2026 Helmholtz – OCPC – Program

for the involvement of postdocs in bilateral collaboration projects

Title of the project:

Multi-Physics Simulation and PINN-Based Surrogate Modelling of Hydrogen Behaviour in Porous Media for Clean Energy Systems

Helmholtz Centre and/or institute:

Karlsruhe Institute of Technology (KIT), Institute of Thermal Energy Technology and Safety

Project leader:

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Description of the project:

Research Background and Scientific Challenges

The efficient and safe utilization of hydrogen in porous media systems faces challenges such as unclear multi-physics coupling mechanisms and difficulties in scale correlation. Existing simulation methods for describing the complex coupling of "flow-reaction-heat transfer-structure" incur high computational costs and are difficult to apply directly at engineering scales. In particular, the relationship between pore-scale mechanisms and system-level performance has not been established, hindering the optimal design and safety assessment of hydrogen engineering equipment. This study integrates multi-physics simulations with Physics-Informed Neural Networks (PINN) to bridge the gap from microscopic mechanisms to macroscopic engineering applications.

Research Objectives

- Establish high-fidelity multi-physics coupling simulation methods for hydrogen in porous media, revealing pore-scale reaction-transport-heat transfer coupling mechanisms.
- Develop PINN-based surrogate models to enable rapid computation and parameter inversion of multi-physics processes.
- Establish cross-scale correlation from pore-scale to engineering-scale, providing a foundation for the design of practical hydrogen-based energy equipment.
- Formulate safety design criteria and performance optimization strategies based on multi-physics mechanisms.

Methodology and Technical Approach

- High-fidelity multi-physics coupling simulation and mechanism research.
- Deep learning-enhanced modeling (PINN applications).
- Cross-scale correlations from microscopic mechanisms to macroscopic engineering.

Expected Outcomes

- A high-fidelity computational framework for multi-physics coupling of hydrogen in porous media.
- PINN-enhanced rapid computation tools.
- Cross-scale correlations and engineering models implemented in CFD code for supporting the optimal design of hydrogen-based energy equipment.

Research Significance and Engineering Value

- Scientific significance: Reveal multi-scale multi-physics coupling mechanisms in porous media.
- Engineering value: Multi-scale optimal design of hydrogen-based energy systems. Safety assessment and leakage prevention for hydrogen systems.
- Industry Support: Provide theoretical and technical support for the large-scale commercialization of hydrogen energy.

Research Plan

Research Duration: October 2026 – October 2028 (24 months), with the possibility of a one-year extension subject to funding availability and research progress.

- Phase 1 (Months 1-10): High-fidelity simulations of multi-physics coupling in porous media; design and preliminary training of the PINN framework.
- Phase 2 (Months 11-17): Establishment of cross-scale correlations; development and validation of engineering foundation models; optimization of PINN tools.
- Phase 3 (Months 18-24): Validation through engineering case studies; tool integration and finalization of outcomes.

Description of existing or sought Chinese collaboration partner institute:

This project welcomes research collaboration with all universities, academic institutions, and public research organizations in China. We are actively seeking to establish partnerships with Chinese research groups whose expertise aligns with the scientific objectives of this initiative, particularly those with demonstrated strength in hydrogen energy, multi-physics simulation, and deep learning-based modelling methods. At present, no specific Chinese collaborating institution has been formally assigned or engaged. This collaboration is envisioned as a long-term, mutually beneficial partnership contributing to the global advancement of clean hydrogen technologies. We look forward to identifying and working with Chinese partners who share our vision and scientific ambition.

Required qualification of the postdoc:

- A Ph.D. in applied physics, mechanical engineering, chemical engineering, energy science, or a closely related interdisciplinary field.
- Extensive hands-on experience with Computational Fluid Dynamics (CFD) software packages.
- Demonstrated capability in developing, modifying, or extending solver functionalities for reactive and multi-physics flows.
- Strong programming proficiency in languages such as C/C++, Python, Fortran, or MATLAB, with experience in high-performance computing environments.
- Excellent collaborative and interpersonal skills, with the ability to work effectively in an interdisciplinary, multicultural research team.
- Exceptional command of written and spoken English.
- Self-motivated, with strong problem-solving abilities and the capacity to conduct independent research.