The AHP results demonstrated that the 'use of nuclear materials verification equipment (NDA, DA)' was the most significant parameter. Other parameters, such as being 'able to attach ID tags to the nuclear material and identify them,' the 'calibration of nuclear material measuring instruments,' and the 'inclusion of sealing and surveillance equipment when designing nuclear facilities,' were also deemed important. These are priority tasks to be performed by IAEA inspectors when verifying nuclear materials at nuclear facilities. Thus, experts classified the tasks necessary for the IAEA inspection as high priority among the safeguardability evaluation parameters and the items assisting the IAEA inspection as low priority.

The safeguardability evaluation parameters and their respective weights, derived in this study, are expected to serve as a tool for integrating safeguards into the design of new nuclear facilities. Designers and operators of nuclear facilities should prioritize parameters with higher weights, as these are the most critical for facilitating DIV, NMA, and C/S. Addressing these higher-priority parameters early in the design process ensures that key safeguard measures are incorporated efficiently. Regulators can also use the prioritized safeguardability parameters to assess the safeguardability of new nuclear facilities during the design and construction phases. If a regulator identifies a safeguardability evaluation parameter that is not adequately addressed, they can request improvements. Focusing on the most critical parameters first ensures that the safeguardability of the facility is enhanced from the earliest stages of design.

We intend to continue our research to develop the safeguardability evaluation program. The parameters and weights derived from this study will be used to develop the FSA program, where SBD can be checked and reviewed for new nuclear facilities in the ROK.

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Cognition-Informed Training for International Nuclear Safeguards

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Abstract:

Each year, the International Atomic Energy Agency (IAEA) spends a significant amount of resources on training incoming nuclear safeguards inspectors. A significant portion of this training is accomplished through the Introductory Course on Agency Safeguards (ICAS). While ICAS and other IAEA safeguards trainings are highly effective, lessons from cognitive science could be applied to safeguards training modules to enhance the successful application of learned skills in various operational environments. In this paper, we review and explain relevant cognitive science literature and provide safeguards-specific recommendations for explaining new concepts, practicing skills, developing effective training environments, reinforcing information, and performing effectively under stress. Many of these recommendations could be implemented with minimal disruption to current curriculum and training approaches. While our recommendations are tailored for safeguards training environments, many are broadly applicable to teaching and training environments spanning the nuclear materials management domain.

Keywords: international nuclear safeguards, cognitive science, human factors, training

1. Introduction

The International Atomic Energy Agency (IAEA) allocates a significant amount of resources to train incoming nuclear safeguards inspectors. One of the primary means of training new inspectors is the Introductory Course on Agency Safeguards (ICAS), a months-long, comprehensive course that seeks to give inspectors all the information and skills they will need to be successful safeguards inspectors. . It is crucial that inspectors be able to transfer new skills from a training environment to the field. While ICAS is highly effective at training safeguards inspectors, lessons and best practices from cognitive science could further enhance the effectiveness of transferring skills learned in training to the field environment, and can also apply to other training within the IAEA Department of Safeguards.

Transfer of training occurs when learned skills are applied successfully in the workplace. Here, we focus on training design and delivery mechanisms to enhance learning, memory, and ultimately transfer of training to the field. We review relevant cognitive science literature on best practices for explaining new concepts, incorporating practice into training, providing realistic training environments, presenting materials in a compelling and memorable way, supporting proper mindset through encouragement of students, and using

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technologies measuring physiological responses to gain deeper understanding of student learning and attention. For each of these areas, we provide distinct lessons relevant for international nuclear safeguards and provide explicit and actionable recommendations that could be considered to support safeguards training. Our intention is not to replace comprehensive reviews in these areas; for a more thorough review on the translation of cognitive and educational psychology practices into classroom strategies, see [1], [2], [3].

