Upgrade of the Python package $\mathrm{lbh15}$ with the integration of liquid-metal thermochemical properties

– Internship proposal –
(ID No. 1000377)

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newcleo SrL, Via Galliano 27, 10129 Torino, Italy

November 30, 2022

Keywords — LMFR, thermochemical properties, chemistry control, Python
Topics — Material corrosion, Elements' solubility, diffusivity and interaction with liquid metals

Location	*new*cleo SrL, Via Galliano 27, 10129 Torino, Italy
Starting date	First or second quarter of 2023
Duration	4 months

Context

Chemical control of the primary coolant in liquid-metal nuclear reactors is of crucial importance during plant operation, preventing alteration or degradation of materials such as steel and other structural alloys by corrosion. Control is usually operated by releasing hydrogen and oxygen within the coolant, and ensuring homogeneous dilution in the mixture. Eventually, the control system considers also purification of the coolant from activation products. Therefore, *new*cleo's activities on lead chemical control are the objects of intensive studies, both in terms of experiments and theoretical modeling. In order to support both types of activities, the Python package $\mathrm{lbh15}$ is under active development to offer an unique and standardized entry point for the use of empirical correlations of physical properties.

Description

$\mathrm{lbh15}$ (**L**ead **B**ismuth **H**andbook 20**15**) is a Python package developed by *new*cleo based on the reference handbook edited by OECD-NEA [1], as contribution to the expert group on heavy liquid metal technologies. The first version of $\mathrm{lbh15}$ was released on September 21 2022,

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implementing a first batch of thermal properties of molten lead (Pb), bismuth (Bi) and of their eutectic alloy (LBE). The package documentation and repository can be found at
`https://newcleo-dev-team.github.io/lbh15/index.html` and
`https://github.com/newcleo-dev-team/lbh15`, respectively.

The properties are implemented as analytical functions from empirical correlations. The package contains also elementary services for function characterization that use the standard Python packages for scientific computation, namely NumPy and SciPy.

During this internship, the student will develop new features in `lbh15`. Specifically, the student will work on the integration of the following topics inside the package:

a) solubility and diffusivity of metallic elements in Pb, Bi, LBE;

b) solubility of oxygen, its diffusivity and interaction with Pb, Bi, LBE;

c) interaction of water with Pb, Bi, LBE;

d) chemistry control and monitoring system.

These topics are covered in chapters 3 and 4 of the above-mentioned handbook.

`lbh15` adopts high quality standards for code development. Hence, the student will develop/consolidate skills in the following aspects of software engineering with Python:

• Object-Oriented programming based on SOLID principles;

• Python Dynamic programming;

• Design patterns (template and factory patterns in particular);

• CI/CD pipelines (including regression tests);

• Write well-documented code for scientific applications.

The student will be followed by the engineering team of *new*cleo that is developing `lbh15`, together with an engineer from the safety team to identify the main correlations that the package shall provide.

Work plan

1) Handbook review and identification of the main correlations to implement

2) Code architecture design

3) Code implementation

4) Test definition and implementation

5) Preparation of a technical report

Applicant profile

Master student in Nuclear, Chemical or Software Engineering; Applied Physics; Chemistry; Computer science.
Skills and background:

• Fundamentals in thermodynamics and chemistry

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- Basic knowledge of software programming (previous experience in Python appreciated but not fundamental)
- Basic knowledge of Linux operative system

Nice to have: experience using git, basic knowledge on liquid metal-cooled fast reactors.

References

[1] C. Fazio et Al. Handbook on Lead-bismuth Eutectic Alloy and Lead Properties, Materials Compatibility, Thermal-hydraulics and Technologies. Technical Report No. 7268, OECD/Nuclear Energy Agency (NEA), Paris, France, 2015.

[2] Ning Li. Active control of oxygen in molten lead–bismuth eutectic systems to prevent steel corrosion and coolant contamination. *Journal of Nuclear Materials*, 300(1):73–81, 2002.

[3] Mariano Anaya. *Clean Code in Python: Refactor your legacy code*. Packt Publishing, Birmingham, 2018.

