

Thermodynamics Properties of Molten Salt Technology Assessment for New Generation Fusion Reactors

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Abstract In this study, some important thermodynamic properties of the fusion reactor have been analyzed. The physical and chemical properties of molten salts have been extensively studied in the nuclear fusion program. In recent years, molten salts technology began to be used in some engineering areas, in the advanced nuclear field and especially in nuclear fusion reactor systems. Nowadays, Aries team has developed advanced designs by using the molten salts technology in order to get high thermodynamic and structural advantage on nuclear technology areas (Tillack et al. in *Fusion Energ Des* 65:215–261, 2003; Tillack et al. in *Fusion Energ Des* 49–50:689–695, 2000; El-Guebaly et al. in *Fusion Energ Des* 65:263–284, 2003). The Aries-St reactors are a 1000 MW fusion reactor system that based on a low aspect ratio ST plasma (Tillack et al. in *Fusion Energy Des* 65:215–261, 2003; Tillack et al. in *Fusion Energy Des* 49–50:689–695, 2000). The Aries team studies especially on liquid walls concepts and this liquid are used to increase neutronic performance of various structures of Aries-St reactors. In this research, candidate molten salts have been studied neutron effects on reactor performance which are the first wall (FW) and blanket. There are various candidate liquids that meet all the criteria such as $\text{Li}_{17}\text{Pb}_{83}$, flibe (Li_2BeF_4) and LiNaBeF_4 , LiSn that are able to breed enough tritium. In this research, we used $\text{Li}_{17}\text{Pb}_{83}$, pure lithium and flibe as candidates that are in the Aries design. Montecarlo n-particle 4b-code is used for neutronics analysis and thermodynamic features. The value of tritium breeding ratio of the Aries-St reactors must be (TBR \geq 1.1). This can be achieved in the region of LiPb /

FW blanket of reactors. Aries-St spherical reactor has high heat flux (0.8 MW/m²) and NWL (6–8 MW/m²) in this region.

Keywords Thermodynamics · Molten salts · Flibe · Aries-St · Fusion reactors

List of symbols

G	Free energy
E	Internal energy
S	Entropy
H	Enthalpy
Mcnp	Montecarlo n-particle
A	Major radius of toroid
a	Minor radius of toroid
$\beta = A/a$	Aspect ratio of plasma
tbr	t6 + t7, Tritium breeding ratio
mhd	Magneto hydrodynamic
Re:Ha ² /N	Reynolds number
Ha	Hartmann numbers

Introduction

Molten salts technology are taken into account at the beginning of research into nuclear energy production. In new fusion applications, reactors technology has been processed with liquid metals and molten salts mixtures at high temperatures and at successful advanced designs. The aim of Aries-St fusion research has been the production of economically and environmentally acceptable nuclear power. The Aries-St investigated as a national US effort to survey the potential of the spherical tokamak concept as a fusion power plant and as a vehicle for fusion development. The 1000 MW Aries-St power plant has an aspect ratio of

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1.6, a major radius of 3.2 m, a plasma elongation (at 95 % flux surface) of 3.4 and triangularity of 0.64 [1–3]. This configuration attains of 54 %, which is 90 % of the maximum theoretical transfer of coolants is very important in toroidal hybrid reactor system, because it remarkably effects the neutronic performance of the reactors. The candidates are given the liquid metals, lithium, $\text{Li}_{17}\text{Pb}_{83}$ and Li-Sn and the molten salts, $(\text{Li}_2\text{BeF}_4)$ and LiNaBeF_4 . The influence of the magnetic field on liquid wall flow characteristics and heat transfer is crucial for both. In the inner blanket of the Aries-ST structure consist of the zones and zone thickness, which is HTS (high temperature shield) and FW (first wall) regions They have ferritic steel structure cooled by helium gas. There is no breeding zone for tritium breeding in the inner blanket must be supplied from the other blanket where four different zones exist (FW, MSZ, HM, LTS) [4, 12, 13]. Particularly during last 30 years a certain number of design studies on fusion reactor have done. In the high temperature, the power flows components are showed in Table 1. In Aries-St fusion, the coolant of $\text{Li}_{17}\text{Pb}_{83}$ is used either as energy carrier or tritium breeder. Recently, montecarlo method is used to obtain analytical solution of the governing differential equations. For the Aries-St fusion reactor, this method is determined the definition of design point. Self-sufficient $T_{br} > 1,1$ has been regarded to designate the upper limit of the proportion of heavy metal salt in the mixture. To supply sufficient tritium breeding, the flowing liquid has to be a lithium containing medium. Figure 1 shows power core and TF coil of Aries-St core cross section of the reactor. The aspect ratio of the ARIES-ST reference equilibrium is achieved by optimizing the value of the engineering q , which is a stable between major fusion power output and minor TF coil dissipation power [5]. Aries-St power core comprises of the essential parts directly surrounding the burning plasma and various important functions. The important properties for these candidate tritium breeders are given in Table 2.