The length, depth, and classroom-style format of ICAS makes it a good candidate for implementing our recommendations to promote the transfer skills learned in a training environment to the workplace. Notwithstanding, safeguards inspectors and other safeguards staff participate in classroom-based trainings throughout their IAEA careers, and many of our recommendations are relevant for those training activities. However, this study does not include a comprehensive overview of safeguards training activities. While we did read relevant literature and interview several subject matter experts in IAEA safeguards training, we did not have access to full training materials or protocols that would have allowed us to provide specific recommendations to change current procedures. Instead, we offer recommendations that we hope the safeguards training community finds relevant, some of which may currently be employed

The paper is organized as follows. Each section provides a high-level concept: explaining, practicing, training environments, presenting materials, encouraging students, and measuring responses. For each section, we provide specific training recommendations with references to cognitive psychology literature and highlight how these recommendations could be applied in safeguards training environments.

2. Explaining New Concepts

Explaining new concepts refers to how trainers present new material to students. It primarily refers to oral explanations, such as classroom lectures. Cognitive psychology research has identified specific strategies that strengthen students' ability to remember new information, understand abstract concepts, and mentally organize new information. Some strategies for enhancing the explanation of new concepts include interleaving related material, relating explanations to in-field duties, providing cues for what is important, and cross-training members of a team.

2.1 Interleave related topics and practice opportunities during instruction to help students identify similarities and differences between concepts.

Interleaving is a strategy in which an instructor switches back and forth between related topics or between example problems and practice problems in a lecture. Interleaving helps students mentally organize information, discriminate between different types of problems or information, and understand the differences between concepts [4, 5]. Instructors can incorporate interleaving by making comparisons between a current topic of focus and a related topic studied previously [5]. In addition, studies have shown that students learn quicker when example problems are interleaved with practice problems [6]. Interleaving teaches students to discriminate between different types of problems or information and understand the differences between them [4, 5]. However, there is little evidence that switching between completely different subjects (such as between mathematics and language arts) is effective for learning; instead, interleaving focuses on similar problem types or solved example problems and practice problems when studying.

Safeguards training recommendations:

- Include intermittent practice opportunities in a lecture, for example with hands-on use of non-destructive assay methods that are being explained.
- Encourage discussion of similar concepts together, for example to compare different safeguards seals and the appropriate application and examination methods for each.

2.2 Explain the "why" or "how" of new information to develop a deeper understanding of new concepts.

Also referred to as elaborative interrogation or explanatory questioning, elaboration is the process of asking and explaining the "why" or "how" of a newly learned concept [5]. Researchers have proposed several possible explanations for the effectiveness of elaboration. One explanation is that elaboration improves learning by promoting the development of connections between new information and existing knowledge, which helps students mentally organize the information [5, 3, 1]. In the classroom, instructors may consider conducting elaboration exercises, in which they ask students to attempt to explain new concepts to themselves (such as writing down an explanation) or to their peers in small groups. However, elaboration is only effective if students' explanations of new concepts are accurate, so it is important that instructors monitor student discussions and provide correct information about new concepts following elaboration exercises [5]. Elaboration may also cause students to slow down while reading and pay more attention to the information being presented [3].

Safeguards training recommendations:

- Continue to present new information within relevant context of its importance to a particular technical objective or to the overall safeguards regime.
- Offer opportunities for safeguards inspectors to engage in explaining concepts as a form of learning and knowledge-check (i.e., correction by trainer if the explanation is incorrect). Self-check opportunities can also be used to provide feedback without pressuring inspectors in front of their colleagues.

2.3 Relate training activities to in-field duties.

Training is more effective when students perceive that what they learn during training will help them perform their jobs or improve their job performance and that the training is relevant to actual workplace tasks. Helping students understand how a training activity relates to job tasks will motivate them to learn the target skill or apply it in the workplace. Training programs could begin with information about how and why the training is relevant to motivate students to pay attention and apply trained skills [7, 8].

Safeguards training recommendations:

- Relate training information to in-field and other safeguards verification tasks by providing context for the overall safeguards mission area.

2.4 Provide examples to explain difficult or abstract concepts.

Illustrating abstract concepts with specific examples helps students understand new ideas [6]. Examples can convey information more concisely and concretely than abstract concepts [5]. Associating an abstract concept with a concrete example can help students recall information, especially with the use of concrete examples that accurately illustrate the concept being taught to avoid confusion.

