Project partners

Project Owner

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Enterprise number	
Partner's role	Both research activity and financing

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Project participants

First name	Last name	Institution/company
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Project info

Project title

Project title	AICCA - Artificial Intelligence for Creating Control Architectures

Primary and secondary objectives of the project

The primary objective of AICCA is to leverage generative AI to create control structures. The secondary objectives are:
-Develop AI models to capture and extend the knowledge in ARC
-Compile a substantial, reliable dataset of expert-generated control structures.
-Create effective representations of control structures.
-Develop novel graph-modified neural network structures.
-Develop advanced training techniques.
-Incorporate human expertise to evaluate and refine AI-generated control structures.

More details, including conditions for how these secondary objectives will be considered met, are given in the attached project description.

Project summary

AICCA aims to leverage generative AI to develop a novel "ChatGPT for control structures" that can generate on-demand control structures for specific industrial cases and includes evaluation by human experts before implementation. This will streamline the design process of control structures and enhance industrial operations' efficiency, safety, and sustainability. Three main challenges need to be addressed to realise such a tool; i) proper training of generative models will require access to a substantial database of pre-trained data, which is currently missing ii) there are currently no suitable machine learning methods to effectively model the unique characteristics of control structure design and iii) methods for explainability and transparency, including human-in-the-loop mechanisms are needed to adopt AI-generated control structures in safety-critical and regulated applications. AICCA is designed to meet these challenges by adopting control systems theory, machine learning, and graph theory. More specifically, the project will use advanced machine learning techniques, particularly Graph Neural Networks for capturing process systems' complex relationships and dependencies. AICCA will furthermore integrate AI-generated models with process simulators to create a reinforcement learning loop, where also ranking by human experts will serve as an additional metric in the reinforcement learning layer. This method will continuously improve the accuracy and reliability of the generated control structures, representing a significant advancement in the application of AI in process control engineering. Case studies will be conducted at two industrial stakeholders to implement and validate AI-generated control structures. In this way the project has the potential to bridge the gap between machine learning and control systems engineering by developing graph representations for control structures and maintain critical expertise in control structure design.

Outcomes and impacts

Potential for academic impact:
AICCA aims to advance process systems engineering by introducing AI-driven methodologies for control structure generation, and will address important scientific challenges, including i) Integration of AI and Control Theory through Graph Representations, ii) Advancement of Graph Neural Networks and iii) Preservation of Expert Knowledge for Educational Purposes.

Potential for societal impact:
AICCAs approach to automating control structure design have the potential to meet societal challenges by enhancing efficiency, cost reduction, safety, and sustainability in industrial processes. AICCA will mitigate the impact of the declining number of ARC experienced professionals and preserve expertise, and have the potential to uncover novel control structures, fostering innovation in process control engineering.

For each project output, the project has a defined exploitation strategy with associated dissemination activities with identified target groups.

Funding scheme

Funding scheme - supplementary info from applicant

Programme / activity	FRIPRO

Application type	Researcher Project

Topic

Thematic Area	Topic
Ground-breaking research	Ground-breaking research

Classification of scientific disciplines

Filter by subject field	Filter by subject	Discipline
Teknologi	Informasjons- og kommunikasjonsteknologi	Teknisk kybernetikk
Teknologi	Kjemisk teknologi	Kjemisk prosessteknologi

Other relevant programmes/ activities/projects	
If applying for additional funding, specify project number	
Is this proposal related to other grant applications or ongoing projects allocated support from the Research Council and/or any other public funding scheme?	No

Progress plan

Project period

From date (dd.mm.yyyy)	31.05.2025
To date (dd.mm.yyyy)	30.10.2029

Main activities and milestones in the project period (year and quarter)

	Milestones throughout the project	From	Quarter	To	Quarter
1	WP1 Dvelopment of representations	2025	2	2027	1
2	D1.1 Dataset established	2025	2	2026	2
3	D1.2 Graph representations established	2025	3	2027	1
4	D1.3 Design features identified	2026	2	2028	1
5	M1: Effective representations established	2025	3	2026	4
6	WP2 Generative Models	2026	4	2028	4
7	D2.1 Generative model based on enhanced GNNs	2026	4	2027	4
8	D2.2 Benchmarking performed	2027	2	2028	3
9	D2.3 Advanced training techniques implemented	2027	4	2028	4
10	M2 Viable control structures established	2028	2	2029	4
11	WP3: Simulators and Expert Evaluation	2027	2	2029	3
12	D3.1 Process simulators integrated	2027	1	2029	3
13	D3.2 RL framework integrated	2027	2	2029	4
14	D3.3 Human-in-the-loop integrated	2028	3	2029	4
15	D3.4 Explainability-transparency integrated	2028	3	2029	4
16	D3.5 Industrial case studies implemented	2028	4	2029	4
17	M3 Control structures validated	2028	2	2029	4

Dissemination of project results

The attached project description provides an overview of key activities contributing to realisation of the potential impacts of the project outputs in AICCA`s, including exploitation strategies, dissemination/communication activities, and target groups. Here, the planned dissemination/communication activities connected to each expected project output are described in more detail:

Project output: AI tool for generating control structures:
Diss/comm: Conferences, industry workshops, webinars, trade shows, academic publications, and case studies.

Project output:: Comprehensive database of control structures:
Diss/comm: Online repositories, data sharing agreements, collaborative projects, and integration with existing industrial and academic platforms.

Project output: Graph representations for control structures:
Diss/comm: Academic papers, conference presentations, guest lectures, training sessions, and technical reports.

Project output: Novel training techniques for GNNs:
Diss/comm: Academic publications, workshops, tutorials at conferences, integration into university courses and research projects.

Project output: Integration of GNNs with reinforcement learning:

Diss/comm: Industry whitepapers, case studies, webinars, workshops, and collaborations with industry partners.

Project output: New GNN architectures for control structure generation
Diss/comm: GitHub repositories, academic publications, AI and ML conferences, developer forums, and hackathons.

Project output: Software and models developed during the project
Diss/comm: GitHub repository, open-source community engagement, developer meetups, hackathons, and online forums.

Project output: Detailed documentation and educational materials
Diss/comm: Online tutorials, step-by-step guides, video tutorials, webinars, and academic course integration.

Project output: Explainability and transparency tools (e.g., GraphFrameX)
Diss/comm: Technical documentation, compliance reports, industry standards publications, and workshops with regulatory bodies.

Budget

Costs per project partner per year (NOK 1000)

	2024	2025	2026	2027	2028	2029	2030	2031	Sum
Institutt for kjemisk prosessteknologi	0	957	3163	3739	3452	1528	0	0	12839
Totals	0	957	3163	3739	3452	1528	0	0	12839

Cost plan (NOK 1000)

	2024	2025	2026	2027	2028	2029	2030	2031	Sum
Payroll and indirect expenses	0	723	2941	3516	3275	1528	0	0	11983
Procurement of R&D services	0	0	0	0	0	0	0	0	0
Equipment	0	0	0	0	0	0	0	0	0
Other operating expenses	0	234	222	223	177	0	0	0	856
Totals	0	957	3163	3739	3452	1528	0	0	12839

Specification

Other operating expenses:

There will be 2 Phds at NTNU who will work with AI. To carry out the work they need high-performance desktops (2 x 50 k NOK).

Access to IDUN-HPC (3 year cpu (56 cores)) - 400 k NOK total (2 Phds). The Idun cluster, a high-availability and professionally administrated compute platform. For rapid testing and prototyping of HPC software.

The rest is for travels of PhDs to conferences.