Table 1 General structural of Aries-St fusion reactors systems [1–3]

Modification	Area (m ²)	Nuclear heating (MW)	Surface heating (MW)	Total power (MW)
Outboard first wall	421	100	195	295
Inboard first wall	67	18	52	70
Inboard shells	54	71	73	144
Inboard shield	–	199	0	199
Divertor	128	201	250	451
Outboard ferritic steel	–	~ 340	–	330
Outboard PbLi	–	~ 1,600	–	1,614
Total	–	~ 2,533	570	3,103

Advanced Design of Molten Salt

The molten salt technology was transmitted to the civilian nuclear programme of the US in the second half of the 1950s. In the 1990s renewed interests in molten salt technology arise from programmes seeking for possibilities for transmutation of actinides [24]. Molten salt is solid canonical temperature and pressure in the liquid stage. It can provide being used as a coolant that is able to be used at high temperatures without hitting a high vapor pressure. Liquid metal breeder blankets have been searched extensively due to numerous advantages including relatively simple design, sufficient tritium breeding ratio, removal of high heat and so forth. Following a step-by-step approach, thorium molten salts fusion reactors technology will endeavor for realizing effective thorium energy production by nuclear energy in nearly 15 years. Because of the fact that thorium is three to four times more abundant in nature than uranium and it is important for supplying energy to the world in a sustainable manner. Recently, a new attractive concept (D,T) fusion reactions fuel cycles are produced high energetic neutron at 14.1 MeV, for which thorium has quasi comparable fission cross sections with uranium so that one fusion neutron will be needed to release fission energy out of neutron. For that purpose, Aries team has been developed advanced multipurpose Aries-St fusion reactor systems. A tokamak is a device which uses a magnetic field to restrain plasma in the shape of a torus. This reactor has various attractive features including high beta and power density, low aspect ratio, low magnetic field, high neutron walls and high self-driven current. In fusion applications, liquid metals are characteristically regarded to be the best working fluids (LiPb, flibe, LiSn, Li). The working liquid has to be a lithium-containing medium as to supply sufficient tritium that the plasma is self-sustained and that the fusion is a renewable energy source. As to flibe free surface flows, the mhd effects which are caused by interaction with the mean flow is negligible, while a fairly uniform flow of thick can be maintained throughout the reactor that based on hydrodynamics calculations. In this research, the molten salt engineering design plasma parameters are defined with respect to Mhd equilibrium and nuclear analysis, thermodynamics properties, head capacity, phase diagram, neutron wall loading, density and viscosity. The Mhd model is the extension of fluid dynamics to electrically conducting fluids like plasmas, with the inclusion of the effects of electromagnetic forces. The MHD equations consist of macroscopic transport equations and magnetic induction equation. In order to design a suitable salt, information is required on the phase diagrams, thermodynamic properties (heat capacity, viscosity, thermal conductivity et al.) and magnetohydrodynamics (mhd) properties.

