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Nucleation, growth and transport modelling of helium bubbles under nuclear irradiation in lead–lithium with the self-consistent nucleation theory and surface tension corrections

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HIGHLIGHTS

- The work presented in this manuscript provides a reliable computational tool to quantify the He complex phenomena in a HCLL.
- A model based on the self-consistent nucleation theory (SCT) is exposed. It includes radiation induced nucleation modelling and surface tension corrections.
- Results informed reinforce the necessity of conducting experiments to determine nucleation conditions and bubble transport parameters in LM breeders.
- Our findings and model provide a good qualitative insight into the helium nucleation phenomenon in LM systems for fusion technology and can be used to identify key system parameters.

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ABSTRACT

Helium (He) nucleation in liquid metal breeding blankets of a DT fusion reactor may have a significant impact regarding system design, safety and operation. Large He production rates are expected due to tritium (T) fuel self-sufficiency requirement, as both, He and T, are produced at the same rate. Low He solubility, local high concentrations, radiation damage and fluid discontinuities, among other phenomena, may yield the necessary conditions for He nucleation. Hence, He nucleation may have a significant impact on T inventory and may lower the T breeding ratio.

A model based on the self-consistent nucleation theory (SCT) with a surface tension curvature correction model has been implemented in OpenFOAM® CFD code. A modification through a single parameter of the necessary nucleation condition is proposed in order to take into account all the nucleation triggering phenomena, specially radiation induced nucleation. Moreover, the kinetic growth model has been adapted so as to allow for the transition from a critical cluster to a macroscopic bubble with a diffusion growth process.

Limitations and capabilities of the models are shown by means of zero-dimensional simulations and sensitivity analyses to key parameters under HCLL breeding unit conditions. Results provide a good qualitative insight into the helium nucleation phenomenon in LM systems for fusion technology and reinforces the idea that nucleation may not be a remote phenomenon, may have a large impact on the system's design and reveals the necessity to conduct experiments on He cavitation.

1. Introduction

Future magnetic confinement D–T fusion reactors, based on liquid metal (LM) eutectic alloy Pb15.7Li as a coolant and breeding material, are supposed to be tritium fuel self-sufficient. Tritium production inside the so called breeding blankets is linked to He production in the LM, that may lead, under the necessary conditions, to nucleation events [1]. Nucleated He bubbles may have a large impact on the self-sufficient principle, heat exchange, T permeation (leakage) and auxiliary systems. The present work intend to be a step forward toward the understanding of the complex phenomena that take place in a breeding blanket, focusing on He nucleation.

Homogeneous nucleation (HON), that is bubble formation in the bulk fluid, turns out to be triggered by neutron irradiation (radiation induced displacements in the LM structure), fluid discontinuities or temperature local peaks. Evidence of such phenomenon has been exposed in Conrad et al. [2], where impact on LM properties and T

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Nomenclature

Abbreviations

CFD	Computational Fluid Dynamics
CNT	Classical Nucleation Theory
DT	deuterium–tritium
EoS	Equation of State
HCLL	Helium Cooled Lithium–Lead
HEN	heterogeneous nucleation
HON	homogeneous nucleation
LM	liquid metal
SM	structural material
T	tritium

Greek characters

α	void fraction
θ	contact angle
π	number pi
ρ	density
σ	surface tension
υ_0	volume of one atom or molecule
ψ	supersaturation ratio

Latin characters

$f(\theta)$	shape factor
Δg	nucleation driving force
k_B	Boltzmann's constant
k_H	Henry's constant
p	pressure
r	radius, radial coordinate
m_0	mass of one atom or molecule
n	number of atoms in a bubble
t	time
$\mathbf{v}$	velocity
x	atomic fraction
C	concentration
D	diffusivity
G	Gibbs free energy
J	diffusion rate, depletion rate
M	molar mass
N_A	Avogadro's number
N_b	number of bubbles per unit volume
R	gas constant
S	source term, nucleation rate
T	temperature
Z	compressibility factor

Subscripts

b	bubble
c	cluster
G	gas phase
He	helium
HEN	heterogeneous nucleation
HON	homogeneous nucleation
L	liquid bulk phase
nuc	nucleation
PbLi	lithium lead Pb15.7Li eutectic
sur	surface
th	thermal
vol	volume, per unit volume

Superscripts

m	molar
sat	saturation
xp	atomic fraction - pressure
0	pre-exponential
*	critical

breeding ratio has been experimentally assessed. A thermodynamically self-consistent nucleation model including radiation effects has not been developed yet. However, many efforts towards the developments of such model have been made for solid irradiated materials, e.g., Trinkaus [3] and references there. Nucleation in LM under neutron irradiation studies are scarce as well as experimental data. Molecular dynamics (MD) studies on He cavitation in liquid lead for Pb15.7Li phenomenon determination have been carried out by Bazhirov et al. [4]: results show significant discrepancies with respect to CNT, which is not acceptable as it underestimates the work of formation due to the surface tension approximation to that of a planar surface. Bazhirov et al. [4] state that the surface tension of a critical cluster, that is a stable cluster that will develop into a gas bubble, has a larger surface tension than that of the planar surface. This fact fully agrees with Tolman [5] surface tension correction, which predicts that surface tension for a droplet increases for increasing droplet sizes, while surface tension of a bubble decreases for increasing bubble sizes.

As has already been mentioned, in a Fusion reactor T is expected to be generated in order to fulfil fuel self-sufficiency requirements at the same rate than He (of the order of 500 g/day for a 3 $\mathrm{GW_{th}}$ DEMO reactor [6]) due to the following nuclear reactions:

$$^{6}\mathrm{Li} + \mathrm{n} \rightarrow {}^{3}\mathrm{H} + {}^{4}\mathrm{He} + 4.78\,\mathrm{MeV}. \quad (1)$$

$$^{7}\mathrm{Li} + \mathrm{n} \rightarrow {}^{3}\mathrm{H} + {}^{4}\mathrm{He} + \mathrm{n} - 2.47\,\mathrm{MeV}. \quad (2)$$

Anticipated results [1], using Classical Nucleation Theory (CNT) showed that He nucleation event, rather than being a remote possibility, may occur under nominal conditions leading to a significant set of effects: flow regime perturbations, heat transfer efficiency reduction, degradation of pumping systems and T permeation reduction. Hence, the issue of He bubbles formation may be highly relevant to fusion reactor design and operation. He bubbles show up to act as a T sink, that may have an impact on T inventory as well as in T breeding ratio. Note that He bubbles may also have a large impact on T effective solubility, as T would be absorbed into the bubbles allowing more T to be present in the bulk LM.

The main aim of this paper is to give insight and to provide a reliable computational tool to quantify the He complex phenomena in a HCLL, in order to assess its potential effect. In the present work, a model based on the self-consistent nucleation theory (SCT) by Girshick et al. [7] is exposed, together with some other major improvements regarding radiation induced nucleation modelling and surface tension corrections. Implementation of the model have been done in the open source CFD code OpenFOAM® (see Jasak [8] and references there) solver.

Note that the presented results deal with nano to micro bubbles upon their formation; at onset conditions and immediately after. Hence, the effect of the bubbles on the LM properties is out of the scope of the presented work and may deserve a dedicated publications taking into account multi phase flow. However it is worth to be noted that if bubbles become large enough, which is not a remote possibility under fusion conditions, LM effective density and viscosity may be affected by a dispersed He gas phase.

2. He nucleation model

Simple models for He nucleation, bubble growth and transport, together with T complex transport phenomena, have been