Safeguards training recommendations:

- Provide specific safeguards scenarios or examples as illustrations of difficult concepts. For example, when discussing the protocol for taking environmental swipe samples, describing the ramifications that would result from cross-contamination of swipe samples could facilitate learning.

2.5 Present materials in multiple formats.

Contrary to popular belief, teaching to an individual's preferred "learning style" (visual, auditory, verbal, and kinesthetic) does not result in better learning outcomes. Instead, all students benefit from being presented material in multiple formats [9, 10, 11, 12]. This concept is related to dual-coding theory, in which words are combined with visuals or other sensory information to enhance learning and memory [12]. Text is most often combined with visuals since images are easier to remember and they convey information more succinctly than text [5, 13, 14]. Dual-coding can help students understand complex processes or systems that would be difficult to understand with only a verbal description. Furthermore, delivering instructional materials in multiple formats can eliminate potential monotony from lectures and maintain audience attentiveness, thereby increasing the ability of students to sustain attention on the lecture [15]. Multiple formats might also support a diverse population of students with varying levels of proficiency in the presentation language.

Safeguards training recommendations:

- Safeguards trainers may consider providing examples in various media forms, such as images, text, video, spoken words, and physical objects, if applicable.
- Present safeguards training information in mixed-media formats, with a focus on audio supported by text.

2.6 Use multimedia elements effectively to reinforce learning.

One way to present in multiple formats is by incorporating multimedia elements such as slideshows, images, and videos into lectures to help students organize information, see examples, and understand processes. Multimedia instruction often involves presenting information in more than one modality at once, but excessive amounts of information presented simultaneously can result in cognitive overload and inhibit learning. Reinforce auditory information with complementary visuals to avoid overloading the audience with text. For example, an animation that also includes on-screen text descriptions overloads visual channels as the student must split their attention between the animation and the text. Swapping on-screen text for auditory narration can reinforce, rather than undermine, learning taking place through visual channels [16, 17].

Safeguards training recommendations:

- Break presentations into segments to allow inspectors time to process and organize information. For example, present information in text form and then show an illustrative animation or image on the next slide [16, 17]. The ideal split will be driven by the concepts to be learned: diagrams with short text labels may be helpful for learning the components of a system, whereas animations with spoken descriptions may be more helpful for learning a new process [18, 19].
- Present corresponding material for a specific safeguards concept together, but do not add extraneous information in the process. Remove irrelevant examples, large amounts of text from slideshows, background music, and text descriptions that do not match narration in videos [16].
- Use human voices rather than computer-generated voices when presenting information, as people learn better from real human voices than from synthesized voices [17, 20].

2.7 Provide students with information about components of a system prior to teaching the system.

When learning about new systems, it is important that students learn the functions of the individual components comprising that system before trying to understand how those components work together to make the system work. For example, it would benefit a student to learn the name and function of computer parts before they attempt to build a computer. Pre-training allows students to understand causal links and complex processes [16].

Safeguards training recommendations:

- Provide reading, videos, or other content to safeguards inspectors to preview prior to the start of related class sessions.
- Introduce new concepts with reminders about the component pieces and how they fit into a broader safeguards concept.

2.8 Provide cues about how to select and organize important information.

Indicate what information is important and how new information fits with previously learned information to help students prioritize and organize knowledge. For example, include an agenda or table of contents to show how information is categorized, use headings to indicate main ideas, highlight the most important points or reiterate them using more than one modality (e.g., through text and narration), write main ideas on a board, or provide an outline of the most important topics [16, 17].

Safeguards training recommendations:

- Provide notes pages with main topics and important safeguards definitions already included.
- Describe learning objectives at the start and end of safeguards training modules to ensure key concepts are identified.