Fig. 1 Power core and Tf coil structural design of Aries-St fusion reactor [1–3, 9]

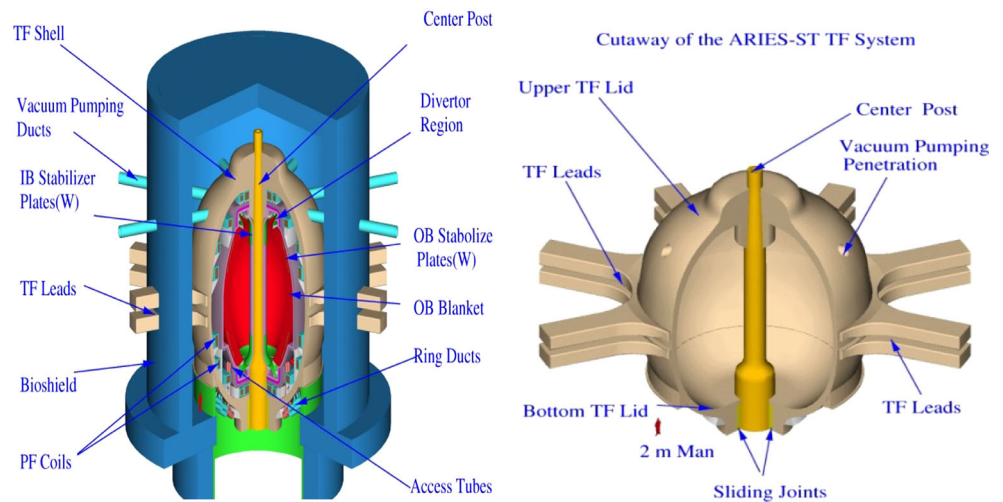


Table 2 The thermodynamic of the candidate molten salt in Aries-St reactor [8, 10]

Composition (% mole)	Melting point (°C)	Liquid density (g/cm ³)		Head capacity (at 700 °C cal/g)	Viscosity		
		$\rho = A - BT(^{\circ}C)$			$\eta = A \cdot e^{B/T(K)}$ 600 °C		
		A	B.10 ⁻⁵		A	B	
Li-BeF ₄ (69–31)	505	2.16	40	0.65	0.118	3,624	7.5
Lif-BeF ₂ (50–50)	350	2.46	40	0.67	0.0189	6,174	22.2
NaF- BeF ₂ (57–43)	360	2.27	37	0.52	0.0346	5,164	12.8
NaF-ZrF ₄ (50–50)	510	3.79	93	0.28	0.0709	4,168	8.4
Lif-NaF-KF 46,5–11,5–42	454	2.53	73	0.45	0.0400	4,170	4.75
Lif-Naf-Bf ₂ (35–27–38)	338	2.22	41	0.59	0.0338	4,738	7.8

Molten salt technology is a catch all phrase that consist some diverse technologies such as; electro-chemistry, heat transfer, chemical oxidation/reduction baths, and nuclear reactors. All of technologies are linked by the general characteristics of molten salts; can serve as solvents and beside that they have a very good heat transfer capacity, function like a fluid can also reach very high temperatures (heat >700 °C), they can conduct electricity, some molten salts have chemical catalytic speciality. Molten salts are used to breed most non-ferrous metals (non-iron like metals aluminum, titanium, etc.). The most important and oldest use of them is the production of aluminum via electrolytic decomposition of alumina (Al₂O₃) [25–27].

Thermodynamics Properties of Molten Salt Technology

One method of defining molten salts is to say that they are melts consisting of positively and negatively charged atoms. Most chemical thermodynamic problems of optical interest are concerned with the equilibrium in reactions, in which more than one phase is present. Heat capacity of molten salt halogen is very important for thermodynamics quantities at constant pressure (C_p) and at constant