Cost code (NOK 1000)

	2024	2025	2026	2027	2028	2029	2030	2031	Sum
Trade and industry	0	0	0	0	0	0	0	0	0
Research institutes	0	0	0	0	0	0	0	0	0
Universities and university colleges	0	957	3163	3739	3452	1528	0	0	12839
Other sectors	0	0	0	0	0	0	0	0	0
Abroad	0	0	0	0	0	0	0	0	0
Totals	0	957	3163	3739	3452	1528	0	0	12839

Funding plan (NOK 1000)

	2024	2025	2026	2027	2028	2029	2030	2031	Sum
Own financing	0	76	267	278	118	100	0	0	839
International funding	0	0	0	0	0	0	0	0	0
Public funding	0	0	0	0	0	0	0	0	0
Private funding	0	0	0	0	0	0	0	0	0
The Research Council	0	881	2896	3461	3334	1428	0	0	12000
Totals	0	957	3163	3739	3452	1528	0	0	12839

Specification

Fellowship

Type of fellowship	From date (dd.mm.yyyy)	To date (dd.mm.yyyy)
Doctoral research fellowship	01.09.2025	31.08.2028
Doctoral research fellowship	01.10.2025	30.09.2028

Allocations sought from the Research Council (NOK 1000)

	2024	2025	2026	2027	2028	2029	2030	2031	Sum
Student fellowships	0	0	0	0	0	0	0	0	0
Doctoral fellowships	0	647	2674	2780	2169	0	0	0	8270
Post-doctoral fellowships	0	0	0	0	0	0	0	0	0
Grants for visiting researchers	0	0	0	0	0	0	0	0	0
Grants for overseas researchers	0	0	0	0	0	0	0	0	0
Researcher positions	0	0	0	458	988	1428	0	0	2874
Hourly-based salary including indirect costs	0	0	0	0	0	0	0	0	0
Procurement of R&D services	0	0	0	0	0	0	0	0	0
Equipment	0	0	0	0	0	0	0	0	0
Other operating expenses	0	234	222	223	177	0	0	0	856
Total amount sought	0	881	2896	3461	3334	1428	0	0	12000

Attachments

Project description

Project description	ES739402_001_1_Prosjektbeskrivelse_20241001
Reference	AICCA - Artificial Intelligence for Creating Control Architectures_Fripro_VF.pdf

Curriculum vitae (CV)

Curriculum vitae (CV)	ES739402_002_1_CV_20240930
Reference	Skogestad_CV_RCN.pdf

Curriculum vitae (CV)	ES739402_002_2_CV_20240930
Reference	Idelfonso_CV_RCN.pdf

1. Excellence: AICCA - Artificial Intelligence for Creating Control Architectures

1.1 State of the art, knowledge needs and project objectives

State of the Art

The field of systems control, encompassing diverse sectors such as the process industry, automotive, aerospace, robotics, and manufacturing, currently employs two main approaches for advanced control: Advanced Regulatory Control (ARC) and Model Predictive Control (MPC). ARC uses standard control elements like PID controllers, while MPC relies on dynamic process models for online optimization. Despite significant advancements in control theory over the last 50 years, its impact has been limited to large-scale operations like refineries and petrochemical plants. The engineering efforts required to install and maintain these systems often outweigh the marginal improvements in control performance. Consequently, most industries and applications still rely on ad-hoc ARC methods designed based on the expertise of seasoned engineers. This design integrates prior knowledge, practical experience, and case-specific analysis, all guided by practical insight into the process. This expertise is usually acquired after a long career experience. This knowledge is slowly disappearing as experienced professionals retire, partly because of the academic focus on MPC as a replacement for ARC[1].

More recently, a large focus has been on using machine learning (ML) within control schemes (including PID, MPC, and ARC). However, the success has been limited since most data is not sufficiently rich (meaning that the input signals are not sufficiently excited) to (indirectly) learn the model, which is needed to do control. This limitation echoes the failure of adaptive control in the 1970s, which also relied on data-based approaches. Therefore, it is believed that the present ARC approaches, based on standard controllers (PID), as well as more advanced multivariable control solutions (MPC), will survive and will not be replaced by ML approaches[1].

AICCA focuses on designing the control architecture for use in ARC with existing control elements, including PID controllers, selectors, cascade control, ratio control, split range control, and more. The focus is on structure/architecture and not on the controller tuning. Important decisions include also the placement of sensors (measurements) and actuators (valves, inputs). ***We strongly believe that the area of control system architectures for ARC is very well suited for ML methods, particularly generative and graph-based methods.,***

To develop the desired tool, the three main challenges are to generate:

C**1)** appropriate data for training,
C**2)** suitable ML methods, and
C**3)** methods for validation and testing of the approach (by human experts or dynamic simulations).

These challenges are addressed in the AICCA project. Regarding C**2)** suitable ML approaches, recent advancements in machine learning, particularly generative models, have demonstrated remarkable capabilities in learning from expert experience and replicating tasks with unprecedented accuracy and speed. Despite these advancements, the application of generative ML in creating ARC structures remains unexplored. Regarding C**1)** data for training - a few works in the literature propose similar ideas for process flowsheet generation (without control loops added) using text-based models. However, these text models, such as T5[2], face challenges due to their reliance on extensive pre-training data, which is scarce for process control structures. In this context, Graph Neural Networks (GNNs) can naturally represent the block diagrams of control structures, where blocks are nodes, and their connections are edges. This graphical representation aligns with the information flow in control structures, allowing GNNs to learn and generate control designs more accurately and effectively, as demonstrated in other applications[3]. Regarding C**3**), the challenge is ensuring that AI-generated control structures meet the high safety and reliability standards required in industrial applications. Furthermore, another challenge is to ensure they are applicable in real-case scenarios.

The alternative to the ML approach for designing control structures is optimization-based approaches, often based on superstructures that include, in principle, all possible combinations. However, these methods have become infeasible due to the exponential growth in possible alternatives. It also requires a dynamic model and the controller tuning for each option[4], which are not needed in the structural approach proposed in AICCA.

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[1] Sigurd Skogestad, Advanced control using decomposition and simple elements, Annual Reviews in Control, Volume 56, 2023.

[2] Hirtreiter E, Schulze Balhorn L, Schweidtmann AM. Toward automatic generation of control structures for process flow diagrams with large language models. AIChE J. 2024

[3] Bruno C.L. Rodrigues, Vinicius V. Santana, Luana P. Queiroz, Carine M. Rebello, Idelfonso B. R. Nogueira, Harnessing graph neural networks to craft fragrances based on consumer feedback, Computers & Chemical Engineering, Volume 185, 2024

[4] Vassilis Sakizlis, John D. Perkins, Efstratios N. Pistikopoulos, Recent advances in optimization-based simultaneous process and control design, Computers & Chemical Engineering, Volume 28, Issue 10, 2004

Knowledge Needs and Challenges

Table 1. Summary of key requirements and knowledge needs for the three challengesC1-C3.

Challenge	Requirement	Data and knowledge needs
C1) Appropriate data for training,	Comprehensive Database	Access to a substantial database of reliable, expert-generated control structures is crucial for training generative models. Furthermore, the control structures and the context in which they are applied are documented in Piping and Instrumentation Diagrams (P&IDs), a crucial element for these databases.
	Data generation	Due to the complexity and interdependence inherent in control systems, high-quality, labeled data is needed to train effectively and overcome issues with scalability and performance. Data for designing these structures is not as deterministic and abundant as chemical data, often influenced by the designer's subjective expertise.
	Effective Representations	Non-existent robust graph representations of control structures and the associated system conditions teach computers what a control structure is. Unlike the well-established SMILES notation in chemistry, there is no analogous pre-training data for control structures.
C2) Suitable ML methods	Computer Vision	P&Ids are visual information. Thus, computer vision tools must be developed to read and tabulate this information into a specific representation.
	GNN Architectures	Currently, no neural network architectures can effectively model the unique characteristics of control structure design. Developing new GNN architectures is crucial to addressing this gap and transitioning from traditional optimization-based approaches to AI methods, overcoming the exponential growth in alternatives and the complexities of tuning each option.
	Training Techniques	Need to develop training techniques to enhance GNNs' performance in generating reliable control structures due to the complexity of this task. Techniques available in the literature for training GNNs might be insufficient, and a combination of techniques might be necessary to be implemented.
C3) Methods for validation and testing,	Explainable and Interpretable Results	Explainability and transparency are critical for successfully adopting AI-generated control structures, especially in safety-critical and highly regulated industries. Transparent AI systems help stakeholders understand, trust, and manage AI decisions.
	Human-in-the-Loop Mechanisms	Incorporating human-in-the-loop mechanisms to evaluate and refine AI-generated control structures is needed to ensure that the designs are practical, reliable, and aligned with real-world requirements.

AICCA is designed to meet these challenges (Table 1) by developing a novel "ChatGPT for control structures" that can generate on-demand structures for specific cases and be evaluated by experts before implementation. This will streamline the design process and enhance industrial operations' efficiency, safety, and sustainability.

Project Objectives

The primary objective of **AICCA** is to leverage generative AI to create control structures. This primary objective will be obtained by fulfilling the following set of sub-objectives:

O1. Develop AI models to capture and extend the knowledge in ARC. Connected with challenge C2), this objective will be considered met when we have successfully developed and validated the AICCA tool to accurately replicate and extend the expertise of seasoned engineers in ARC.

O2. Compile a substantial, reliable dataset of expert-generated control structures. Connected with challenge C1), this objective will be considered met when we have compiled a minimum of 3000 examples of P&Ids in a dataset, i.e., 10x more examples than our baseline reference[5].

O3. Create effective representations of control structures. Connected with challenge C1), making them suitable for machine learning **models.** This objective will be considered met when an algorithm capable of translating system diagram information into graphs is fully functional. It can provide the adjacency matrix for any system diagram input to the model.

