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D3.1 – Compact Heat Exchanger for High Temperature Heat Pump Preliminary Design

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Author: KTH Royal Institute of Technology

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Reviewer(s)	Silvia Trevisan (KTH), Rafael Guedez (KTH)
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Executive summary

The deliverable, D3.1: Compact Heat Exchanger for High Temperature Heat Pump Preliminary Design, has been developed in the context of WP3 under the responsibility of KTH, with broad interaction with ENERIN, and collecting inputs from all partners. This deliverable describes the current state of work on the preliminary sizing and design of a compact Helium to ternary molten salt heat exchanger for the integration between the high temperature heat pump and the thermal storage loop. The main scope of the deliverable is twofold: 1) identify the main boundary and key operating conditions for the heat exchanger; and 2) identify main design alternatives and perform initial optimizations aimed at maximizing the heat transfer coefficient offered by the HX between the two media.
The methodology involves a combination of analytical 1D predictions coupled with an iterative design and CFD based study to identify the key design parameters of influence such as piping arrangement and specific dimensioning toward optimization of the key performance parameters: pressure drop, and heat transfer coefficient. The preliminary results and the down selection of heat exchanger design for a range of flow conditions will be further exploited in a detailed optimization strategy as is proposed under D3.2 (WP3). Additionally, preliminary consideration in terms of material selection and manufacturing options are presented.

This work forms the basis towards a comprehensive heat exchanger design, optimization and prototype manufacturing which is to be carried out throughout the following tasks of WP3 and in the I-UPS project.

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Contents

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1. Introduction

1.1 Scope

This deliverable describes the current state of work on the preliminary sizing, design and simulation of a key component of the I-UPS system that is the heat exchanger (HX). As part of WP3 (D3.1) the HX design shall support its integration within the high temperature heat pump (HTHP) and promote an exchange between the pressurized gas and molten salt. The thermal-hydraulic performance quantification of the HX will lead to an optimization of designs and exploring advanced manufacturing techniques towards the further tasks within WP3 and I-UPS as a whole.

1.2 Structure

The first section of the deliverable outlines the key geometrical design parameters and constraints associated with the compact heat exchanger model. The design considerations in this deliverable are taken in accordance with the proposed specifications of the heat exchanger from D2.1 such that a full integrated heat pump system can be achieved. A few key geometric parameters of interest are identified, and design iterations are performed within the tolerance projections to satisfy the expected simulation outcomes. The latter section focusses on a 2D CFD modelling of the shortlisted design cases. Simulation parameters are varied under favourable operating conditions and the model scenarios pertaining to an optimum range of thermal-hydraulic performance are proposed. Subsequently a brief overview of material preference is provided and the HX manufacturing methodologies using AM techniques are discussed.

1.3 Relation to other deliverables

The outcomes from this deliverable are projected to aid into a full-scale design optimization strategy that forms D3.2 in WP3. Additionally, the preference of component materials and advanced manufacturing techniques such as the highly preferred Additive manufacturing (AM) methods are a key relevance to the tasks 3.3 and 3.4. Crucially, the geometric design includes significant inputs from the ongoing activities in WP2, T2.1 and the development of the heat exchanger design with lead to a potential modification of the HTHP design to ensure a seamless integration of the HX within the system.

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2. HX Design Strategy

This section describes the preliminary HX design and sizing strategy with an overview of the geometry with a 3D CAD model and the 2D design considerations. The design strategy follows an adoption of the existing pressurised gas to water heat exchanger developed by the project partner ENERIN for their HTHP. The objective of this direction is to limit the needs for the overall geometric modifications such that the manufacturing associated costs and complexity are minimised.

2.1 Preliminary 3D model overview

The preliminary heat exchanger design is subjected to the design considerations undertaken by the HTHP such that its direct integration in the unit is achieved seamlessly. The design criteria as enlisted in D2.1 are briefly described as follows:

- He flow in pipes and salt flow in shell side
- Main HX diameter equivalent to current configuration and relative helium seal
- Length of the HX along the main axis in the range 150-400 mm
- Tube inner diameter below 5 mm
- Number of tubes between 400 to 800
- Ensure drainability of the unit with inclined installation (also beneficial for the mechanical stability of the HTHP and the balancing of shank active forces during operation) and with a salt drain port at the lowest point

Additionally, for the prototype to be tested in I-UPS the below key sizing targets are also identified:

- Heating capacity target: ~40 kW delivered to molten salt
- Delta T for molten salt over the heat exchanger < 5K
    - Which will be further reviewed based on the specific HX optimization and the system level assessment in terms of operability of the unit.