volume(C_v).Best of calorimetric measurements of heat capacity are made at constant pressure. For most fluid-flow calculations C_p is used even though may be pressure variation in the fluid. For enthalpy change at constant pressure are defined as flows; H₂ – H₁ = $\int_{T_1}^{T_2} C_p dT$, when both pressure and temperature change, the enthalpy change is given by $dH = C_p dT + [-T\delta/\delta T(1/\rho) + 1/\rho]$, the last term gives the change in enthalpy due to pressure changes. Heat capacities at constant pressure of some common liquids metals and molten salt halogen. The thermodynamic activity of knowledge will be assumed of elementary thermodynamics together with the following thermodynamic functions and variables, free energy change (G₁ – G₂) for ideal gases are related by equation; $G_1 - G_2 = RT \ln(P_1/P_2)$, where P₁ and P₂ pressure [24–26]. Many experimental methods involving the measurement of thermodynamic quantities for molten salt mixtures result in the evaluation of partial molar quantities for one component. For a solution consisting of only two components, it is in fact necessary to measure partial molar quantities pertaining to one component only. For the other, the quantities can be evaluated by means of the Gibbs–Duhem equation. The Gibbs–Duhem equation defines the relationship between changes in chemical potential for components in a

thermodynamically system. It is clear that intensive properties are not independent but related in thermodynamics which are making it a mathematical statement of the state postulate. The Gibbs–Duhem equation is given by, $N_1 dG_1 + N_2 dG_2 = 0$ [24–26]. N_i describes the number of moles of component and this equation i., $d\mu_i$ the infinitesimal increase in chemical potential for this component, where S is the entropy, T is the absolute temperature, V is volume and P is the pressure. Frequently used thermodynamic relationship is $G = H - TS$. G is the potential energy and H is enthalpy [24–26].

In the studies of Aries-St Reactors, the temperature profile in the near-surface layer plays an important role in the structural phase changes, which is constant heat flux on the free surface $C = (-\Gamma \partial E / \partial y)_{\text{surface}}$. The non-dimensional temperature is described as; $T(x, y, z, t) = \{ \langle E_W \rangle_{x,z} - E(x, y, z, t) \} / E_\tau$, where E_W and E_τ are respectively wall temperature and friction temperature. This method is adopted to channel flow and loop flow. The gradient of the Bulk temperature $T_m = \langle T \rangle_{x,y,z}$ is given by $\frac{dT_m}{dx} = \frac{2C}{\rho v h}$, where v is the mean bulk velocity [8, 10].

The equivalent heat capacity is defined by $C_p(r, T) = C_p(r, T) + S(r) f(T - T_m)$, where $S(r)$ is the latent heat of fusion and $f(T - T_m)$ is dirac-delta function. There are important two coolant in the concept blanket design, which are He at the 8 MPa and LiPb in the Fig. 2. It is shown cross section of the LiPb blanket FW/Blanket/Manifolds. The He cools the FS structure. The LiPb transports the nuclear heating from FW to the blanket at high temperatures. It has both good tritium breeding potential and self-cooled concept. This liquid walls succeeded in phases of inertial fusion reactors within the possibilities of present day technology. This research is required to demonstrate the feasibility of a liquid wall protected chamber for magnetic fusion and on the feasibility of a conducting liquid metal flowing along field lines. Widespread analysis on the thermohydraulics and mhd effects of different types of liquid protection have been related. And this following liquid wall concept has more advantages than the solid first wall concept has and it also expands the life-span of reactor. This study can be clearly summarized as; (1) high power density (2) the surface of renewable first wall (3) decreasing radiation damage and activation in structural materials (4) produced tritium breeding potential [1–3, 9]. In the concept of the integrated blanket coil, liquid lithium subserves as a conductor, a producing material, a coolant with the joule losses directly in the coolant and it is partially recovered by the power conversion system [16–19, 23]. The liquid wall idea developed during the apex study into numerous concepts that have some common features but also have greatly different issues and virtues. These concepts can be classified as it is shown in Table 2.