O4. Develop novel graph-modified neural network structures. Connected with challenge C2), tailored to the specific needs of control structure design, ensuring accurate modeling of control systems. This objective will be considered met when a graph neural network structure is trained to receive the graph representations, plus any additional information considered important (such as process time constants). This objective does not consider the model's accuracy but only whether we can train the model.

O5. Develop advanced training techniques. Connected with challenge C2), to improve learning and performance. This objective will be considered met when the control structures consistently show an accuracy of 95% compared to expert designs.

O6. Incorporate human expertise to evaluate and refine AI-generated control structures. Connected with challenge C3), ensuring practical applicability, safety, and reliability. This objective will be considered met when a structured feedback loop involving domain experts is established and functional. This results in at least two iterative refinements of the AI-generated control structures that demonstrate improved safety, applicability, and reliability in real-world scenarios.

1.2 Research questions and hypotheses, theoretical approach and methodology

Research Questions and Hypotheses

Our hypotheses are:

1. **Generative AI models can learn from expert-generated control structures and replicate them accurately:** By training on a comprehensive dataset of expert-generated control structures, generative AI

[5] Hirtreiter E, Schulze Balhorn L, Schweidtmann AM. Toward automatic generation of control structures for process flow diagrams with large language models. AIChE J. 2024

models will be able to understand and replicate the intricate patterns and decisions made by human experts, achieving high accuracy and reliability in the process. 2. **Graph representations will provide a robust framework for training generative AI models, capturing the essential features and relationships within the control systems:** Graph representations of control structures, including the specific requirements, characteristics, and constraints of the systems they are applied to, will provide a robust framework for training generative AI models. Utilizing GNNs to represent control structures and their context as nodes and edges will enable the AI models to effectively capture and learn the complex relationships and dependencies inherent in control systems. This approach will lead to more precise and effective control structure generation. 3. **Coupling AI-generated control structures with simulators in a reinforcement learning loop will continuously improve the models' performance:** By integrating AI-generated control structures with process simulators and using reinforcement learning, the AI models can receive continuous feedback and iteratively improve their performance, leading to increasingly accurate and effective control structures. 4. **Implementing training techniques can significantly enhance GNNs' performance in generating reliable control structures:** Implementing advanced training techniques, such as feature masking, next structure prediction tasks, and bidirectional training, will significantly enhance GNNs' performance in generating reliable control structures. This methodology will enhance learning efficiency and performance, producing more robust and reliable AI-generated control structures. 5. **Incorporating human-in-the-loop mechanisms will enhance the practical applicability and reliability of AI-generated control structures:** By involving human experts in evaluating and refining AI-generated control structures, the project will ensure that the generated designs are theoretically sound, practically applicable, and reliable in real-world scenarios. 6. **AI-based solutions can navigate the vast design space more effectively than traditional optimization-based approaches:** AI models, particularly those leveraging GNNs and GANs, can explore and identify optimal control structures more efficiently than traditional optimization methods, reducing computational overhead and improving scalability. 7. **The project will uncover novel and unconventional control structures that human designers might overlook:** The generative AI approach has the potential to discover control structures that are not apparent to human designers, leading to new and improved solutions for process systems engineering.

Methodology

The theoretical foundation will include Control Systems Theory, Machine Learning, and Graph Theory. **AICCA** is structured to systematically address the critical challenges (C1-C3) by designing advanced regulatory control (ARC) systems using generative AI. To achieve this, the project is divided into three comprehensive work packages (WPs) as follows:

WP 1: Development of Representations (addressing C1 and contributing to O1, O2 and O3)

Task 1.1: Data Extraction from P&IDs Using Computer Vision Techniques and Data Curation (M1-M12). Participants: S. Skogestad, I. Nogueira, PhD1-collecting and generating data, PhD2-developing computer vision tool.

To address the first hypothesis, we will start by compiling a comprehensive dataset of expert-generated control structures from various industrial, academic, and in-house sources. The main source will be P&IDs in academic textbooks, papers, and industrial records. Computer vision techniques will extract data from P&IDs, such as Optical Character Recognition (OCR) for text extraction and Convolutional Neural Networks (CNNs) for object detection and classification. OCR will be applied to identify and digitize textual information such as process labels and equipment specifications. Concurrently, CNNs, trained on annotated P&ID datasets, will detect and categorize components such as control elements, valves, pumps, and sensors and their interconnections. We will also use image segmentation algorithms to delineate individual elements and their relationships. This integration of OCR and CNNs will facilitate the conversion of P&IDs into structured data, enabling the creation of a database of control structures and contextual information.

Task 1.2: Develop Detailed Graph Representations (M6-M18). Participants: S. Skogestad, I. Nogueira, PhD1- stressing representations against challenging cases, PhD2-developing graph representations.

The process information and control structures from the P&Ids extracted in Task 1.1 will be used to build the graph representations for the GNNs, as they will need comprehensive input data about the process application to generate adequate control structures. Furthermore, complementary expert knowledge not annotated in the P&Ids will be extracted from operation documentation (e.g., manuals, logs, reports collected together with the P&IDs) and added to this data, including: Type of process unit (e.g., reactors, distillation columns, heat exchangers, storage tanks); Operational objectives and constraints; Through-put manipulator location; Available measurements (e.g., temperature, pressure, flow rates); Manipulated variables (e.g., valve positions, flow rates); Interaction between variables (input/output pairings). The collected information will be translated into graph representations. In these graphs:

Input Graphs: Nodes represent the process units and their associated instrumentation. Each node will include attributes detailing the type of process unit, operational parameters, and variables. Edges will represent the connections and interactions between the available variables to inform the model of the information flow available in the process, carrying contextual information about operational relationships and constraints.
Output Graphs: Nodes represent control elements, and edges denote the connections and interactions within the control structure. In graph-to-graph learning, the goal is to map the input and output graphs.

Task 1.3 Feature Selection and Analysis (M14-20). Participants: S. Skogestad, I. Nogueira, PhD1-developing mechanism for critical analysis evaluation and PhD2-developing tool.

We will analyze the collected data to identify key features for control structure design, using Principal Component Analysis (PCA) to reduce dimensionality and highlight the most relevant variables. Partial Least Squares (PLS) will model the relationships between system variables and control structures, pinpointing those with the greatest impact. Integrating PCA and PLS will enhance GNN training efficiency and performance, ensuring the models focus on the most critical features for generating effective and reliable control structures.

WP 2: Developing and Training Generative Models (Addressing C2 and contributing to O1, O4 and O5)

Task 2.1 Development of Generative Model Based on Enhanced GNN Architectures (M18-M30). Participants: S. Skogestad, I. Nogueira, PhD1-applying generative tool and analyzing outputs and PhD2-developing new generative model.

To address the third hypothesis, we will develop Generative Adversarial Networks (GANs) with GNNs at their core to generate control structures. The GNNs within the GANs will feature modified architectures to capture the relationships within control structures and their context. This includes the introduction of a Laplacian matrix instead of the usual adjacency matrix. The Laplacian matrix L is defined as $L = D - A$, where D is the degree matrix (a diagonal matrix where each entry D_{ii} represents the degree of node i), and A is the adjacency matrix. We believe this modification comes with several advantages:

- **Enhanced Feature Representation**: L captures the degree of each node and the graph's connectivity, providing a richer and more informative representation of the graph's structure. This helps capture the relationships and dependencies within control structures and their context.
- **Spectral Properties**: L has well-defined spectral properties beneficial for graph learning tasks. It will be used to perform spectral clustering, which is useful for identifying clusters or communities within the graph. This capability is valuable for understanding complex control structures where different components may have varying levels of interaction and dependencies.
- **Improved Convergence**: L can improve convergence properties in GNN training. The normalization inherent in the Laplacian helps stabilize the training process, especially when dealing with graphs of varying sizes and densities.
- **Smoothness**: L promotes smoothness in the learned representations, meaning connected nodes are encouraged to have similar feature representations. This is crucial for control structures where the behavior of one component can significantly influence its neighbors.

These advantages will be validated in AICCA. GANs are effective in creating synthetic data that closely mimics original datasets, and by embedding GNNs within GANs, we can better learn complex patterns in control structures. This synthetic data will address data scarcity and enhance GNN robustness. To improve performance, we will tackle the pooling problem by evaluating traditional methods like sum and mean pooling alongside advanced techniques like Set Transformer pooling, which captures complex node interactions without losing critical information. This approach is especially useful for transfer learning, preserving graph structure integrity. We will compare GNN performance across different pooling methods to enhance their reliability and accuracy.

Task 2.2 Benchmarking New Structure with Traditional GNNs and FNNs (M28-M40). Participants: S. Skogestad, I. Nogueira, PhD1-implement traditional models, and benchmarking.

