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Post-Doctoral Research Associate in AI-Driven Process Modelling and Control

Department/Division/Faculty:	Department of Computing, Faculty of Engineering
Campus/Location:	South Kensington, London
Job Family/Level:	Research Job Family, Research Associate (Research salary scale)
Responsible to:	Dr Calvin Tsay
Line management for:	N/A
Key working Relationships:	Internal staff and students within the Departments of Computing and Chemical Engineering, and the industry partner
Contract type:	Full-time, Fixed term for 12 months from January 2027 (flexible starting date)

Purpose of the Post

We are looking for a Research Associate (post-doctoral) to conduct research in AI-enabled process modelling and optimisation, as part of a new collaboration between Repsol S. A. and Imperial College London. We will study two interlinked objectives: (1) the automated generation of dynamic process models using large language models (LLMs), and (2) the data-driven discovery of control strategies trained on those models, focusing on the sim-to-real transfer gap. The work will be validated using real-world industrial case studies and is designed to produce both publishable scientific contributions and deployable engineering/software tools.

The successful candidate will collaborate with Dr Calvin Tsay in the Department of Computing, along with Dr Antonio del Río Chanona and Dr Mehmet Mercangöz in the Department of Chemical Engineering, and with relevant process modelling teams at Repsol S.A., who will provide access to real-world operating data and case studies. Furthermore, they will be a member of the broader Sargent Centre for Process Systems Engineering at Imperial College London.

Alongside research and publication, the Research Associate will be expected to contribute to developing, documenting, and maintaining software tools arising from the project, with the aim of releasing stable AI-enabled workflows. This role may include:

- Building frameworks to couple AI models with process simulators.
- Designing learned representations for dynamic process systems.
- Studying data-driven and hybrid control systems.
- Conducting independent and collaborative research within the group.
- Publishing results in leading venues across applied AI (e.g., Engineering Applications of Artificial Intelligence, AAAI), process control (e.g., IEEE CDC, Journal of Process Control), and process systems engineering (e.g., Computers & Chemical Engineering).
- Contributing to research projects involving optimisation and machine learning.
- Contributing to the life and development of Calvin Tsay's group, including weekly meetings, presentations, maintaining the website and other resources.
- Delivering tutorials at conferences and summer schools.
- Mentoring PhD and MSc students.
- Presenting research at international conferences and workshops.
- Contributing to grant proposals and collaborative research initiatives.

Further information on the research of Drs del Río Chanona, Mercangöz, and Tsay, as well as the Sargent Centre can be found at https://www.optimlpse.co.uk, https://profiles.imperial.ac.uk/m.mercangoz, https://www.doc.ic.ac.uk/~ctsay/, and https://www.imperial.ac.uk/process-systems-engineering/.

The post will be based in the Department of Computing at Imperial College London at the South Kensington Campus. The Department of Computing is a leading department of Computer Science in the UK and the world and has consistently been awarded the highest research rating. In the 2021 REF assessment, the Department claimed the top spot for computer science and informatics. Overall, Imperial College London ranked first in the UK for research outputs, first in the UK for research environment, and first for research impact among Russell Group universities.

The position is fully funded for 12 months in the first instance, with extension subject to funding. This project includes funding for equipment and travel.

Key Responsibilities

Main Duties:

- To plan and carry out scientific research in accordance with project aims.
- To propose and investigate new techniques and frameworks for AI-enabled process modelling.
- To conduct data analysis and always ensure the validity and reliability of data.
- To collaborate and cooperate with researchers and industrial partners of the project.
- To maintain organised, accurate, and complete records of all findings.
- To write reports for submission to research sponsors.
- To present findings to colleagues and at conferences.
- To submit publications to refereed journals .
- To attend relevant workshops and conferences as necessary.
- To develop contacts and research collaborations within the College and Sargent Centre community.
- To promote the reputation of the Group, the Department, and the College.