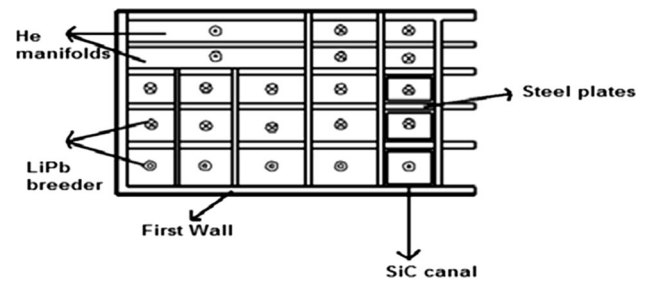


Fig. 2 Cross section of the LiPb blanket FW/Blanket/Manifolds [1, 2, 9]

Flibe(Li₂BeF₄) Properties and Molten Salt Technology

Flibe is a combination of lithium fluoride (LiF) and beryllium fluoride (BeF₂). Flibe has been greatly researched in the Oak Ridge National Laboratory (USA) for molten-salt reactor experiment (MSBR). Like a molten salt, this is projected as a coolant which is nuclear reactor. The 2:1 mixture with rates of Li₂BeF₄ has 460 °C melting point, 1,430 °C boiling point, and 1.94 g/cm³ density. As water, its heat capacity is 4,540 kJ/m³ which is more than four times that of sodium, and also more than 200 times that of helium at ordinary reactor conditions. The eutectic mixture is a bit greater than 50 % BeF₂ and has 360 °C melting point. Differently from sodium or potassium metals that can also be used as high-temperature coolants, it does not violently react with air or water. The low atomic weight of lithium, beryllium and to a lesser extent fluorine make flibe an effective neutron moderator. As natural lithium contains ~7.5 % Li-6, which tends to absorb neutrons producing alpha particles and tritium, nearly pure Li-7 is used to give the flibe a small cross section. Table 3 shows physical properties of working liquid structure for Aries-St fusion reactor. For Aries-St, the problem associated with tritium permeation are even more severe. Because, this is the coolants are He and Pb₈₃-Li₁₇. The tritium solubility in Pb₈₃-Li₁₇ is very low. The Aries-St studies liquid walls concept, although containing many common aspects, the variability related to the liquid used. In this study, candidate molten salts have studied neutron effects on reactor performance [27].

A salt is normally liquid even at standard temperature and although technically molten salts are a class of ionic liquids, pressure is generally called a room temperature ionic liquid. Molten salts have a variety of uses. Molten chloride salt mixtures are usually used as baths for numerous alloy heat treatments, like tempering and annealing of steel. A fluoride salt is used as a solvent for aluminum oxide in the production of aluminum in the process. Fluoride, chloride, and hydroxide salts can be used as solvents in preprocessing of nuclear fuel. Molten salts (fluoride, chloride, and nitrate) can also be used as heat

Table 3 Working liquid properties of compared with flibe [10–12]

Properties	Li	Li ₁₇ Pb ₈₃ (lithium lead)	Flinabe	Li ₂₀ Sn ₈₀	Li ₂ BeF ₄ (Flibe)
melting point (°C)	180	235	300	330	459
density (g/cm ³)	0.48	8.98	2.00	6.20	2.00
Li density (g/cm ³)	0.48	0.062	0.12	0.09	0.28
Tritium solubility	High	Very low	Very low	–	–

transfer fluids as well as for thermal storage [27]. Their ability to conduct electricity is one of the exciting features of molten salts. Because of the fact that it is exposed to the highest neutron, gamma ray, X-ray, and charged particle currents, that are produced in the fusion chamber, the highest material damage occurs in the first wall in the fusion structure. When a viscous flows in a closed conduit, the boundary layer extends from the wall to a point in the fluid where the velocity is maximum. The boundary layer does not form immediately at the entrance of the conduit but it builds in the entrance region At the point where the fluid enters the conduit, the boundary layer has zero thickness. If we compare the two different velocity profiles affecting on the mass transfer in reactor fist wall and assuming the velocity profile is linear.