Development of a Python package with thermal-hydraulic correlations for LMFR – $\mathrm{lmth23}$

– Internship proposal –
(ID No. 1000378)

Daniele Tomatis [*] and Daniele Panico

newcleo SrL, Via Galliano 27, 10129 Torino, Italy

November 30, 2022

Keywords — LMFR, physical correlations, heat exchange, friction factor, fuel bundles, Python
Topics — Heat transfer, thermal-hydraulics, frictional pressure loss, python programming

Location	*new*cleo SrL, Via Galliano 27, 10129 Torino, Italy
Starting date	First or second quarter of 2023
Duration	4–5 months

Context

*new*cleo is preparing a large experimental campaign of thermal-hydraulic experiments to support the design activities for new LFR units. A compilation of the available empirical correlations from literature in a single and comprehensive library is currently on-going to characterize heat transfer and thermal-hydraulic phenomena with liquid metals. This library will also collect the results from the future experiments. This internship position focuses on the literature review about the existing correlations and supports the development of this library.

Description

Several empirical correlations are available in literature to describe heat transfer, thermal-hydraulics and pressure drop phenomena occurring in presence of liquid metals, which are used as coolant for nuclear fast reactors. Every physical correlation comes with its validity range given in terms of dimensionless numbers, flow conditions, and for particular geometrical configurations. The use of a correlation outside the validity range does not guarantee accurate

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predictions of the quantity of interest. So a careful check about the correlation's appropriateness must be done before use.

Some correlations yield directly dimensionless numbers, expressing the importance of a given phenomenon with respect to other competing ones, like in the case of the Nusselt number that measures the ratio between heat transfer by convection and heat transfer by conduction alone. Indeed, heat transfer and pressure drop correlations (Darcy factor for instance) are fundamental for the design of heat exchangers, which constitutes a large part of the forthcoming experimental program planned by *new*cleo.

Unfortunately, it is difficult to find a comprehensive and compact tool to make such correlations readily available for engineers when designing LFR components. For this reason, *new*cleo is implementing a Python package as unique and standardized entry point for evaluating all the empirical correlations needed for general LMFR applications. Moreover, this package will be used to support the next experimental campaign, including possible implementation of the new correlations arising from it.

During this internship the student will participate to the development of the Python package `lmth23` (Liquid-Metal Thermal-Hydraulics).

In particular, the correlations for the friction factor and for the Nusselt number in LMFR fuel bundles and once-through heat exchangers with cross-flow will be considered. A wide list of correlations for the friction factor can be found in [1]. Instead, correlations for the Nusselt number are given in [2]. The first release of the package will provide the desired quantity given the characteristic geometric parameters and coolant velocity at input to calculate the Reynolds number appropriately. In addition to reviewing and implementing the physical correlations, the student will focus on implementation techniques and high quality standards for code development. This will make the package easier to maintain and extend in the future, serving both uses in industry and research. Therefore, the student will develop/consolidate skills in the following aspects of software engineering in Python:

- Object-Oriented programming based on SOLID principles;
- Python Dynamic programming;
- design patterns (template and factory patterns in particular);
- CI/CD pipelines (including regression tests);
- write well-documented code for scientific applications.

The internship will be supervised by an engineer from R&D team of *new*cleo.

Work plan

1) Literature review and identification of the main correlations to implement
2) Code architecture design
3) Code implementation
4) Definition and implementation of tests
5) Preparation of a technical report

Applicant profile

Master student in Nuclear, Mechanical or Aerospace Engineering; Applied Physics; Informatics and Computational Sciences.
Skills:

- Fundamentals in thermal-hydraulics and heat transfer

- Basic knowledge of software programming (previous experience in Python is very appreciated)

- Basic knowledge of Linux operative system

Nice to have: experience using git, basic knowledge on liquid metal-cooled fast reactors.

References

[1] S.K. Chen, N.E. Todreas, and N.T. Nguyen. Evaluation of existing correlations for the prediction of pressure drop in wire-wrapped hexagonal array pin bundles. *Nuclear Engineering and Design*, 267:109–131, 2014.