2.9 Present examples or instructions conversationally, in relation to the student.

Using conversational language helps students learn and remember information because such language personally connects the student with new material. For example, say, "When you use this piece of equipment, you have to calibrate it first to make sure your readings will be accurate," instead of, "This piece of equipment must be calibrated prior to operation to ensure accurate readings" [17]. An overview of studies indicated broad findings that that content presented in a conversational style compared to a formal style increased performance for information retention and transfer [21].

Safeguards training recommendations:

- Use a conversational, but professional, tone.
- Present material in the first or second person ("I" and "you"), as opposed to the third person ("one, he, she").

2.10 Teach members of a team about their teammates' roles and responsibilities to create more communicative and effective teams.

Cross-training is a training strategy in which every member of a team is trained in the duties of their teammates such that each team member understands the others' roles, tasks, and responsibilities [22]. The goal of cross-training is to create teams that can communicate, coordinate, anticipate each other's needs, and assist each other effectively. Studies have found that two- and three-person cross-trained teams outperformed non-cross trained teams by engaging in more teamwork behavior, communicating more effectively, having higher success rates on team based-tasks [23, 24], and developing shared mental models [25].

Safeguards training recommendations:

- Train all members of inspection teams on all tasks that might be required.
- Training across safeguards tasks could also be considered for non-inspector participants in safeguards verification activities, such as analysts or technicians that support inspection efforts.

3. Practicing

Practicing refers to opportunities for students to apply their new knowledge or skills in a supervised way. The repetition and course-correction that occurs while students practice target skills increases students' ability to perform effectively outside of training environments. Practicing can include hands-on activities, practicums, or applications, as well as classroom discussions. It can also include more formal mechanisms of practice such as quizzes and exams.

3.1 Provide opportunities to practice information recall.

Retrieval occurs when a student recalls a piece of information. Practicing retrieval by drawing information from long-term memory into working memory strengthens knowledge of that information [5]. For this reason, tests and quizzes can enhance one's knowledge while checking for successful retention of information [26]. Students tested more than one time retain more information long-term than those that are tested only once [27]. To enhance this effect, instructors could give students a series of quizzes prior to a final exam to give students multiple opportunities to practice retrieval. Furthermore, providing feedback on quizzes and tests promotes learning because students have an opportunity to review and learn from mistakes [26].

Safeguards training recommendations:

- Encourage self-testing, such as by creating flashcards, for inspectors to practice retrieval and discover what they know and what they do not know. Best practice for self-testing with flashcards includes practicing with both sides of the cards (concept and definition, for example), and shuffling after each run-through of the deck.
- Provide low-stakes opportunities for inspectors to practice retrieving information, such as through quizzes or discussions that include feedback, so they can identify concepts to review. The use of game-like elements to support learning objectives has also been shown to increase learning outcomes (though, typically only small increases) and could provide low-stakes and engaging opportunities for practice [28].

3.2 Give students opportunities to observe and practice skills.

Observation and practice are critical for learning and remembering new information and skills [7]. During training, explanations of the behaviors to be learned can help students understand new behaviors and skills. This could include the trainer displaying effective and ineffective implementation of target skills (i.e., what to do and what *not* to do) and providing students with opportunities to practice and receive feedback on those skills.

Safeguards training recommendations:

- Demonstrate correct and incorrect execution of desired safeguards skills.
- Provide opportunities for safeguards inspectors to practice new skills with oversight and feedback from trainers.

3.3 Space practice over time.

Spaced practice involves revisiting previously learned information multiple times over the course of several days, weeks, or months. Distributing learning over several days significantly increases the amount of information that a student will retain compared to presenting the information in one learning session [27]. Spaced practice results in longer-term retention of information, likely because revisiting information at different times strengthens a student’s ability to retrieve that information from memory [5]. Practice can also continue once the training period is over, for example through opportunities for continued learning, skill maintenance, and long-term goal setting, that will help students maintain their skills.

Safeguards training recommendations:

- Review prior, related content at the start of new lesson modules to provide multiple spaced exposures to safeguards information.
- Provide homework or external assignments that require inspectors to draw on prior information.
- Interleaving safeguards concepts (e.g., differences between seal types) can give inspectors multiple opportunities to learn concepts within a lesson.