Numerical Calculation

Design of Aries-St

In this study, we used Mcnp-4b computer code and Endf library for design of Aries-St. The Aries-St reactors of inner region include vacuum and plasma. After this it follows first liquid wall, blanket, ferritic steel, shield, stainless steel and ferritic steel zone take place. The Aries-St reactor has 1000 MW a fusion power and an aspect ratio of 1.6, a major radius of 3.2 m [2, 7, 8]. A monte carlo method is generally described as a statistical method used in simulation of data. Monte Carlo is a numerical process and it is frequently used for solving mathematical problems by the simulation of random variables. The statistical simulations are operated by the monte carlo method by using the randomly generated numbers. Mcnp is a overhead goal monte carlo n-particle code and it can also be used for neutron, electron, phroton for or coupled neutron/photon-electron transport. Mcnp has run for approximately $8,6 \times 10^5$ particle histories per calculation. By using Mcnp-4b computer code, we have calculated cross-sectional view of Aries-St designed [14, 20–22]. It is shown in

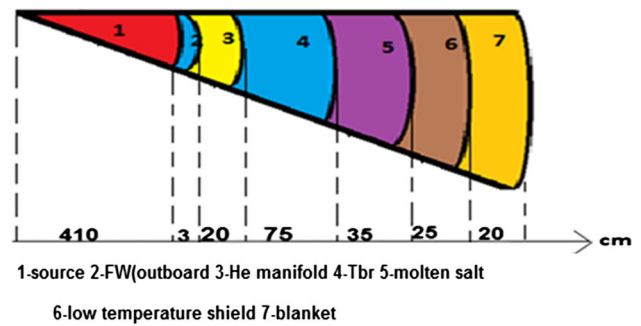


Fig. 3 Cross-section of Aries-St fusion reactor with mcnp-4b code [6, 7, 13]

the Fig. 3 In contrast to the analytical approximations; simulation models are more successful in modeling. These models are also more succeeding in solution of complicated problems. Monte Carlo technique is the technique of randomly number selection from one or more probabilistic distribution in a special trial or simulation study. The Mcnp-4b code has been used for calculations and reactor designs. The integral of f(x) function has becomes by randomly [8, 10, 11]. The random of data is given this formulae,

$$I = \int_R f(x)dx = \Delta x^d \sum_{i_1=1}^N \sum_{i_2=1}^N \dots \sum_{i_d=1}^N f(x_{i_1}^1, \dots, x_{i_d}^d),$$

As it is shown in Fig. 3, the outboard structure of reactor has numbered in details. Plasma region is the 1 region and it is source and region of plasma. The first liquid wall region follows it. And this region is cooled with He. Especially in the region of 4 and 5, the speed of the production of tritium increases The primary source of nuclear data used by Mcnp4b-code is evaluations from the evaluated nuclear data file (Endf) evaluated nuclear data files system. The effects of the first load wall layer thickness and of different blanket configurations and the various mixture compositions of molten salt and heavy metals on many parameters of fusion reactor, such as tritium production rate, energy multiplication factor, fissile fuel breeding, first wall material radiation damage, and heat deposition were investigated.

Thermophysical Properties of Aries-St

With regards to our thermodynamic data the vapor pressure of Li₁₇-Pb₈₃ and pure Li (0–120 %) mol composition have been calculated for temperature range (200–1,000 K), which involve a representative operating temperature range of Aries-ST reactor. Flibe, Li₁₇-Pb₈₃, LiNaBeF₄ and pure Li phase diagram have been measured by Aries team [1–3, 9]. Aries-St reactor design has different zones which are the inboard and outboard [4, 8, 13]. They are very different