To evaluate the GNN architecture modified with the Laplacian matrix, traditional GNNs and Feedforward Neural Networks (FNNs) will be identified and coupled with GANs as benchmarks. The following comparative analysis will provide a clear understanding of the effectiveness of the new GNN architecture compared to established methods:

Identification and Implementation: Traditional GNN and FNN architectures will be identified based on established research[6], existing implementations, and the proposed representation of the control structures. These traditional architectures will be implemented and integrated with the GAN.

[6] Bruno C.L. Rodrigues, Vinicius V. Santana, Luana P. Queiroz, Carine M. Rebello, Idelfonso B. R. Nogueira, Harnessing graph neural networks to craft fragrances based on consumer feedback, Computers & Chemical Engineering, Volume 185, 2024

Training and Testing: Both traditional GNNs and FNNs will be trained using the same dataset and context-rich graph representations. This will ensure that all models are evaluated under the same conditions.

Performance Evaluation: The performance of traditional GNNs and FNNs will be compared to the proposed modified GNNs with the Laplacian matrix. Key metrics will include accuracy and robustness of the generated control structures, training efficiency and convergence rates, ability to capture complex relationships, and flexibility and generalization across various control scenarios.

Task 2.3 Advanced Training Techniques for GNNs (M30-M42). Participants: S. Skogestad, I. Nogueira, PhD2-developing and testing training algorithms.

With the comprehensive and well-represented data, we will train enhanced GNNs to generate viable control structure options. We will implement training techniques to enhance GNN performance and address the fourth hypothesis and advanced pooling methods. Additionally, we will implement bidirectional training to improve further the flexibility and validation capabilities of the GNN models. The training techniques will involve:

Feature Masking: Deliberately obscuring specific features within the graph forces the model to learn underlying structures and relationships rather than relying on superficial patterns. This technique enhances the model's robustness and ability to handle incomplete or noisy data.

Next Structure Prediction Tasks: Splitting process graphs into subgraphs and training the model to predict whether pairs of subgraphs originate from the same original graph. This task improves the model's understanding of structure continuity and the relationships between control system parts.

Bidirectional training: To enhance the flexibility, robustness, and validation capability of the GNN models. By training the GNNs to perform both forward and reverse predictions, we can ensure that the models can generate control structures from process information and infer process information from control structures. This dual capability is crucial for several reasons:

- **Validation and Consistency:** Bidirectional training allows us to validate the generated control structures by ensuring they can be accurately traced back to their corresponding process configurations. This helps in verifying the consistency and accuracy of the designs.
- **Improved Learning:** Training the GNNs in both directions helps the models learn more comprehensive representations of the data, more effectively capturing the intricate relationships between process units and control structures.
- **Flexibility in Application:** With bidirectional training, the models become versatile and capable of addressing a wider range of design and analysis tasks in process systems engineering.

To implement bidirectional training, we will train the GNNs to perform two tasks:

1. **Forward Prediction:** Generate control structures from the given process information. The input graphs (process units and their interactions) will be mapped to output graphs (control structures). This ensures that the GNNs can effectively design control structures based on specific process parameters and constraints.
2. **Reverse Prediction:** Infer process information from given control structures. The control structure graphs will predict the corresponding process unit graphs. This capability is important for validating the generated control structures and ensuring they align with the intended process configurations and requirements.

WP 3: Integration with Simulators and Expert Evaluation (Addressing C3 and contributing to O1 and O6)

Task 3.1 Integration of AI Models with Process Simulators (M28-M50). Participants: S. Skogestad, I. Nogueira, PhD1-implementing process simulator and integrating with developed AI tool, Researcher-supporting coding activities.

To address the fifth hypothesis, we will integrate AI-generated control structures with process simulators to create a reinforcement learning loop. This work is structured to meet the following two main requirements:

Seamless Interface Development: We will establish a seamless interface between the GNN-based generative control structures and high-fidelity process simulators like Aspen HYSYS or Aspen Plus. These commercial simulators offer robust platforms for simulating complex industrial processes. The interface will facilitate the smooth transfer of control structures to the simulator and efficiently retrieve performance metrics. The process flowsheet will be built within the simulator, with the interface feeding the flowsheet into the generative model while collecting the resulting control structures. This development involves utilizing programs such as Python to interact with HYSYS simulations. Two key methods will be employed:

- **Aspen Simulation Workbook (ASW) Method:** In this method, HYSYS simulation results are exported to an Excel workbook, which Python scripts can then read, process, and use to refine the control structures generated by the GNN model further.

- **Component Object Model (COM) Interface Method:** This approach automates and controls HYSYS directly from Python, providing another avenue for seamless data exchange and process control.

Iterative Performance Evaluation: The interface will enable the transfer of AI-generated control structures to the simulator and the retrieval of key performance metrics such as stability, robustness, and efficiency. These metrics will be crucial in evaluating and iteratively improving the control structures. The process simulators will emulate real-world industrial processes, offering a dynamic and realistic environment to effectively test and refine the generative AI tool. This structured approach ensures that a robust and well-integrated interface supports the reinforcement learning loop, capable of enhancing AI-generated control structures through continuous feedback from high-fidelity process simulations.

Task 3.2: Reinforcement Learning Loop with Simulated Feedback (M36-M50). Participants: S. Skogestad, I. Nogueira, PhD2-implementing RL, Researcher-polishing codes, supporting RL implementation, and developing user interface.

The RL framework will be integrated to provide continuous feedback and iterative improvement of the GNN models. Initially, GNN models will generate control structures based on input process data, which will be tested in a process simulator against metrics like stability, robustness, efficiency, settling time, overshoot, and energy consumption. These performance metrics will feed back into the RL algorithm, which will iteratively optimize the control structures by adjusting them according to the reward signals from simulation outcomes. A weighted reward system prioritizes control structures that align with operational goals, such as superior stability in dynamic environments or reduced energy consumption in energy-intensive operations. This approach ensures that the AI models generate tailored and efficient control solutions. This iterative process enables the AI models to continuously learn from simulation results, progressively improving their ability to produce effective and reliable control structures.

Task 3.3: Human-in-the-Loop Evaluation and Refinement (M40-M54). Participants: S. Skogestad, I. Nogueira, PhD1-evaluating and providing insights to improve the tools.

Human experts will be incorporated into the evaluation and refinement process of AI-generated control structures to test the sixth hypothesis. The experts (team members and invited members from the industry) will assess the generated designs' practicality, reliability, and compliance with industry standards. The evaluation process will begin with the experts reviewing and ranking the AI-generated control structures based on their coherence with expert knowledge and practical applicability. The ranked control structures will then be fed back into the process simulators for further evaluation, using the simulation outcomes to refine the models. The ranking will serve as an additional metric in the reinforcement learning layer and will be carried out as an iterative process. This step will incorporate the possibility of human intervention in the tool.

Task 3.4: Enhancing Explainability and Transparency (M40-M54). Participants: S. Skogestad, I. Nogueira, PhD1-critically evaluating insights, PhD2-support explainability implementation, Researcher-implement explainability and transparency tools.

To enhance the explainability of AI-generated control structures, we will integrate **GraphFrameX** into our solution. This framework will be embedded directly within our system to offer insights into the decision-making processes of GNNs. Specifically, GraphFrameX will help highlight critical features, such as the importance of node and edge, and identify key subgraph structures through community detection and motif analysis. These insights will enable a transparent view of how control structures are generated and refined. The integration involves leveraging GraphFrameX's visualization tools and explainability metrics, such as SHAP values (SHapley Additive exPlanations) and LIME (Local Interpretable Model-agnostic Explanations), to ensure the AI-generated models are interpretable and align with industry standards.

The SHAP values will be implemented for feature attribution, while LIME will be used for model interpretability, consistency, and stability metrics to assess decision reliability and transparency index to rate the overall clarity of AI decisions. The explainability metrics and tools will be integrated into the evaluation criteria for AI-generated control structures. During the model development, GraphFrameX will identify and highlight critical features and interactions within the graph, ensuring that the model focuses on the most relevant parts of the control structure. Models will be iteratively refined based on insights from explainability tools, ensuring that decisions become more transparent and justifiable over time. This task will monitor explainability metrics during the Task 3.5 to maintain transparency and trust in AI decisions. Deviations in scores will prompt investigation and model adjustments, while stakeholder feedback will refine the tools. Detailed reports for regulatory and compliance checks will document the decision-making process, ensuring alignment with standards and best practices. This approach ensures AI-generated control structures are effective, transparent, and trustworthy, building confidence, facilitating regulatory approvals, and promoting AI adoption in control systems engineering.

Task 3.5: Industrial Case Study Implementation (M42-M54). Participants: S. Skogestad, I. Nogueira, Researcher-implementation and documentation.