[2] Konstantin Mikityuk. Heat transfer to liquid metal: Review of data and correlations for tube bundles. *Nuclear Engineering and Design*, 239(4):680–687, 2009.

[3] Mariano Anaya. *Clean Code in Python: Refactor your legacy code*. Packt Publishing, Birmingham, 2018.

Assessment of neutronic data for the calculation of LFR fuel rods by TRANSURANUS

– Internship proposal –
(ID No. 1000360)

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November 15, 2022

Location	*new*cleo SrL, Via Galliano 27, 10129 Torino, Italy
Starting date	As soon as possible
Duration	3–4 months

Context

*new*cleo is designing new Lead-cooled Fast Reactor (LFR) units for small and modular reactors using MOx fuel. At *new*cleo, fuel performance analysis is performed by the thermo-mechanical computer code TRANSURANUS (TU) distributed by the Joint Research Center of the European Commission based in Karlsruhe, Germany. *new*cleo has started a careful review of the code in order to ensure its suitability and fitness for the applications with LFR fuel rod types that are currently under design. Such work is also meant producing an upgraded version of the code to extend its range of applications, and in particular, to provide reliable predictions when modelling LFR fuel rods. The goal of this internship is to produce new neutronic data by Monte Carlo calculations that is needed for the TU calculations of LFR fuel rods.

Description

During this internship, the student will perform Monte Carlo calculations of LFR fuel rods by the computer code OpenMC to prepare neutronic data needed by the simplified burnup models implemented in TU. The data represent microscopic one-group reaction rates for the nuclides

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considered in the reduced decay chain of TU. The calculations are requested for both fresh and irradiated fuel, and at different exposure periods. The approach of data preparation will be validated against existing TU data used for LWR fuel types.

Among the target data, the student will have to find feasible and valid means to estimate the radial power distribution inside the hollow fuel pellets by fine tallies, still achieving narrow statistical uncertainty around the expected values in reasonable time. Approximation in the definition of the problem to match the expected critical conditions at operation will be necessary. The production of a technical report is expected at the end of the internship to describe the work done by the student and to compile the analysis of the results.

Work plan

1. Problem discussion and definition
2. Setup of calculations by OpenMC
3. Validation of the approach by comparisons with existing data
4. Analysis of results
5. Preparation of a technical report

Applicant profile

Master or PhD student in Nuclear Engineering. Students in theoretical Physics and applied Mathematics will also be considered for the position.
Background: *fundamentals in Monte Carlo methods for neutral particle transport*.
Required computer skills: Python programming, linux, FORTRAN and LaTeX scientific editing (optional).

References

[1] K Lassmann. TRANSURANUS: a fuel rod analysis code ready for use. *Journal of Nuclear Materials*, 188:295–302, 1992.

[2] K Lassmann and H Blank. Modelling of fuel rod behaviour and recent advances of the TRANSURANUS code. *Nuclear Engineering and design*, 106(3):291–313, 1988.

[3] Paul K Romano, Nicholas E Horelik, Bryan R Herman, Adam G Nelson, Benoit Forget, and Kord Smith. OpenMC: A state-of-the-art Monte Carlo code for research and development. *Annals of Nuclear Energy*, 82:90–97, 2015.

[4] Jerome Spanier and Ely M Gelbard. *Monte Carlo principles and neutron transport problems*. Dover Publications, Inc., Mineola, New York, 2008.

Modeling of once-through thermal channels with phase separation by centrifugal force

– Internship proposal –
(ID No. 1000073)

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[2] *Politecnico di Torino, Dipartimento Energia, Corso Duca degli Abruzzi 24, 10127, Torino, Italy*

September 27, 2022

Location	*new*cleo SrL, Via Galliano 27, 10129 Torino, Italy
Starting date	As soon as possible
Duration	5–6 months

Context

*new*cleo has planned an experimental campaign with external partners in order to optimize the design of components for lead-cooled fast reactors. In this framework, mathematical models of the components are needed to reproduce accurately their physical behavior, with the aim of supporting design studies. This internship is proposed to students attending the last year of the Master program in Nuclear Engineering with particular interest in thermal-hydraulics and heat transfer. This internship work could possibly continue with a PhD program.