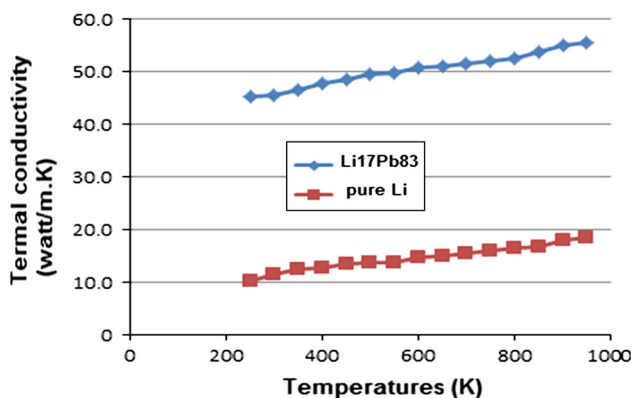


Fig. 4 Thermal conductivity of candidates molten salts in the liquid state

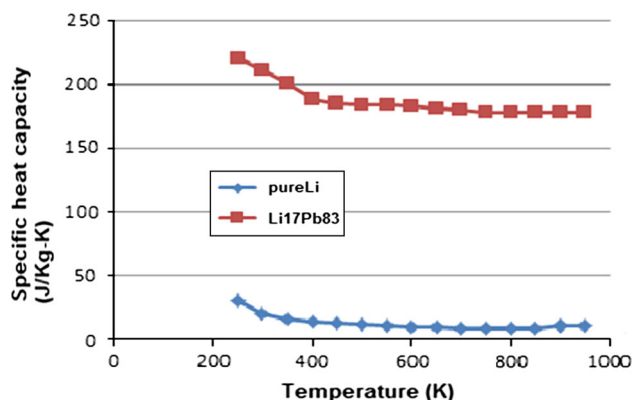


Fig. 5 Specific heat candidates of molten salts in the liquid state

design constraints. Both for inboard and outboard use He is a coolant of ferritic steel structural. Coolant pressure of first wall is 12 MPa and it has total 542 m² surface area. Aries-St structure consist of the zones and zone thickness, which is HTS (high temperature shield) and FW (first wall) regions [4, 23]. On the other hand FW has average NWL 4.1 MW/m² and average first wall heat flux is nearly 0.48 MW/m². In Fig. 4 are shown, thermal conductivity (watt/mK) of Li₁₇-Pb₈₃ and pure Li in the liquid state. Lithium lead(PbLi)/FW are put forward for use both an energy productions and tritium gain material in blanket for Aries-St. In terms of these problems which will occur in case of structural materials being used, liquid first wall (FW) concept is more suitable choice in fusion reactors. Molten salts have been used in many industries as a high temperature heat transfer medium. It is salt which is solid at standard temperature and in pressure in the liquid phase due to elevated temperature. In Fig. 5 these are shown Specific heat candidates of molten salts in the liquid state.

Neutron Wall Loading

An complete evaluation of the neutron wall loading is vital for determining the radiation damage to the structure and magnet, for designing the various components of the power core, and for assessing the radiation environment around the torus. In Fig. 6 these are given, variation of neutron wall loading vertical distance from mid-plane. Tritium producing depends exactly on the blanket structure 1. Plasma support systems can ability cover 10–20 % of the first wall are. By the reason of symmetry, the upper half of the first wall and divertor have modeled for the Mcnp-4b code to generate the poloidal distribution. The machine generates a fusion power of 2,860 MW. The first wall's total surface area and divertor plates amount to 700 m which results in a machine average pik NWL of 3.7 MW/m². In Fig. 6 briefly illustrates the poloidal change of NWL for

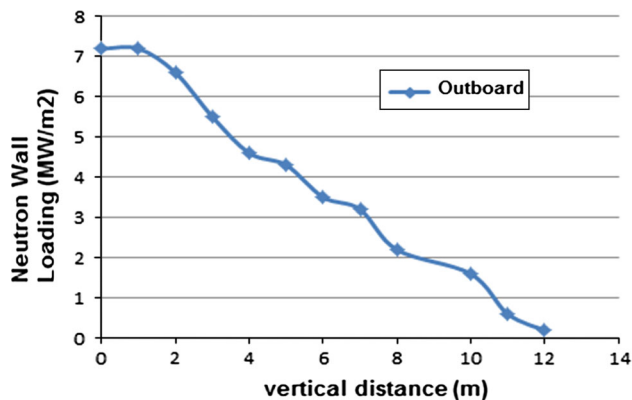
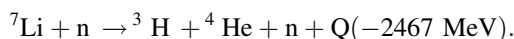
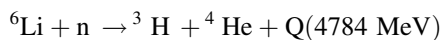


Fig. 6 Variation of neutron wall loading vertical distance from mid-plane

outboard and outer divertor plate. The neutron wall loading peaks at 6.4 MW/m² at the mid-plane of the outboard FW.