Case studies will be conducted at ABB and Perstorp to implement and validate AI-generated control structures. ABB and Perstorp will provide detailed process flowsheets of specific industrial processes where they aim to install new control structures or improve current ones. The flowsheets will include operational parameters, constraints, and control requirements toensure they accurately reflect the current process conditions and configurations. Using the AI tool developed in this project, we will generate control structure proposals tailored to the specific requirements and constraints of the case study. The AI-generated control structures will be implemented in ABB and Perstorp's process environments, followed by thorough testing to evaluate their performance, stability, and efficiency. Performance metrics, including throughput, quality, energy consumption, and safety improvements, will be monitored and documented. Based on the feedback and performance data , the control structures will be refined if necessary to ensure continuous improvement.

Risk Management

The main risks include data limitations, model inaccuracies, implementation challenges, safety and reliability concerns, compliance with regulatory standards, and ethical issues. Table 2 outlines these risks and the strategies to mitigate them, ensuring AI-generated control structures' robustness, reliability, and ethical adherence.

Table 2: Risk Management Strategy and Mitigation Measures

Risk	Description	Mitigation Strategy
Data Limitations WP1	Lack of extensive and high-quality training data.	Use web scraping and data extraction to build a comprehensive database. Employ data augmentation techniques, such as leveraging GANs to generate synthetic data, ensuring diversity and completeness. Perform cross-validation to identify and rectify data imbalances, enhancing the dataset's robustness.
Model Inaccuracies WP2	AI models may generate suboptimal or incorrect control structures.	Implement rigorous testing protocols, including unit, integration, and end-to-end tests. Continuously monitor performance metrics. Develop reliability scores based on the frequency and severity of failures or malfunctions in the control structures. High-reliability scores will indicate robust and dependable performance.
Implementation Challenges WP3	Integrating GNN models with existing control systems.	Develop robust APIs and middleware to facilitate seamless integration. Use adaptive strategies, such as incorporating large language models (LLMs), to enhance natural language processing capabilities, thereby improving the GNNs' performance.
Safety and Reliability WP2 & WP3	AI-generated structures may not meet the required safety and reliability standards.	Extensive simulations and real-world tests can be conducted using commercial process simulators like Aspen HYSYS. Stress testing and failure mode analysis can be included to ensure that control structures can withstand various operational scenarios.
Compliance with Regulatory Standards WP2 & WP3	Non-compliance with regulatory standards can lead to legal and operational issues.	Engage with regulatory bodies and industry stakeholders to align project outcomes with safety and ethical guidelines. Perform regular audits and compliance checks to ensure adherence to these standards.
Ethical Concerns WP1, WP2 & WP3	Ensuring the safety and reliability of AI-generated control structures.	Adhere to ethical standards and regulatory requirements. Involve experts in the evaluation process. Develop and implement rigorous testing protocols, validation procedures, and continuous monitoring mechanisms.

1.3 Novelty and ambition

Potential for developing new knowledge beyond the current state-of-the-art

This project aims to push the boundaries of generative AI applications in process and control engineering by developing innovative methods for automatically generating control structures for process systems. By leveraging advanced machine learning techniques, particularly Graph Neural Networks (GNNs), this project will introduce several significant advancements:

Graph Representation of Control Structures: Unlike other methods, this project will develop and utilize graph representations for control structures. This involves identifying the fundamental building blocks of a control structure, determining the contextual elements that influence the type of control structure, and translating these elements into string or graph representations. This approach is more suitable for capturing process systems' complex relationships and dependencies.

Transition from Text Models to GNNs: A key issue with text/language models is the need for extensive pre-training data, which is unavailable for process control structures. Therefore, moving from text models to GNNs is essential. According to graph theory, the blocks in a control structure's block diagram can be represented as nodes and their connections as edges, aligning well with the information flow in control structures.

Integration of Reinforcement Learning: The project will integrate AI-generated models with process simulators to create a reinforcement learning loop. This method will continuously improve the accuracy and reliability of the generated control structures, representing a significant advancement in the application of AI in process control engineering.

AI-Driven Process Engineering: By automating the generation of Piping and Instrumentation Diagrams (P&IDs) from Process Flow Diagrams (PFDs), the project will significantly reduce the time and effort required in process design, leading to faster development cycles and reduced costs.

Particular novel and Ambitious Aspects of the project

The project stands out due to several particularly novel, original, and ambitious aspects:

- **End-to-End Control Structure Generation:** Inspired by transformer-based human language translation models, the project will treat control structure generation as a translation task, converting PFDs without control structures into PFDs with control structures. This approach is unprecedented in the field and promises to streamline the design process significantly.
- **Hybrid Data Solutions:** The project will develop hybrid AI solutions that can adapt to various industrial applications by combining synthetic data generation with real-world fine-tuning. This dual approach ensures robustness and applicability in real-world scenarios.
- **Integration with Simulators for Reinforcement Learning:** Coupling the AI-generated models with process simulators to create an RL loop represents a significant advancement. This continuous improvement mechanism will enhance the accuracy and reliability of the generated control structures over time.

Interdisciplinary Approach

The project will integrate control systems engineering, machine learning, and computer science to create a comprehensive and effective methodology. This interdisciplinary approach is essential for tackling the complex challenges of process control design.

By pioneering these approaches, the project aims to develop a tool akin to "ChatGPT for control structures," providing on-demand generation of control structures tailored to specific cases. This innovation can revolutionize process engineering by making advanced control methods more accessible and practical.

2. Impact

2.1 Potential for academic impact of the research project

This project aims to advance the field of process systems engineering by introducing AI-driven methodologies for control structure generation. The anticipated outputs of this project will address important scientific challenges:

Integration of AI and Control Theory through Graph Representations (WP1, WP2): The project will bridge the gap between machine learning and control systems engineering by developing graph representations for control structures. These representations will capture process systems' relationships and dependencies, providing a framework for modeling control structures. By leveraging these graph representations, the project will introduce new methodologies for control structure design that are both theoretically grounded and practically applicable. This approach will improve interpretability and consistently create understandable control structures using standard elements.

Advancement of Graph Neural Networks (WP2, WP3): The project will advance GNNs in control structures, impacting both machine learning and process control engineering. By developing specialized GNN architectures, like those using Laplacian adjacency functions, the project aims to capture complex system interactions better. Novel training techniques like feature masking and next-structure prediction will enhance model robustness and accuracy. Integrating GNNs with reinforcement learning and tools like GraphFrameX will improve the reliability and interpretability of control structures. These advancements could also benefit process flowsheet generation, chemical optimization, and circuit design.

Preservation of Expert Knowledge for Educational Purposes (WP2, WP3): The AI tool developed in this project will encapsulate critical expertise in control structure design, which is at risk due to the retirement of seasoned professionals. By automating the generation of control structures, the tool will preserve this knowledge and make it accessible for educational use. Engineering students and professionals can use the AI tool to learn about various control structure designs, understand the underlying principles, and receive real-time feedback. This will enhance the learning experience by providing practical, hands-on exposure to advanced control methodologies, ensuring that vital knowledge is retained and disseminated effectively within the academic community.

2.2 Potential for societal impact of the research project

AICCAs innovative approach to automating control structure design and the related outputs will have the potential to meet several societal challenges by enhancing efficiency, safety, and sustainability in industrial processes, as summarised below:

Efficiency and Cost Reduction: Automating control structure design will significantly reduce development time and operational costs. McKinsey reports state that using AI for scheduling and optimization can reduce engineering hours by 130%[7], while Deloitte highlights that AI and advanced analytics can decrease timeline deviations by 10-20% in construction projects[8,9]. This automation minimizes manual rework, enhances accuracy, and allows for continuous improvement, significantly accelerating development cycles compared to traditional methods.

Safety and Reliability: AI-generated control structures will enhance safety and minimize errors related to control structure design. Typically, a company reports 10 safety incidents and 20 control errors annually related to traditional control structures[10]. AI-generated structures can reduce these incidents and errors by 40% to 60% due to improved accuracy, consistency, and error-checking capabilities. Studies have shown that AI systems reduce unsafe behaviors and accidents, supporting these potential improvements[11,]. The project addresses critical industrial safety challenges and reduces the risk of accidents and incidents by improving safety and reliability.

Sustainability: Improved process control will reduce energy consumption and lower emissions, contributing to environmental sustainability. As reported by Aspen Technology, the implementation of well-positioned Advanced Process Control can reduce energy usage by 10%[12]. Enhanced control structures will optimize resource use and minimize waste, aligning with sustainability goals. The project will support efforts to combat climate change and promote sustainable industrial practices by fostering more efficient and environmentally friendly industrial processes.