3.4 Allow students to make and correct mistakes during training.

Error management is a strategy in which students are permitted to make mistakes during training. Instructors help students learn from their mistakes by correcting them, informing them of other errors that could occur, and describing the negative consequences of errors. Error management facilitates transfer of knowledge by teaching students how to anticipate issues before they arise and to manage problems if they occur [7].

Safeguards training recommendations:

- Provide opportunities for supervised practice, which can include reinforcement or corrections on a new skill. This could include supervised practice using safeguards equipment, applying or examining safeguards seals, or other important inspection tasks.
- Include low-stakes opportunities for inspectors to practice and fail in order to correct skill performance or recall through additional support from trainers. These low-stakes opportunities include supervised practice opportunities, self-testing, and working with small peer groups in which participants can support each other in mastering a skill.

3.5 Train critical skills for high anxiety scenarios repeatedly.

Increased anxiety (e.g., time pressure, threat of personal harm) in a situation can change decision-making, causing people to make faster and less accurate decisions [30]. This has been found in settings as varied as parachute jumps, piloting an aircraft, simulated firefighting (reviewed in [31]) and simulated police settings [29]. In high stress situations, people tend to fall back on overlearned strategies that they can pull from long term memory [31]. While experts often perform better under high stress situations [32, 33], both experts and novices have been shown to have degraded performance in high stress situations that require a creative response.

Safeguards training recommendations:

- Anticipate high stress scenarios and provide extra training on critical skills needed to mitigate those scenarios. This could include things like safeguards equipment troubleshooting, safety procedures, or emergency protocols.

Other training procedures to support stressful environments are covered in Section 4.

4. Training Environments

IAEA safeguards inspectors are likely to experience moderate levels of stress during inspections. They may face fatigue from lengthy travel and jetlag, discomfort from heat or noise within a facility, and high workload and time pressure from a long list of inspection tasks. Despite the presence of stress, inspectors must perform at consistently high levels. Training to prepare for stress may support this high-performance requirement.

4.1 Train in environments that resemble the field.

Trained skills are more likely to transfer to the workplace when the training environment closely resembles it. Having the training environment mirror the workplace helps students contextualize scenarios in which new skills may be applied in the workplace. Methods to create realistic training environments include the provision of training opportunities in the field and the incorporation of field-relevant environments (such as location, noise, or time pressure) [7].

Safeguards training recommendations:

- Continue to provide in-field training opportunities at realistic or operational nuclear facilities.
- For classroom-based training, include field-relevant environments related to time constraints, space restrictions, operator negotiation, or other relevant elements. These elements could be as simple as introducing timed practice for seal examination and application exercises, or more complex and realistic scenario-based training.

4.2 Educate students on factors that may impact their performance in the field such as performing repetitive tasks, multi-tasking, and sleep deprivation.

When people must perform a low-effort, sustained monitoring task over a long period of time, performance of that task declines [34]. However, some promising work has shown that briefly switching to a different mental operation can offset these detrimental effects [35]. One theory is that the ability to pay attention to one task over time can be "reset" by this brief task-switch. It is also well known that trying to multi-task, or perform multiple similar operations at once, can hurt task performance. This is true both in simple laboratory tasks [36] as well as in real-world situations, like using a cell phone while driving [37]. For a review of factors that could affect the performance of safeguards practitioners, see [38].

Safeguards training recommendations:

- Include a training module on factors influencing safeguards inspection performance, and support inspectors on being able to assess their own state-of-being.
- Provide information on mitigation strategies for performance inhibitors that are common for safeguards inspections such as jetlag, multitasking, or time pressure.

4.3 Educate students on the effects of environmental stressors and mitigation techniques.

The environment in which someone is working can significantly impact their performance. Environmental stressors like noise [39, 40] and temperature (extreme heat [41] or cold [42, 43]) can degrade performance on certain tasks. In some cases, individuals can take action to reduce environmental stressors that can improve their own performance. For example, studies of noise and performance have found that reducing noise levels in work settings improves productivity [44] and reduces human error [45], accidental damage to material and absenteeism [46], and workplace accidents [47, 48].