Limited temperature changes along the HX are beneficial for the operation of the Stirling HTHP, thus leading to higher resulting COP. However, slightly wider temperature increments would provide benefits to the molten salts system integration facilitating the storage charging operation. A more detailed optimization will consider not only the specific HX design but also its influence on the overall operation of the system and its flexibility also considering activities in WP5.

Finally, the below key performance indicators (KPIs) have been considered, as stated in the Grant Agreement:

- Overall heat transfer coefficient ≥ 100 W/m2K (KPI-9)
- Thermal power density ≥ 30 W/cm3 (KPI-10),
- Specific power ≥ 20 kW/kg (KPI-11),
- Pressure drop ≤ 1% of the inlet working pressure (KPI-12)

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Taking into account the key specifications requirement of the heat pump a preliminary 3D CAD model was developed to obtain an estimate of the overall sizing of the compact heat exchanger. A shell and tube heat exchanger design is considered wherein the pressurized Helium gas flows through a tube bank and the molten salt circulates within the shell side.

Figure 2-1 shows an isometric view of the heat exchanger model placed at a 45° inclination. The pressurized He gas side is illustrated and represents the flow direction within the tube bank. The molten salt circulates along the shell side with colinear ducts directing its flow.

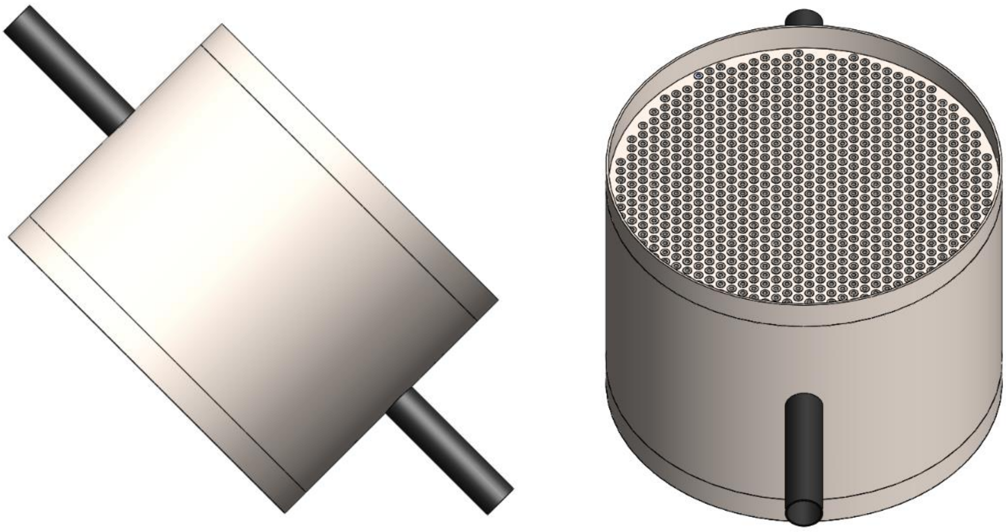

Figure 2-1: 3D CAD model views of the compact shell and tube heat exchanger.

The Figure 2-2 presents a sectional view of the 3D CAD that illustrates the internal volume and clearances of the shell and tube HX.