Operational Benefits: The project will enable industries to operate closer to constraints, allowing higher throughput (production rates) and profit gains (up to 5%)[13]. Benefits include reduced downtime, better quality products, fewer off-spec products, reduced energy usage, and lower CO2 emissions. Less manual control will lead to savings in plant economics and reduced operator fatigue and stress.

Innovation and Knowledge Preservation: The project will uncover novel and unconventional control structures, fostering innovation in process control engineering. According to WIPO, more than 54,000 Generative AI inventions were filed globally between 2014 and 2023[13], with over 25% of these patents filed in 2023 alone. Based on these trends, it is estimated that approximately 15% to 25% of AI-generated control structures will be novel and unconventional. By introducing new control structures, the project will drive technological advancements and support the continuous improvement of industrial processes.

Mitigating the Decline in ARC Expertise: The project will mitigate the impact of the declining number of ARC experienced professionals and preserve critical expertise. AI systems will effectively replicate expert knowledge and generate solutions aligned with established standards. Studies have shown that AI can achieve high accuracy rates, with systems in healthcare diagnostics reaching up to 95% accuracy compared to expert diagnoses[14]. Our AI-generated ARC strategies aim for a 95% match rate with expert-designed solutions for standard problems (O5). This preservation of knowledge will ensure the continuity of expertise and support the training of future professionals.

Contribution to UN Sustainable Development Goals: The project aligns with several UN Sustainable Development Goals (SDGs), as follows. **Goal 9:** The project advances **industrial innovation** by automating control structure design with AI, specifically through Graph Neural Networks tailored for this purpose. Integrating synthetic data with real-world fine-tuning ensures robust AI models adaptable to various applications. A reinforcement learning loop with process simulators continuously improves the accuracy and reliability of these AI-generated control structures. **Goal 12:** The project promotes **sustainable production** by enhancing process efficiency and reducing waste and energy consumption. AI-driven methods improve safety, reliability, and operational efficiency, resulting in higher throughput, better product quality, less downtime, and lower CO2 emissions. By reducing manual control, the project also decreases operator fatigue, supporting more sustainable industrial operations.

2.3 Measures for communication and exploitation

Open Science Practices

To ensure early and open sharing of research outputs, the project will adopt the following practices:

Table 3: Open science practices in AICCA

[7] McKinsey & Company. "Unlocking the promise of AI in industrials." McKinsey Insights, 2021.
[8] Deloitte. "The Age of With… AI in construction and infrastructure." Deloitte Insights, 2020.
[9] **Boston Consulting Group (BCG)**. "Reduce Carbon and Costs with the Power of AI." BCG Insights, January 26, 2021.
[10] McKinsey & Company. "Improving Industrial Safety Performance." McKinsey Insights, 2020.
[11] U.S. Chemical Safety Board (CSB). "Process Safety Incidents Report, 2006-2010." U.S. Chemical Safety Board, 2011.
[12] Advanced Process Control Maximize profitability by maintaining optimal operating conditions 100% of the time, Aspen Technology, Inc., 2020.
[13] World Intellectual Property Organization (WIPO). "WIPO Technology Trends 2023: Generative AI." WIPO, 2023.
[14] Topol, E.J. High-performance medicine: the convergence of human and artificial intelligence. *Nat Med* **25**, 44–56 (2019).

Aspect	Description
FAIR Data Principles	All project data will adhere to FAIR principles, ensuring interoperability through standardized formats like JSON, XML, and CSV. Datasets will be shared in open repositories such as Zenodo, GitHub, or Figshare, with detailed metadata covering data source, collection methods, schema, and processing steps for effective use.
Open Source Software and Models	Algorithms, models, and software developed will be released under open-source licenses like MIT or Apache 2.0. Platforms like GitHub and GitLab will host them, offering version control and enabling community collaboration, benefiting researchers in control systems, process engineering, and machine learning.
Transparent Methodologies	Detailed documentation of methodologies and protocols will be provided, including step-by-step guides, tutorials, and example use cases to facilitate reproducibility. The documentation will cover all project aspects, from data collection to model deployment.
Step-by-Step Guides	Detailed instructions on data preprocessing, GNN model setup, and training and evaluation processes, including command-line instructions, configuration files, and troubleshooting tips.
Example Use Cases	Comprehensive examples demonstrate methodologies' application in real-world scenarios, including case studies, AI vs. traditional control structure comparisons, and performance improvement analyses.
Video Tutorials and Webinars	Visual and interactive learning opportunities, including step-by-step implementation, data preparation, model training, deployment, and process simulator integration. Webinars will include live Q&A sessions to address community questions.

Table 4 describes the activities contributing to realizing AICCA's key outputs, including an overview of exploitation strategies, dissemination activities, and target groups. More details related to the dissemination activities are included in the dissemination plan in the on-line submission portal.

Table 4: Overview of scope and plan for dissemination, communication and engagement activities linked to the key project outputs..

Key project output	Exploitation strategy	Dissemination/communication/engagement	Target groups
AI tool for generating control structures	Commercialization through partnerships with industry leaders like ABB and Perstorp, licensing to other industries.	Conferences, industry workshops, webinars, trade shows, academic publications, and case studies.	Industry professionals, academic researchers
Comprehensive database of control structures	Open access through FAIR data principles and collaboration with academic and industrial partners for continuous improvement.	Online repositories, data sharing agreements, collaborative projects, and integration with existing industrial and academic platforms.	Researchers, industry experts
Graph representations for control structures	Publication in high-impact journals, presentation at international conferences, integration into academic curricula, and professional training programs.	Academic papers, conference presentations, guest lectures, training sessions, and technical reports.	Academic researchers, educators, industry professionals
Novel training techniques for GNNs	Sharing methodologies through academic journals and conferences, incorporating findings into advanced machine learning courses.	Academic publications, workshops, tutorials at conferences, integration into university courses and research projects.	Academic researchers, ML practitioners, educators
Integration of GNNs with reinforcement learning	Demonstrating applications in industrial case studies, partnering with industries for pilot projects.	Industry whitepapers, case studies, webinars, workshops, and collaborations with industry partners.	Industry professionals, researchers
New GNN architectures for control structure generation	Open-source release of GNN architectures, collaboration with the AI research community for further development and refinement.	GitHub repositories, academic publications, AI and ML conferences, developer forums, and hackathons.	AI researchers, developers, industry professionals
Software and models developed during the project	Release under open-source licenses (e.g., MIT, GPL) to encourage widespread adoption and community contributions.	GitHub repository, open-source community engagement, developer meetups, hackathons, and online forums.	Developers, researchers, industry professionals
Detailed documentation and educational materials	Educational partnerships, incorporation into university courses, and professional development programs.	Online tutorials, step-by-step guides, video tutorials, webinars, and academic course integration.	Educators, students, industry trainers
Explainability and transparency tools (e.g., GraphFrameX)	Collaboration with regulatory bodies to ensure compliance and integration into industry standards.	Technical documentation, compliance reports, industry standards publications, and workshops with regulatory bodies.	Regulators, industry professionals, researchers

3. Implementation

3.1 Project manager and project group

Project Manager: Prof. S. Skogestad at NTNU, an internationally recognized expert in process control with significant contributions to the field, will lead the project. His extensive academic and industry experience, highlighted by numerous awards, makes him ideally suited for this role. **Project Team:** Assoc. Prof. I. B. R. Nogueira is an expert in AI-based industrial solutions at NTNU, with extensive experience in Graph Neural Networks, generative networks, and reinforcement learning. Two PhD students will join the team, one focusing on machine learning under Nogueira's supervision and the other on control systems under Skogestad. In the third year, a researcher will be hired to integrate methodologies into an open software platform and implement the industrial case studies. Further details are in the WP descriptions in section 1. **Complementarity of Expertise:** Skogestad and Nogueira's complementary expertise uniquely positions the team to achieve the

project's ambitious goals. Skogestad's deep experience in advanced process control structures ensures a solid strategic foundation, balancing proven principles with innovation. Meanwhile, Nogueira's expertise in AI drives the development of novel AI-based control structure generation methods.

3.2 Project organisation and management

The work plan

The project is designed to span five years, as described in the Gantt chart below, with a clear division between the research and development phases and the application and dissemination of results. The timing of activities is structured to ensure that each phase builds on the previous one, leading to a successful and impactful project.

First Three Years - Research and Development Focus:

1. **Rationale:** The initial three years are dedicated to developing AI-based control structures and methodologies. During this period, the project team will focus on data extraction, model development, and refinement. This timeline is realistic, given the complexity of the tasks and the need for rigorous testing and validation of the developed models.
2. **Feasibility:** The availability of extensive data sources, computational resources, and a highly experienced team ensures this phase can be executed effectively. The two PhDs, specializing in machine learning and control systems, will drive the core research under the close supervision of Prof. Skogestad and Assoc. Prof. Nogueira ensures that the research is innovative and grounded in proven principles.

