The Journal of Open Source Software

lbh15: a Python package for standard use and implementation of physical data of heavy liquid metals used in nuclear reactors

Gabriele Ottino [1¶], **Daniele Panico**[1], **Daniele Tomatis** [1], and **Pierre-Alexandre Pantel**[2]

1 *new*cleo Srl, via Giuseppe Galliano 27, 10129 Torino, Italy 2 *new*cleo SA, 9 Rue des Cuirassiers, 69003 Lyon, France ¶ Corresponding author

DOI: 10.xxxxxx/draft

Software

- Review
- Repository
- Archive

Editor:

Submitted: 08 January 2024
Published: unpublished

Summary

lbh15 is a Python package that provides function correlations for the physical properties of the liquid metals used as coolant in GEN-IV liquid metal fast reactors (*LMFR*), such as those cooled by molten lead and lead-bismuth eutectic alloy. The package implements the correlations contained in the reference handbook edited by OECD/NEA (Fazio, 2015), also offering the possibility of adding new customized properties with minimal effort for the user. The properties of the liquid metal are uniquely defined by its thermo-dynamic state, namely by the temperature and the pressure values. In addition, the value of several other properties can be used at liquid metal object's instantiation, provided that the inverse of the corresponding correlation has at least one root in the validity range (*injective function* property).

lbh15 package is released under the *GNU Lesser General Public License v3.0*.

Statement of Need

Thermal-hydraulic analysis is a key factor for the design and safety studies of *LMFR*s. It involves the implementation and use of several numerical methods and physical data that are employed in different computer tools. With a growing community of users and considering quality assurance needs for the engineering studies, a standardization of the approaches becomes necessary to guarantee homogeneity, reproducibility and comparability of the numerical results. This is an essential point to ensure work effectiveness and successful projects in both industry and research environments, especially for nuclear science and engineering. As well, *new*cleo pursues efforts for data standardization to develop new units of lead-cooled fast reactors (*LFR*).

In this context, standard libraries providing the physical correlations for thermal-hydraulic computer tools are needed.

Implementation

lbh15 package takes inspiration from the iapws[1] Python package, that implements the water-related *IAPWS* full standard (International Association for the Properties of Water and Steam, 2018). However, lbh15 follows a different implementation approach.

The efficiency and the effectiveness are assured by the *Object-Oriented* and the *Dynamic Loading* approaches, that have been applied throughout the entire development process. lbh15

[1] https://pypi.org/project/iapws/ - *Iapws 1.5.3* - jjgomera - 2022

relies on the abstract liquid metal class: all classes describing the different metals inherit from it. The abstract class does not implement directly the property correlations, but it instantiates the property objects and provides the property values. In other words, the abstract liquid metal class acts as both *factory* of the property objects and *proxy* of the property values (Giridhar, 2016). This allows the user to add new custom properties without modifying the existing implementation of the liquid metal class.

Use

There are two main ways to use the package, that is, either by instantiating a liquid metal object to access its related properties, or by instantiating an object for each specific property. The former approach provides one single entry point to all the liquid metal properties, which are evaluated at the specified thermo-dynamic state after checking its validity (temperature between the melting and the boiling values, and positive pressure). In addition, the former approach allows to manage the properties correlations in a simpler way, by acting either on a single or on all liquid metal instances at the same time. The latter approach is best suited to cases where only a few specific properties are required for an individual thermo-dynamic state, i.e., where it may be too much to know the values of all the properties of the liquid metal at once.

Implemented Properties

The properties implemented so far can be subdivided into two groups:

- *thermo-physical* (saturation vapour pressure, surface tension, density, thermal expansion coefficient, speed of sound, isentropic compressibility, specific heat capacity, specific enthalpy, dynamic viscosity, electrical resistivity, thermal conductivity, Prandtl number);
- *thermo-chemical*, including the diffusivity and the solubility of Oxygen and of the impurities within the liquid metals, the Oxygen partial pressure, the molar enthalpy, the molar entropy, the Gibbs free energy and the range of the Oxygen concentration values where a corrosion-protective oxide layer on metallic structure is assured.

Implementation History

The release of version *1.1.0* of the package `lbh15` was described in (Panico & Tomatis, 2023). This version implemented only the thermo-physical properties.

The current version *2.0.0* implements the thermo-chemical properties and updates the documentation accordingly. It improves the performance and the readability. Moreover, solutions have been adopted improving performance and usability (enforced vectorisation over the whole implementation and use of the Horner scheme to evaluate polynomials (Hildebrand, 1974)). It includes a tutorial focusing on a volume of lead that is subjected to time-varying thermal loads, where the Oxygen concentration is controlled to fall in the range where the protective oxide layer formation is assured, see (Fazio, 2015). Great attention is paid to the code quality and readability. *PEP8* guidelines[2] are ensured by the *pycodestyle* utility. In addition, the automatic static analysis of the code has been performed by applying the *pylint* tool throughout the entire development, achieving a score higher than 9 out of 10.

The implementation of irradiation-related properties with new tutorials is planned as future improvement.

[2] https://www.python.org/dev/peps/pep-0008/ - *Style Guide for Python Code. PEP 8.* - G. van Rossum, B. Warsaw, and N. Coghlan - 2001

Documentation

The documentation of `lbh15` is generated by `Sphinx` and published on `lbh15` *Github Pages* at the following address:

`https://newcleo-dev-team.github.io/lbh15/index.html`.

It is composed of parts addressed separately to the developers and to the users. An advanced use of the package needs skills in Python software development. The documentation is completed with examples for the users, starting from basic use up to short tutorials for more advanced applications.

References

Fazio, C. et al. (2015). *Handbook on lead-bismuth eutectic alloy and lead properties, materials compatibility, thermal-hydraulics and technologies*. OECD/Nuclear Energy Agency (NEA), Paris, France.

Giridhar, C. (2016). *Learning python design patterns*. Packt Publishing.

Hildebrand, F. B. (1974). *Introduction to numerical analysis*. McGraw-Hill.

International Association for the Properties of Water and Steam. (2018). *Revised release on the IAPWS formulation 1995 for the thermodynamic properties of ordinary water substance for general and scientific use* (IAPWS R6-95(2018)).

Panico, D., & Tomatis, D. (2023). lbh15: A python package implementing lead, bismuth, and lead-bismuth eutectic thermophysical properties for fast reactor applications. *Proceedings of 20th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-20), Washington DC, USA*, 1–12.