Description

During this internship, the student will develop a mathematical model of a once-through heat exchanger of bayonet type presenting innovative features capable of preventing possible unstable operation. Such exchangers are made of coaxial tubes, as schematically shown in Figure 1. Subcooled water enters from the top of the inner tube and flows downwards. After, it enters the

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outer tube, where it flows upwards while being heated by the surrounding lead, eventually leaving the system as superheated steam. The flow boiling occurs in helicoidal parallel channels within the outer tube, so that inertial phase separation is expected radially because of the centrifugal force. The outer tube constitutes an inert zone filled by helium to guarantee separation between water and lead. The physical model must describe the different flow boiling regimes encountered within the outer tube, accounting for the presence of inertial phase separation due to the centrifugal force. The full technical details will be provided during the internship, after acceptance of the candidate.

A complete literature review is requested to find the most appropriate physical correlations characterizing the flow and the heat transfer in the channels. The heat exchange between neighbouring channels can be neglected as first approximation (adiabatic assumption). The student will derive the conservation equations to describe the thermal-hydraulic model of the system, and check the validity of suitable closure relations and physical correlations used in the model. The development of a Python code solving the identified equations is requested, with the verification of the numerical solution on simplified case problems. Finally, preliminary investigations about the validation of the model are expected at the end of the internship, despite the complete validation against other computer codes is postponed for future work. At the end of the internship, the preparation of a technical report is expected to describe the work done by the student and to compile the analysis of the results.

This internship will be supervised by an engineer from *new*cleo and the academic staff at PoliTo. This study supports the preparation of an experimental facility whose construction is planned in 2023.

Work plan

1. Literature review and retrieval of the existing work
2. Discussion of the problem
3. Derivation of conservation equations in the channel (adiabatic conditions among channels)
4. Assessment of the physical correlations to characterize the flow and the heat transfer
5. Implementation and verification of the numerical solution
6. Analysis of results and proposal of validation plan
7. Model upgrade with intra-channel heat exchange (optional)
8. Preparation of a technical report

Applicant profile

Master or PhD student in Nuclear, Mechanical or Aeronautical Engineering.
Fundamentals in thermal-hydraulics and heat transfer, multiphase flow.
Required computer skills: Python programming, linux (optional).

References

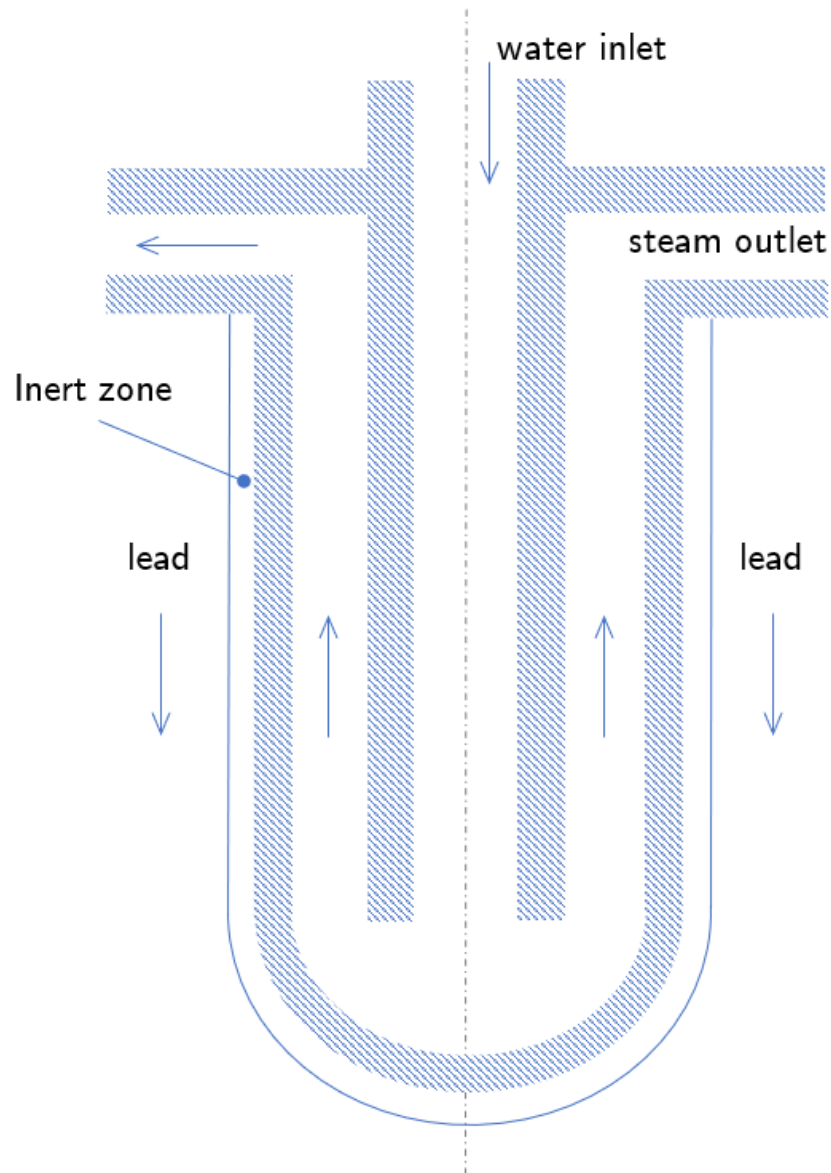[1] N. E. Todreas and M. S. Kazimi. *Nuclear systems Volume I: Thermal hydraulic fundamentals*. CRC press, 2021.