- To provide guidance to UG and PhD Students as required.
- To actively participate in the research group, including research meetings and internal seminars.
- To comply with the College, Division, and Unit safety practices and to attend courses on safety when appropriate.
- Any other duties as may be deemed reasonable by the PI as well as Head of Division / Department / Section.

Other Duties:

- To undertake any necessary training and/or development.
- To undertake appropriate administration tasks.
- To attend relevant meetings.
- To contribute to bids for research grants.

Where Imperial or funder conditions necessitate, you will be required to complete timesheets for your work on projects in a timely manner.

About Imperial. Imperial College is globally recognized, consistently ranking among the top 10 universities worldwide and holding high accolades for research excellence. The Department of Computing is rated 1st in Research Intensity and has been recognized as "Excellent" in the national assessment of teaching quality. This is your opportunity to be part of a world-leading institution driving forward computational sciences.

Person Specification

Requirements Candidates/post holders will be expected to demonstrate the following:	**Essential(E)/ Desirable (D)**
Education	
Hold a PhD (or be close to completion) in an area pertinent to the subject area, i.e., Computer Science, Chemical Engineering, Operations Research, or a closely related discipline. **Candidates who have not yet been officially awarded their PhD will be appointed as Research Assistant.*	E
Experience	
Practical experience within a research environment and publications in top conferences or journals in the field.	E
Experience of dealing with industry partners and research collaborators	D
Experience in applied AI, process systems engineering, mathematical optimisation, and/or applied mathematics	E
Practical experience in a broad range of techniques for data-driven control, including data-driven MPC, system identification, and/or reinforcement learning	D

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Knowledge

Knowledge of research methods, experimentation and statistical tests. Knowledge of AI and LLMs, and excellent skills in coding.	E
Strong foundations in process systems engineering (especially dynamic process modelling, simulation, and control)	E
Familiarity with process modelling tools, e.g., CasADi or gPROMS	D

Skills & Abilities

Ability to conduct a detailed review of recent literature	E
Ability to develop and apply new concepts	E
Creative approach to problem-solving	E
Excellent verbal communication skills and the ability to deal with a wide range of people	E
Excellent written communication skills and the ability to write clearly and succinctly for publication	E
Ability to organise own work with minimal supervision	E
Ability to prioritise own work in response to deadlines	E
Advanced tools for writing and experiment tracking, including LaTeX and frameworks like Weights and Biases.	D
Willingness to work as part of a team and to be open-minded and cooperative	E
Flexible attitude towards work	E
Discipline and regard for confidentiality and security at all times	E
Willingness to undertake any necessary training for the role	E
Willingness to travel both within the United Kingdom and abroad to conduct research and attend conferences	E
Willingness to work out of normal working hours (to a reasonable extent) if the requirements of the project demand	E

Further Information

Please note that job descriptions cannot be exhaustive, and the post-holder may be required to undertake other duties, which are broadly in line with the above key responsibilities.

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- Respect
- Collaboration
- Excellence
- Integrity
- Innovation

Employees are also required to comply with all Imperial policies and regulations.

We are committed to equality of opportunity, to eliminating discrimination and to creating an inclusive working environment for all. We encourage candidates to apply irrespective of age, disability, marriage or civil partnership status, pregnancy or maternity, race, religion and belief, gender reassignment, sex, or sexual orientation. You can read more about our commitment on our webpages.

Imperial is a proud signatory to the San-Francisco Declaration on Research Assessment (DORA), which means that in hiring and promotion decisions, we evaluate applicants on the quality of their work, not the journal impact factor where it is published. For more information, see https://www.imperial.ac.uk/research-and-innovation/about-imperial-research/research-evaluation/

Imperial believes that the use of animals in research is vital to improve human and animal health and welfare. Animals may only be used in research programmes which are ultimately aimed towards finding new treatments and making scientific and medical advances, and where there are no satisfactory or reasonably practical alternatives to their use. Imperial is committed to ensuring that, in cases where this research is deemed essential, all animals in our care are treated with full respect, and that all staff involved with this work show due consideration at every level. Find out more about animal research at Imperial.

November 2026