Safeguards training recommendations:

- Include education on environmental stressors and their impacts on performance, with the aim to help inspectors identify when they are in scenarios of potentially compromised performance. This will allow inspectors to better judge their own ability to complete tasks and request help from their inspection team as needed.

- Include potential mitigation strategies for safeguards inspection environmental stressors, such as using disposable ear plugs, orienting tasking according to temperature (e.g., working outdoors early on a hot day, and moving to indoor tasks during hotter parts of the day, and vice versa for cold climates), and knowing what accommodations they can seek from facility operators regarding environmental conditions.

4.4 Expose students to field-relevant stressors during training.

Stress inoculation training (SIT; also sometimes called stress exposure training) is a targeted three-phase training approach intended to teach individuals about stress and how to manage it [49]. SIT is organized into three phases: In Phase 1, students learn about stress effects and stressors they are likely to encounter in the workplace; in Phase 2, students learn techniques to cope with stress; in Phase 3, students practice using coping skills in increasingly stressful environments [50]. The objectives of SIT are to increase students' familiarity with stressors and stress symptoms, teach them skills to overcome stress effects, and build confidence in their ability to perform at a high level despite stress [50]. SIT has been shown to improve performance in real-life high-pressure situations, such as law enforcement settings [51].

Safeguards training recommendations:

- Implement aspects of SIT into safeguards inspection training. Headquarters-based training could include Phases 1 and 2, to identify stressors and learn techniques to cope with them. Field activities, such as APEX training, are good candidates for Phase 3 practice (and to the authors' understanding, is currently being used this way).

4.5 Create immersive training environments via augmented reality (AR) and virtual reality (VR) to replicate settings that would be too unsafe, costly, or otherwise untenable for in-person training.

Augmented reality (AR) refers to an immersive visual environment in which digital displays are superimposed over images of the participant's actual environment; virtual reality (VR) refers to a fully immersive 3D display, generally blocking out all elements of the real world. The use of AR/VR in training environments could have many potential benefits, including offering immersive, safe, and low-cost ways to expose people to high-risk or otherwise difficult-to-replicate environments during training, under the assumption that training in such environments will enhance transfer of the learned skills to the real-world environment (for review, see [52]). Some potential drawbacks of AR/VR for training include the cost of equipment and development of the virtual training environment, the inability to collaborate with others in real time, and the limited range of motion permitted by many AR/VR setups. Additionally, the quantitative benefits of AR/VR training to real-world performance remain unclear. In a recent meta-analysis, Kaplan et al. [53] found equally good task performance in real-world settings following AR/VR training and traditional training across a variety of cognitive and physical tasks.

Safeguards training recommendations:

- Have new inspectors practice performing inspection tasks in a simulated environment first, such as a new unfamiliar facility, or a more complicated facility than one they have previously visited. Having the opportunity to practice inspection tasks in these varied environments may help them to learn and/or remember the steps better than simply reading about it in the classroom or watching a video.
- Replicate stressful aspects of the real environment that inspectors may encounter via AR/VR, following the research that learning under stressful environments likely improves recall in a real-world stressful environment. In these cases, environmental stress could be caused by issues such as equipment malfunction, uncooperative facility operators, or a safety incident.

5. Encouraging Students

Motivation refers to a student's desire to learn a new skill or reach a goal. Motivation is closely linked to self-efficacy, which is a person's confidence in their abilities. Students with higher self-efficacy believe that they can learn new skills and that learning new skills will result in positive outcomes or benefit them in the workplace [7]. Building appropriate self-efficacy supports student learning.