Figure 1: Schematic of a bayonet tube heat exchanger.

[2] N. E. Todreas, M. S. Kazimi, and M. Massoud. *Nuclear systems Volume II: Elements of thermal hydraulic design*. CRC press, 2021.

[3] A. Bersano, N. Falcone, C. Bertani, M. De Salve, and B. Panella. Conceptual design of a bayonet tube steam generator with heat transfer enhancement using a helical coiled downcomer. *Progress in Nuclear Energy*, 108:243–252, September 2018.

[4] D. Rozzia, A. Toti, M. Tarantino, L. Gramiccia, D. Vitale Di Maio, and F. Giannetti. Double-wall bayonet tube steam generator for LFR application – preliminary characterization. Technical Report NNFISS-LP3–032, ENEA Ricerca Sistema Elettrico, Italy, 2011.

Development of the thermal model of a once-through steam generator with spiral geometry and cross-flow

– Internship proposal –
(ID No. 1000303)

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[2] *NEMO group, Dipartimento Energia, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129, Torino, Italy*

October 26, 2022

Location	*new*cleo SrL, Via Galliano 27, 10129 Torino, Italy
Starting date	As soon as possible
Duration	5–6 months

Context

*new*cleo has planned an experimental campaign in collaboration with external partners in order to optimize the design of the components for the next units of lead-cooled fast reactors. In this framework, mathematical models of the components are needed to reproduce accurately their physical behavior, with the aim of supporting the design studies.

Description

During this internship, the student will develop a mathematical model of a once-through heat exchanger that presents innovative features to achieve a compact design. The exchanger is made of many layers, each containing a single spiral-shaped tube, arranged in a staggered lattice along the axial direction. The tubes are all immersed in molten lead, which flows outwards from the center to the periphery of the exchanger. The exchanger can be described in cylindrical geometry with the spirals representing the tubes lying in parallel polar planes. Subcooled

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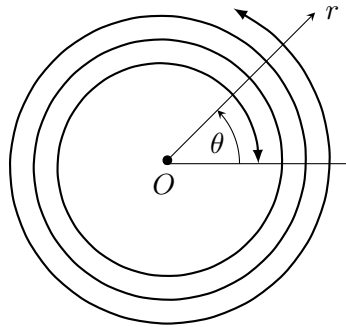newcleosrl@pec.it   *new*cleo

Figure 1: Archimedean spiral.

water enters the spirals at the periphery of the exchanger, flowing inwards inside the tubes, and exits as superheated steam, see Figure 1. The Archimedean or arithmetic spirals are drawn according to the following equation:

$$r = a + b\theta, \tag{1}$$

where a is the centerpoint offset and b is the ratio of the pitch between two consecutive arms of the spiral (pitch) over 2π.