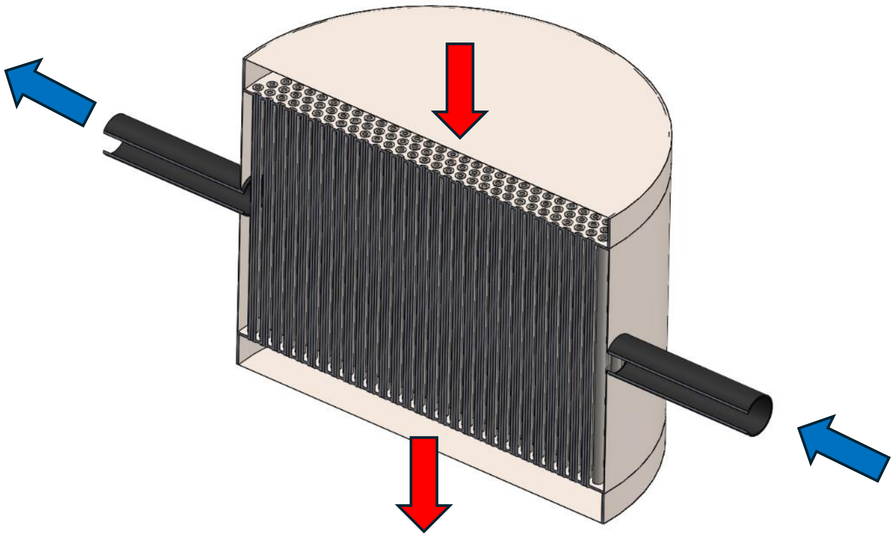

Figure 2-2: Sectional view of the 3D CAD model showing the tube bank and the internal volume. Red arrows indicate the flow of pressurised He gas through the tube bank and blue arrows indicate the flow of molten salt across the shell periphery.

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The 3D CAD model presents the following preliminary geometric parameters in accordance with the specifications provided:

- Overall dimensions:
    - Outer diameter of the shell – 263 mm
    - Duct diameter – 25 mm
    - Length of the HX – 203 mm
- Tube side details:
    - Inner tube diameter – 3 mm
    - Outer tube diameter – 6 mm
    - Number of tubes – 786
    - Pitch to pitch distance – 8.5 mm
    - Pitch layout pattern – 60° triangular

2.2 Geometric case variations

For simplification of preliminary simulation analysis, 2D CAD models are developed with wide ranging geometric parameters and to analyse their interdependencies on the HX performance.

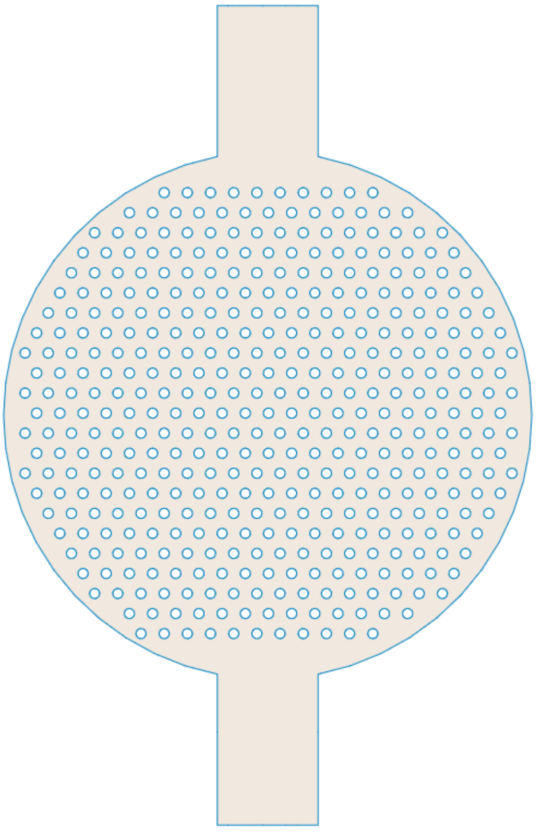

Figure 2-3: 2D CAD model of the shell and tube heat exchanger used for CFD simulations.

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The Figure 2-3 is one of the example cases of a shell and tube HX with colinear ducts which is based on the following geometric parameters:

- Shell diameter – 262 mm
- Duct width – 50 mm
- Duct length – 75 mm
- Tube external diameter – 5 mm (incorporates the wall thickness)
- Tube – tube pitch distance – 11.5 mm
- Distance from the shell side wall – 3 mm
- Pitch layout pattern – 60° triangular
- Number of tubes – 420

Several geometric parameters are varied within a prospective range in accordance with the design specifications and the structural integrity of the HX system are as suggested in D2.1 and Section 2.1 above. However, the shell side outer diameter and the 60° triangular layout pattern of tubes are maintained as a constraint.
The variables are described as follows:

Tube layout pattern (in no of tubes)	420
	535
	655
	766
Tube external diameter	4 mm
	5 mm
	6 mm
Duct diameter	25 mm
	50 mm

In order to vary the tube layout pattern within a fixed shell side outer diameter, the tube pitch to pitch distances are varied in the range of $8.5 \leq \text{pitch distance} \leq 11.5$.