5.1 Promote trainees' confidence in their abilities.

A student's belief in their ability to learn and apply new skills is strongly linked to positive training outcomes. Students with higher confidence in their abilities are more likely to persevere despite challenges, while those with lower confidence are likely to be discouraged by challenges and reduce effort. Self-efficacy can be developed through skill mastery (practicing a skill to increase comfort level), modeling (watching others perform a skill so that it becomes more predictable and makes sense in context), encouragement, instruction, feedback from instructors, and post-training goal setting [7, 54, 8]. Giving positive feedback when students perform a skill correctly reinforces the skill and can increase trainees' beliefs about their competency with a skill [55]. Goal setting can also increase self-efficacy by giving students specific benchmarks to work toward and the ability to self-monitor their progress. Strong goals are specific to the trained skill, and are challenging but attainable [56].

Safeguards training recommendations:

- Give positive feedback and supportive corrections to inspectors as warranted by their performance.
- Provide multiple opportunities for inspectors to practice, fail, and correct their performance through hands-on activities and classroom exercises.

5.2 Encourage peer support.

Peer support has been found to be just as impactful on student development as supervisor support [7, 8]. Peers can provide each other with encouragement, feedback, coaching, and behavior modeling, and play a significant role in a student's transfer of training to the workplace.

Safeguards training recommendations:

- Encourage inspectors to work together on problem-solving.
- Provide opportunities for inspectors to recognize the strengths and accomplishments of their peers.

6. Measuring Physiological Response

Specialized techniques can be used to assess learning and/or enhance training by collecting physiological data during task performance. Physiological data refers to data collected about the body (e.g., heart rate, brain activity) that can be used to infer something about cognition. These physiological measures can provide a way to study aspects of cognitive processing during performance, without asking the individual to stop and respond to questions. When collected together with behavioral data, these measures can be used to both understand and enhance training and performance. Selected technologies are described below based on their relatively easy implementation in operationally relevant environments. Because the technologies discussed below require cognitive science expertise to execute in the proper experimental settings and interpret the data appropriately, we do not recommend these technologies for immediate implementation for international safeguards training. Instead, we highlight these techniques to demonstrate that it is possible to measure trainees' stress levels, cognitive load, learning, and focus during training. This data could be used in the future by safeguards trainers to identify challenging or stressful training tasks that may require additional practice.

- **Electrodermal activity (EDA)**, a physiological measurement of the electrical conductance of skin, can give insights about a person's psychological state in response to a stressor [57, 58]. EDA could be used in safeguards training to identify training scenarios that produce stress in trainees for the development of stress-reducing interventions.
- **Heart rate (HR**) and **heart rate variability (HRV)** can be used to measure cognitive workload and fatigue [59, 60, 61, 62]. For safeguards training, HR and HRV measurements could be used to assess workload demands of a particular tool or procedure.
- **Eye-tracking** is used to measure the eye gaze location of people performing visual tasks, such as reading, viewing an image, or using an interface [63, 64, 65, 66]. Novice safeguards inspectors could study the eye gaze behaviors of senior inspectors to identify task-relevant areas to focus their attention on and learn which cues experts use to guide their attention during difficult tasks.
- **Electroencephalogram (EEG)** is the measurement of brain electrical activity using electrode sensors placed on the scalp, and event-related potentials (ERPs)are portions of the EEG signals that are time-locked to specific stimulus events [67, 68]. EEG and ERP data could help trainers

identify safeguards tasks that produce higher cognitive workload – and are therefore more difficult to learn – and design trainings that give extra practice time for more challenging tasks.

7. Conclusion

In this work, we highlighted specific training techniques that cognitive psychology research has identified as having positive effects on the transfer of training and described how these techniques could be applied to international nuclear safeguards training environments. Many of these techniques could be implemented in existing training programs like ICAS for minimal cost and could significantly increase students' knowledge retention and transfer of training from the classroom to the field. In particular, giving students opportunities to practice target skills, spacing exposure to materials over time, delivering material in multiple formats, and exposing safeguards staff to some stressors during training could significantly improve learning and knowledge retention. By making small changes to the ways that they explain information, present materials, and set up training environments, trainers can improve the effectiveness of their trainings and set up students for greater successin the workplace.

Other valuable contributions that support learning and human performance could come from domains such as social psychology and anthropology. Future studies should address lessons from these domains, as well as deeper analysis of current safeguards training practices to provide the most actionable recommendations.

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