Molten lead flows radially outwards exchanging heat with the water that flows inside the tubes, and can be considered as uniformly distributed along the azimuthal coordinate θ when encountering the first spiral loop. Lead has a very low Prandtl number, so that thermal diffusion shall be taken into account, both radially and azimuthally. Flow-boiling occurs inside the spiral-shaped tubes, and phase separation is expected in the section of the tube because of the centrifugal force applied by the curvilinear motion. Different correlations for heat transfer between lead and water are expected at the two sides of the tube as a consequence of phase separation. Heat-transfer phenomena in presence of phase separation have been extensively studied for helical configurations in the past, but not for spiral configurations. The student will perform a review of the existing literature to find appropriate physical correlations for heat transfer between lead and water in the configuration at hand. New correlations for the distributed friction in cross-flow are expected to become available during the internship thanks to the first results of the experimental campaign.

The student will derive the conservation equations to describe the thermal-hydraulic model of the system, and check the validity of suitable closure relations and physical correlations used in the model. The development of a Python code solving the identified equations is requested, with the verification of the numerical solution in simplified case problems. Finally, preliminary investigations about the validation of the model are expected at the end of the internship, despite the complete validation against other computer codes is postponed for future work. At the end of the internship, the preparation of a technical report is expected to describe the work done by the student and to compile the analysis of the results.

This internship will be supervised by an engineer from *new*cleo and the academic staff at PoliTo. This study supports the preparation of an experimental facility whose construction is planned in 2023.

Work plan

1. Literature review and retrieval of the existing work

2. Problem discussion and definition
3. Derivation of the conservation equations in the spiral-like tube
4. Assessment of the physical correlations to characterize the flow and the heat transfer
5. Implementation and verification of the numerical solution
6. Analysis of results and proposal of validation plan
7. Preparation of a technical report

Applicant profile

Master or PhD student in Nuclear, Mechanical or Aeronautical Engineering. Students in theoretical Physics and applied Mathematics will also be considered for the position.
Background: *fundamentals in thermal-hydraulics and heat transfer, multiphase flow*.
Required computer skills: Python programming, linux, LATEX scientific editing (optional).

References

[1] N. E. Todreas and M. S. Kazimi. *Nuclear systems Volume I: Thermal hydraulic fundamentals*. CRC press, 2021.

[2] N. E. Todreas, M. S. Kazimi, and M. Massoud. *Nuclear systems Volume II: Elements of thermal hydraulic design*. CRC press, 2021.

[3] Vincenzo Luci and Vittorio Vaiarelli. THEST: an in-house tool for spiral-tube steam generator design and verification. Technical report, *new*cleo SrL, Turin, Italy, 2021. LFR-000-NC-A-T-25-0002.

[4] Andrew Michael Fsadni and Justin P.M. Whitty. A review on the two-phase heat transfer characteristics in helically coiled tube heat exchangers. *International Journal of Heat and Mass Transfer*, 95:551–565, 2016.

[5] Paisarn Naphon and Somchai Wongwises. A review of flow and heat transfer characteristics in curved tubes. *Renewable and Sustainable Energy Reviews*, 10(5):463–490, 2006.

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Validation of ECCO calculations of LFR fuel assemblies by Monte Carlo calculations

– Internship proposal –
(ID No. 1000247)

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November 30, 2022

Keywords — LFR, V&V, ECCO, lattice calculations, cross section preparation
Topics — Physical modeling, neutronics, fuel design

Location	*new*cleo SrL, Via Galliano 27, 10129 Torino, Italy
Starting date	As soon as possible
Duration	5–6 months

Context

*new*cleo is designing new units of lead-cooled fast reactors (LFR) aiming to increase the utilization of plutonium produced by the many light water reactors that are currently operating worldwide. The fuel elements are exposed to a fast neutron spectrum favoring fission of heavier actinides. The reactor is cooled by molten lead that shows low neutron absorption and shields radiation protecting the core vessel.