Final Two Years - Industrial Case Studies and Dissemination:

1. **Rationale:** In the last two years, the project will apply the developed AI in real-world industrial settings and test and validate the findings. This phase is essential for validating the research in practical applications and ensuring that the project's outputs have a tangible impact.

2. **Feasibility:** By the second half of the second year, a researcher will be hired to integrate the methodologies into a cohesive software platform and engage with industrial stakeholders. This allows sufficient time to conduct thorough testing and refine the solutions. Additionally, showcasing the results through workshops and industry engagement for the broader adoption of the project's innovations will mainly take place during the final year.

Research infrastructure and other resources

The **AICCA** project is well-equipped with the necessary research infrastructure and resources to ensure its success. NTNU provides all required software licenses, including those for Python, TensorFlow, PyTorch, Aspen HYSYS, and MATLAB. The project utilizes P&IDs from academics, available in the scientific journals, which access is provided by NTNU, industrial sources, operational data from industries like ABB and Perstorp, and synthetic data generated using the expertise within the consortium. These comprehensive data sources ensure robust training and validation. The budget includes access to NTNU's High-Performance Computing Laboratory for computationally intensive tasks, ensuring efficient handling of simulations and data processing.

Organisation and management structure

The project team will hold weekly meetings to assess progress, plan the next steps, and address key risks, ensuring well-informed daily decisions. Monthly online meetings will include broader academic involvement (such as Ph.D.s/Postdocs from the process systems engineering community), focusing on updates, recommendations, and idea exchanges. Twice a year, in-person discussions with industries like ABB and Perstorp and academic experts will align the project with strategic goals and address major challenges.

Short curriculum vitae – Sigurd Skogestad

Role in the project Project manager ☒ Project partner ☐

Personal information

First name, Surname:	Sigurd Skogestad		
Position	Professor Norwegian University of Science and Technology		
Date of birth:	14-08-1955	Sex:	Male
Nationality:	Norwegian		
Researcher unique identifier(s) (ORCID, ResearcherID, etc.):	ORCID: 0000-0001-6187-8261 Reseatcherid: c-1449-2008		
URL for personal website:	https://folk.ntnu.no/skoge/		

Education

Year	Faculty/department - University/institution - Country
1987	Ph.D. in Chemical and Biological Engineering, California Institute of Technology, USA
1978	Master (siv.ing.) in Chemical Engineering, NTNU (former NTH), Trondheim. Norway

Positions - current and previous

Year	Job title – Employer - Country
1987-Current	Professor in Chemical Engineering, NTNU, Trondheim, Norway
1983-1987	PhD student and Research Assistant, California Institute of Technology, USA
1980 –1983	Research Engineer, Norsk Hydro' s Research Center, Porsgrunn, Norway
1979	Military Service, Norwegian Defence Research Center (FFI)

Career breaks - Mobility

Year	Job title – Employer - Country
1994 -1995	Visiting Professor, Departments of Chemical Engineering and Mechanical Engineering, University of California, Berkeley, USA (12 months).
2001-2002	Visiting Professor, Departments of Chemical Engineering, University of California, Santa Barbara, USA (5 months).

Project management experience

Year	Project owner - Project - Role - Funder
1987 - current	As is clear since I have supervised 47 PhD students to completion and have had many postdocs, I have been involved In a large number of projects over the years, and in most cases as the project manager and principal investigator. Funding has come from the

	Norwegian Research council (about 60%), NTNU (about 18%), Industry (about 18%) and EU (about 4%).
2015 - 2024	The by far largest project is the SFI SUBPRO where I was Director for 9 years. This highly successful PhD program had a total finding of 264 million NOK from the Norwegian Research Council (36%), industry (48%) and NTNU (16%).

Supervision of students 1987-2024

(Total number of students supervised to completion as main supervisor)

Master students	Ph.D. students	University/institution - Country
210	47	Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway

Other relevant professional experiences

Year	Description - Role
1994-1998	Chair of the University committee for all engineering PhDs at NTNU
1994-1998	Founding chair of the Nordic Process Control Working group (and still a member)
1994-2018	Head of NTNU/SINTEF's strong point center in process systems engineering (PROST)
1987-present	Member of numerous editorial boards and IPCs for conferences, including Editor of Automatica 1996-2002, IPC Chair for the PSE-ESCAPE conference in Trondheim (1996), NOC chair for the IFAC DYCOPS conference in Trondheim (2016), IPC Chair for the IFAC conference on Automatic control in offshore oil and gas production, Denmark (2018).
1999-2009	Head of Department of Chemical Engineering, NTNU
2019 – Current	Study Director for the 5-year Master (siv.ing.) program in Chemical and Biochemical Engineering at NTNU (about 100 new students per year).

Fellowships and awards

1979 *Instilling* awarded for the *Siv.ing* degree (result communicated to the Norwegian King)

1983 Fullbright Fellowship (travel grant) awarded for graduate studies at Caltech

1983 *Utdanningsstipend* awarded from Univ. of Trondheim for graduate studies at Caltech

1989 *Ted Peterson Best Paper Award* by the CAST division of AIChE (The American Institute of Chemical Engineers)

1990 *George S. Axelby Outstanding Paper Award* by the Control System Society of IEEE (The Institute of Electrical and Electronic Engineers)

1992 *Hugo Schuck Best Paper Award* by the American Automatic Control Council
2006 *Best t paper award* for paper published in 2004 in *Computers and chemical engineering*
2019 *Best paper award at the ESCAPE 2019 Symposium (Eindhoven, June 2019)*

2019 *Computing in chemical engineering award from the American Institute of Chemical Engineers (Orlando, 12 Nov. 2019)*

Membership of scientific societies

1988 Elected Member to the Norwegian Academy of Tehnical Sciences (NTVA)

1991 Elected member to Det Kongelige Norske Vitenskapers Selskab

2008-2014 Member of IFAC Technical Board

2011 Elected member of Process Automation Hall of Fame, Delaware, USA

2012 Elected Fellow of American Institute of Chemical Engineers (AIChE)

2014 Elected Fellow of International Federation of Automatic Control (IFAC)

2015 Elected member to *The Norwegian Academy of Science and Letters*, Oslo

2015 Honorary member of *Norwegian Society of Automatic Control*

Track record

- I have published about 230 international journal publications and 330 conference publications
- H-index (Web of Science): 54 (2024).
- H-index (Google scholar): 76 (2024)
- Author of 2 international text books. (1) S. Skogestad and I. Postlethwaite, ``Multivariable feedback control -analysis and design,'' Wiley (1996); 2nd Edition (2005). (2) S. Skogestad, ``Chemical and energy process engineering'', CRC Press (2009).
- No. of citations to book Multivariable feedback control: 12161 (Google scholar, 2024)

Recent Publications

2024

1. Optimal measurement-based cost gradient estimate for feedback real-time optimization. LF Bernardino, S Skogestad Computers & Chemical Engineering, 108815 2024
2. Reinforcement learning based MPC with neural dynamical models S Adhau, S Gros, S Skogestad. European Journal of Control, 101048 2024
3. Primal-dual feedback-optimizing control with override for real-time optimization R Dirza, S Skogestad. Journal of Process Control 138, 103208 3 2024
4. Decentralized control using selectors for optimal steady-state operation with changing active constraints. LF Bernardino, S Skogestad. Journal of Process Control 137, 103194 5 2024
5. Understanding Temperature Profiles of Distillation Columns LM Ranger, IJ Halvorsen, T Grutzner, S Skogestad Industrial & Engineering Chemistry Research 63 (10), 4533-4546 2024
6. Model Predictive Control for Bottleneck Isolation with Unmeasured Faults EM Turan, S Skogestad, J Jaschke.IFAC Adchem conference, 2024

2023

1. The theoretical basis of ratio control S Skogestad 2023 AIChE Annual Meeting 1 2023
2. Steady-state and dynamic model for recirculating aquaculture systems with pH included AM dos Santos, LF Bernardino, KJK Attramadal, S Skogestad Aquacultural Engineering 102, 102346 5 2023
3. Home Energy Management with Dynamic Tariffs and Tiered Peak Power Charges D P�rez-Pi�eiro, S Skogestad, S Boyd arXiv preprint arXiv:2307.07580 2023
4. Transformed inputs for linearization, decoupling and feedforward control S Skogestad, C Zotica, N Alsop. Journal of process Control 122, 113-133 13 2023
5. Advanced control using decomposition and simple elements S Skogestad Annual Reviews in Control 56, 100903 24 2023
6. Bidirectional inventory control with optimal use of intermediate storage and minimum flow constraints LF Bernardino, S Skogestad IFAC-PapersOnLine 56 (2), 2665-2670 5 2023
7. Decentralized control for optimal operation under changing active constraints LF Bernardino, S Skogestad Computer Aided Chemical Engineering 52, 1699-1704 2023