2.3 Analytical estimations

Prior to the CFD study with the abovementioned geometric designs, analytical calculations are performed to determine the flow characteristics.

The thermo-physical properties of ternary molten salt (YARA MOST) are modelled as a temperature dependent relationship.

- Density (ρ) (kg/m^3) : $(-0.0006705 \times T + 2.187) \times 1000$
- Heat capacity (c_p) (KJ/kg·K) : $1.53084 + 1.10431 \times (0.97496)^T$
- Dynamic viscosity (μ) (Pa·s) : $1372144977 \times T^{-3.36406}/1000$
- Thermal conductivity (k) (W/m·K) : 0.52

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Flow characteristics:

Hydraulic diameter of the duct is calculated based on:

$$D_h(rectangular\ duct) = \frac{2a \cdot b}{a+b} = 0.05\ or\ 0.1\ (\mathrm{m}) \tag{1}$$

Where "*a*" corresponds to the duct width of 25 mm and 50 mm, "*b*" refers to an unity value since a 2D study is performed.
Reynolds number is calculated to determine the flow characteristics of the shell side fluid i.e., molten salt.

$$Re = \frac{4 \times \dot{m}}{\pi \times D_h \times \mu} = 350 \le Re \le 7000 \tag{2}$$

$$Re < 2300 - \text{Laminar}$$
$$Re > 2300 - \text{Turbulent}$$

Wherein "$\dot{m}$" refers to the mass flow rate of the molten salt and is varied between 0.5 kg/s to 10 kg/s thus leading with Reynolds numbers of approx. 350 to 7000 respectively that cover a flow regime of both laminar and turbulent.

Pressure drop (ΔP) is typically associated with the hydraulic performance of a HX and is computed by taking a difference of the average inlet and the outlet pressure values on the duct side.

Heat transfer characteristics:

Several parameters are used to quantify the thermal performance of HX.
Heat supplied to the fluid on the shell side (*Q*) determines the heat transfer rate of a HX:

$$Q = \dot{m} \times c_p \times \Delta T \tag{3}$$

Where ΔT is the temperature difference between the inlet and outlet temperature in the ducts with molten salt.

A heat transfer coefficient (h_{sh}) is a quantitative characteristic of shell side convective heat transfer between the fluid medium and the surface flowed over by the fluid. For the current work, it involves the regions within the shell and the surface area surrounding the heated tube bank.

$$h_{sh} = \frac{Q}{P_t \times N \times (T_{t,wall} - T_{b,avg})} \tag{4}$$

Where, P_t refers to the perimeter of a tube, *N* is the number of tubes, $T_{t,wall}$ is the wall temperature of the tubes and $T_{b,avg}$ is the average molten salt bulk temperature (computed as the difference between the inlet and outlet duct temperatures).

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3. HX CFD Simulations

A 2D CFD simulation model is developed using ANSYS Fluent package to analyse and quantify the thermal-hydraulic characteristics of a compact shell and tube HX incorporating He and molten salt.
The model consists of a refined mesh in the near boundary regions to capture the recirculation zones generated from the cases involving turbulence. The total cell count varies on a case-by-case basis as a result of geometric modifications an approximately is 200k.

3.1 Boundary conditions & Assumptions

For simplification of the model and to delve into more understanding with the dynamic behaviour of molten salt performance, the He gas on the tube bank side of the HX is modelled as a uniform wall temperature boundary condition.