The computer code ECCO (European Cell COde) from the ERANOS 2.3N code suite is used for all the activities of fuel design. ERANOS is a system of computer codes developed in the 1990s for the calculation of fast reactors. ECCO solves the neutron transport equation by the collision probability method using the subgroup method to shield the cross sections of the resonant nuclides. This internship focuses on the validation of the results obtained by ECCO on typical hexagonal fuel assemblies using the Monte Carlo computer code OpenMC.

Description

The fuel assemblies used in LFRs are built upon a hexagonal lattice with hollow fuel pellets inside the fuel rods. A typical fuel assembly for LFR is shown in Fig. 1. The fuel is made of

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mixed uranium and plutonium oxides. The rods can also contain poorly-enriched fuel along the axis that makes breeding zones for the optimization of the core cycle. A metallic wire is helically wrapped around the cladding of the fuel rods to avoid mechanical contact between neighboring rods. The assemblies are boxed and immersed in molten lead, which removes the heat released by nuclear reactions while flowing through the assemblies.

During this internship, the candidate will calculate a set of fuel assemblies by the Monte Carlo code OpenMC in order to compare pin-wise reaction rates and integral quantities like the neutron multiplication factor with the corresponding quantities obtained with the calculations performed by ECCO. Simplified calculation schemes are generally adopted with ECCO, thus introducing physical approximations in the problem to solve, but with the advantage of achieving fast calculations. Instead, Monte Carlo calculations introduce fewer approximations but at the cost of longer calculations. They are then used to validate the deterministic calculations in a representative set of cases, featuring different assembly types. Comparisons of reaction rates in the typical 33-group energy mesh of ERANOS are also requested to validate the self-shielding step done by ECCO. The validation will be performed with fresh fuel, and optionally after exposure at different burnup steps.

Finally, the student will study the anisotropy effects for this kind of assemblies, especially in presence of a central cooling tube. At the end of the internship, the preparation of a technical report is requested to describe the work done by the student and to compile the analysis of the results. This internship will be supervised by engineers from *new*cleo.

Work plan

1. Retrieval of the existing work about ECCO calculations
2. Setup and installation of OpenMC
3. Analysis of the test cases
4. Problem discussion
5. Calculation of the different cases by OpenMC
6. Analysis of results
7. Preparation of the technical report

Applicant profile

Master or PhD student in Nuclear Engineering, Theoretical or applied Physics.
Background: *fundamentals in reactor physics, neutronics and Monte Carlo methods*.
Required computer skills: Python programming (intermediate level), Linux, LATEX scientific editing (optional).