2022

1. Experimental validation of distributed feedback-based real-time optimization in a gas-lifted oil well rig R Dirza, J Matias, S Skogestad, D Krishnamoorthy Control Engineering Practice 126, 105253 4 2022
2. Deoiling Hydrocyclones: An Experimental Study of Novel Control Schemes M Vallabhan KG, C Holden, S Skogestad SPE Production & Operations 37 (03), 462-474 6 2022
3. Real-time optimization as a feedback control problem, A review. D Krishnamoorthy, S Skogestad Computers & Chemical Engineering 161, 107723 45 2022
4. Bidirectional inventory control with optimal use of intermediate storage C Zotica, K Forsman, S Skogestad Computers & Chemical Engineering 159, 107677 7 2022
5. Real-time optimal resource allocation using online primal decomposition R Dirza, M Rizwan, S Skogestad, D Krishnamoorthy IFAC-PapersOnLine 55 (21), 31-36 2 2022
6. Online Feedback-based Optimization with Multi-input Direct Constraint Control R Dirza, S Skogestad IFAC-PapersOnLine 55 (7), 149-154 2 2022
7. Control of steam bottoming cycles using nonlinear input and output transformations for feedforward disturbance rejection C Zotica, RM Montanes, A Reyes-LUa, S Skogestad IFAC-PapersOnLine 55 (7), 969-974 8* 2022
8. Comparison of simple feedback control structures for constrained optimal operation LF Bernardino, D Krishnamoorthy, S Skogestad IFAC-PapersOnLine 55 (7), 883-888 4 2022
9. Optimal control of water quality in a recirculating aquaculture system AM dos Santos, KJK Attramadal, S Skogestad IFAC-PapersOnLine 55 (7), 328-333 6 2022
10. Soft Sensor of Key Components in Recirculating Aquaculture Systems, using Feedforward Networks AM dos Santosa, E Karlsen, S Skogestad, KJK Attramadal Computer Aided Chemical Engineering 51, 1495-1500 2022
11. Systematic Pairing Selection for Economic-oriented Constraint Control R Dirza, S Skogestad Computer Aided Chemical Engineering 51, 1249-1254 2 2022
12. Optimal operation of heat exchanger networks with changing active constraint regions LF Bernardino, D Krishnamoorthy, S Skogestad Computer Aided Chemical Engineering 49, 421-426 4 2022
13. Primal-dual feedback-optimizing control with direct constraint control R Dirza, D Krishnamoorthy, S Skogestad Computer Aided Chemical Engineering 49, 1153-1158 3 2022

Short curriculum vitae

Role in the project Project manager ☐ Project partner ☒

Personal information

First name, Surname:	Idelfonso Bessa dos Reis Nogueira		
Position	Associate Professor Norwegian University of Science and Technology		
Date of birth:	13-02-1988	Sex:	Male
Nationality:	Brazilian		
Researcher unique identifier(s) (ORCID, ResearcherID, etc.):	ORCID: 0000-0002-0963-6449 Scopus: 57035118100		
URL for personal website:	https://www.ntnu.edu/employees/idelfonso.b.d.r.nogueira		

Education

Year	Faculty/department - University/institution - Country
2018	Ph.D. in Chemical and Biological Engineering Faculty of Engineering/ Department of Chemical Engineering, University of Porto, Portugal
2016	Master in Industrial Engineering Polytechnic Institute/ Department of Chemical Engineering, Federal University of Bahia/ Post-graduation Program in Industrial Engineering, Brazil
2012	Master in Chemical Engineering Faculty of Engineering/Department of Chemical Engineering, University of Porto, Portugal

Positions - current and previous

Year	Job title – Employer - Country
Current	Associate Professor in Process Systems Engineering Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway
2021 – 2022	Invited Assistant Professor Department of Biological and Chemical Engineering, University of Minho, Portugal
2021 – 2022	Invited Assistant Professor Polytechnic Institute/Department of Chemical Engineering, Federal University of Bahia, Brazil
2018 – 2022	Contracted Researcher LSRE-LCM, Department of Chemical Engineering, Faculty of Engineering, University of Porto, Portugal
2016 – 2017	Visiting Researcher Tampere University of Technology/Department of Automation Science and Engineering /Finland
2013 – 2014	Invited Assistant Professor Polytechnic Institute/ Department of Chemical Engineering, Federal University of Bahia, Brazil

2013 – 2014	Project Engineer WG Projects LTDA, Brazil
2012 – 2012	Chief of Production IDEBA, Brazil

Project management experience

Year	Project owner - Project - Role - Funder
2024 - current	Belmont Forum. SCENTinel | Climate Changes and Scent Heritage: The Urgent Need for Capturing and Preserving Olfactory Landscapes in a Changing World. Project Coordinator.
2024 - current	Water4All. A smart process for water harvesting from air and water distribution based on eco-friendly MOFs. Funding: RCN/Horizon Europe. Coordinator pilar 1, and WP leader.
2024 - current	Marie Skłodowska-Curie Actions Doctoral Networks. Smart Integration of Process Systems Engineering & Machine Learning for Improved Process Safety in Process Industries. Funding: Horizon Europe. Partner and Member of Supervisors Board.
2024 - current	Hydrogeni. Centre for Environment-friendly Energy Research, FME. AI-Driven Flowsheet Innovation for Sustainable Blue Hydrogen: Design and Optimization for Energy and Emission Reduction. Project Supervisor.
2024 - current	Petrobras. Dynamic modelling of decision-making processes in technological development. Technical Coordinator.
2022 - current	Petrobras, Intelligent Control System for Artificial Elevation in offshore fields, Coordinator of NTNU team.
2022 - current	Simoldes/NTNU, Development of Solid State Batteries, Coordinator
2022 – 2023	Investment and Development Agency of Latvia, Scent reproduction by AI, Coordinator
2021 – 2023	MIT-FCT, Cyber-physical oriented chemical process for the separation of biopharmaceutical compounds from natural extracts, Supervisor
2021 – current	MIT-FCT, A novel Cyber-physical prototype for on-demand perfume optimal design and production, Supervisor
2018 – 2021	FCT, A disruptive Cyber-Physical System-oriented autonomous chemical plant: a virtualizable, cooperative, self-manageable, and green approach, Coordinator.
2018 – 2022	Korea Research Institute of Chemical Technology, Development of package process of reaction and separation in refinery and petrochemical industry, Team member.

Supervision of students

(Total number of students)

Master's students	Ph.D. students	University/institution - Country
22	13	Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway

		Doctoral Program in Chemical and Biological Engineering, Department of Chemical Engineering, Faculty of Engineering, University of Porto, Portugal Postgraduation Program in Industrial Engineering, Department of Chemical Engineering, Federal University of Bahia, Brazil Postgraduation Program in Mechatronics, Department of Control and Automation Engineering, Federal University of Bahia, Brazil Postgraduation Program in Chemical Engineering, Department of Chemical Engineering, Federal University of Rio de Janeiro, Brazil

Other relevant professional experiences

Year	Description - Role
2022 – current	International Federation of Automatic Control (IFAC) - Technical Committee 6.1- Chemical Process Control, Member
2020 – current	Founding Member, Coordinator, Research Network "A*rtificial Intelligent oriented Cyclic Adsorption Separation and Reaction Processes Optimization and Control (AICySPrOC)*"
2020 – current	External Member, Polytechnic Institute/ P2S - Processes and Sustainable Products, Federal University of Bahia/ Brazil
2013 – 2016	Manager Member, Polytechnic Institute/Group of Research in Uncertainty GI-UFBA, Federal University of Bahia/ Brazil
2021	Scientific Cometee, 4rd International Conference on Machine Learning and Intelligent Systems (MLIS 2022) Seoul, Republic of Korea
2020	Scientific Cometee, 3rd International Conference on Machine Learning and Intelligent Systems (MLIS 2022) Online
2019	Scientific Cometee, 2rd International Conference on Machine Learning and Intelligent Systems (MLIS 2022) China
2019	Scientific Cometee, International Conference on Machine Learning and Intelligent Systems National Dong Hwa University – Taiwan.
2019	Program Cometee, 2nd Sensor Networks and Signal Processing (SNSP 2019), Hualien, Taiwan
2018 – Current	I have been acting as a reviewer in several renewed international journals such as: Soft Computing, Computers & Chemical Engineering, Chemical Engineering Science, Processes, AI. Furthermore, I have been an editor and guest editor of several special issues.

Track record

- I have published over 75 manuscripts, ~70% in Q1 Scimago rank and ~25% in Q2 Scimago rank. 884 citations, h-index: 16 (Google Scholar)