Tritium Breeding Ratio (TBR)

Tritium breeding ratio (Tbr) is described as the ratio of the rate of tritium production in the system to the rate of tritium burned in plasma. In order to provide adequate tritium breeding, the flowing liquid must be a lithium containing medium. Mcnp 4b simulation results to give that the overall TBR is for %60 a enriched Li The tritium production reactions are as follows;



The Fig. 7 shows tritium production rate (TBR) of exchange with % heavy metal liquid Li₁₇Pb₈₃ has both tritium generating material and multiplier in the blankets of fusion power plans. Li₁₇Pb₈₃ eutectic permits the use of relatively enriched or pure Li and has a relatively low cost

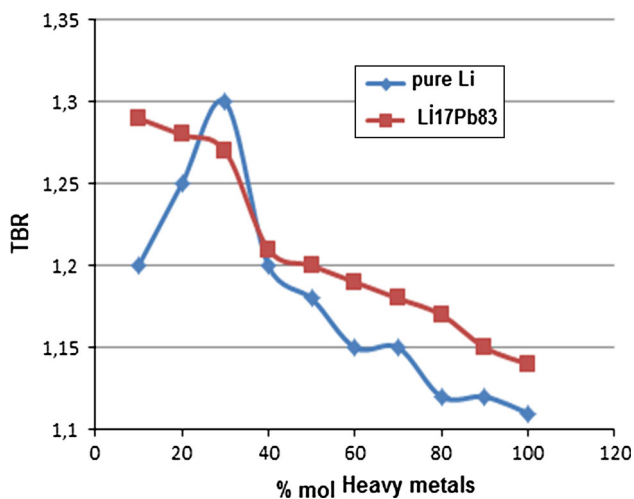


Fig. 7 Tritium production rate (TBR) of exchange with % heavy metal liquid

in comparison with other tritium breeding. If the eutectic is kept at temperatures 300–350 °C in the blanket, continuous tritium extraction is possible. General Aries-St study has shown that the St concepts lead to attractive fusion power plants in fusion and hybrid reactors, it is necessary to provide the $TBR > 1.1$, terms so as to provide the continuity of the operation of the reactors [4, 10, 13, 14].

Conclusions

The fusion molten salt technology can be used for fuel processing and spent fuel recycling, for heat transfer, as a homogeneous fuel and as a breeder mater in fusion systems [24–26]. Controlled nuclear fusion is a very essential energy choice for humankind in the future by virtue of both being environmentally friendly and having limitless fuel reserves. But besides this, it also needs a long time period in order to be commercialized. Development of nuclear energy has become one of the strategic focuses of fusion molten salt reactor systems. The fusion molten salt reactors have characteristics including thorium–uranium energy utilization, hydrogen production at high temperature, water-free cooling and modular design. General the Aries-St study has shown that the St concepts lead to challenging fusion power plants in fusion and hybrid reactors, it is necessary to provide the $TBR > 1.1$ terms [2, 10, 13, 14]. So as to supply the continuity of the operation of the reactors, one of the important tasks in Aries-St is to achieve tritium self-sufficiency. The He has used to cool in the first wall structure. A specially $Li_{17}Pb_{83}$ composition is transported the nuclear heating for the blanket and has at the high temperature. $Li_{17}Pb_{83}$ composition is an breeding material, which has both good tritium breeding potential

and self-cooled concept. Design and calculations of Aries-ST have carried out as 3D Spherical torus by using Mcnp-4b computer code/Endf library [6, 7, 14] Compatibility between materials at high temperature increases so much concern both inside of the blanket and in the heat transport loop [8, 9, 12]. The mhd model is the extension of fluid dynamics to electrically conducting fluids such as plasmas, with the inclusion of the effects of electromagnetic forces [10, 23]. Turbulent models based on Navier–stokes–Maxwell equations are applied to be calculated simultaneously with other flow quantities thick and thin liquid wall concept [5, 8, 15, 20].

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