References

[1] Paul K Romano, Nicholas E Horelik, Bryan R Herman, Adam G Nelson, Benoit Forget, and Kord Smith. Openmc: A state-of-the-art monte carlo code for research and development. *Annals of Nuclear Energy*, 82:90–97, 2015.
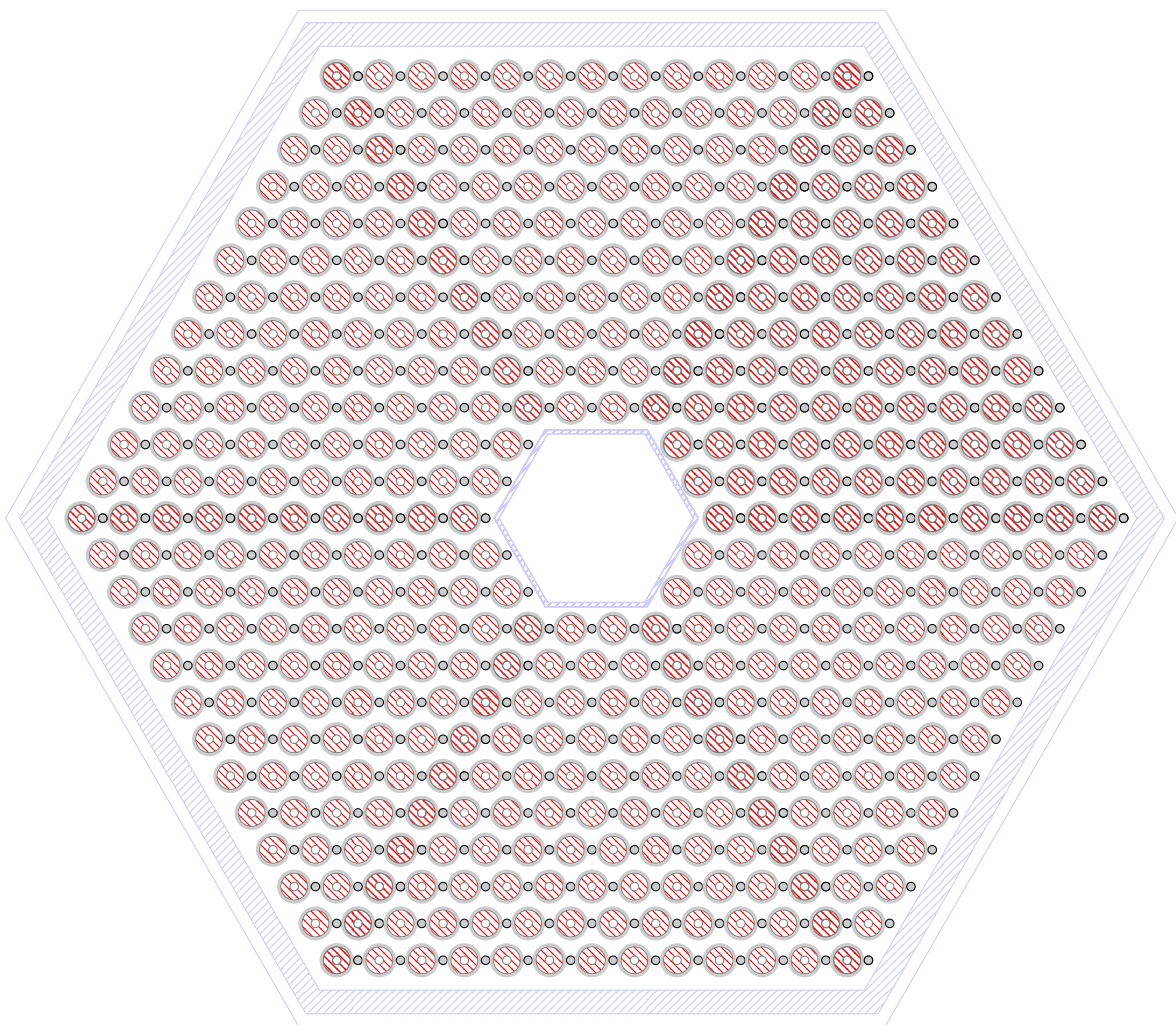
Figure 1: Section of a boxed fuel assembly with central tube.

[2] Gérald Rimpault, Danièle Plisson, Jean Tommasi, Robert Jacqmin, Jean-Marie Rieunier, Denis Verrier, and Didier Biron. The ERANOS code and data system for fast reactor neutronic analyses. In *Proc. Int. Conf. on the New Frontiers of Nuclear Technology PHYSOR2002: Reactor Physics, Safety and High-Performance Computing, Seoul, South Korea*, Oct 7-10 2002.

[3] E Garcia, P Sciora, T Kooyman, G Rimpault, H Guo, and B Faure. Flux distribution of the Superphénix start-up core for the validation of neutronic codes. *Annals of Nuclear Energy*, 133:889–899, 2019.

[4] Kenneth Allen, Travis Knight, and Samuel Bays. Benchmark of advanced burner test reactor model using mcnpx 2.6. 0 and eranos 2.1. *Progress in Nuclear Energy*, 53(6):633–644, 2011.

[5] Siyu Lyu, Daogang Lu, and Danting Sui. Neutronics benchmark analysis of the ebr-ii shrt-45r with sac-3d. *Nuclear Engineering and Design*, 364:110679, 2020.