- Several scenarios are generated with a wide range of molten salt flowrates at the inlet side of the duct based on the pumping specifications.
- The molten salt is specified with a fixed inlet temperature and an operating pressure of 101325 Pa (1 bar equivalent).
- All other HX walls are considered adiabatic and heat loses aren't accounted.
- The effect of gravity is not considered in the 2D geometry.
- Variation of standard laminar model and a $k{-}\epsilon$ turbulence model with near-wall treatment is adopted based on the quantification of Re flow regimes.
- Baffles are not considered in the CFD simulations for the 2D design cases as the flow distribution was determined to be satisfactory with the expectations.
- The simulation plane is considered along the horizontal axis of the geometry and thus the effect of inclination is not incorporated

3.2 Scenarios implemented

Five distinct scenarios are simulated with flow and geometric variations to determine the optimum range of HX performance. Results of pressure drop are averaged and computed based on the difference between the inlet and outlet duct pressure. Relative pressures are determined based on the difference of the duct outlet pressure and the operating pressure. A prime objective of WP3 is to maintain the pressure drop within $\leq 1\%$. The outlet temperature refers to the average temperature of molten salt at the exit of the heat exchanger and is determined at the outlet duct along the transverse direction.

Following modelling constraints are considered to calculate the dependencies on other variables as described:

- As a standard duct width of 50 mm
- A fixed molten salt inlet temperature of 493.15 K and tube bank wall temperature of 523.15 K is considered across the scenarios unless otherwise treated as a variable.

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Molten salt mass flow rates

In all the below cases the tube pattern is with fixed 420 nos of tubes and external tube diameter of 5 mm. The influence of the MS mass flow rate is investigated.

Case #	Mass flow (kg/s)	ΔP (Pa)	Outlet T (K)	Q (kW)	h_{sh} (W/m².K)	% $rel. P$	ΔT	Flow
1	0.5	1.32	522.04	22.10	215.37	0.001	28.89	Laminar
2	2	6.59	513.70	62.87	483.06	0.007	20.55	Laminar
3	3.5	13.53	509.37	86.84	601.30	0.013	16.22	Laminar
4	***5***	***21.92***	***506.77***	***104.18***	***680.96***	***0.022***	***13.62***	***Turbulent***
5	7.5	39.04	504.39	128.92	801.46	0.039	11.24	Turbulent
6	10	59.93	502.90	149.16	899.82	0.059	9.75	Turbulent

An optimal mass flow rate range of $3.5 \leq \dot{m} \leq 5$ kg/s is determined to attain suitable values of pressure drop that are in the range of $13.5 \leq \Delta P \leq 21$ Pa and corresponding heat transfer rates of $86 \leq Q \leq 104$ kW which are the desired characteristics for the molten salt operating pumps and the HTHP requirements as stated from Section 2 and D2.1.

Tube layout patterns (number of tubes)

In all the below cases the external tube diameter of 5 mm and the molten salt mass flow rate of 5 kg/s is fixed. The influence of tube layout patterns (number of tubes) is investigated.

Case #	Tube nos	ΔP (Pa)	Outlet T (K)	Q (kW)	h_{sh} (W/m².K)	% $rel. P$	ΔT
4	***420***	***21.92***	***506.77***	***104.18***	***680.96***	***0.02***	***13.62***
7	535	36.46	510.63	133.70	748.26	0.04	17.48
8	655	50.14	515.92	174.19	1113.52	0.05	22.77
9	766	65.35	515.94	174.31	1114.76	0.06	22.79

The ideal thermal-hydraulic performance is obtained for the case #4 with lower tubes number layout i.e. 420 compared to the higher tube numbers which present a substantial increase in pressure drop.

Tube diameters

In all the below cases, the tube pattern with 420 number of tubes and molten salt mass flow rate of 5 kg/s is fixed. The influence of tube diameter's is investigated.

Case #	Tube diameter (mm)	ΔP (Pa)	Outlet T (K)	Q (kW)	h_{sh} (W/m².K)	% $rel. P$	ΔT
10	4	15.95	501.88	66.81	493.76	0.02	8.73
4	***5***	***21.92***	***506.77***	***104.18***	***680.96***	***0.02***	***13.62***
11	6	32.52	509.84	127.68	744.78	0.03	16.69

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An optimal range of tube diameters between the test cases of 4 and 5 is determined to present satisfactory performance with a gain in the heat transfer for the 5 mm tube diameter albeit with a small increase in the pressure drop.

Molten salt duct width

In all the below cases, the tube pattern with 420 number of tubes, tube diameter of 5 mm and mass flow rate of 5 kg/s is fixed. The influence of molten salt duct width is investigated.

Case #	Duct width (mm)	ΔP (Pa)	Outlet T (K)	Q (kW)	h_{sh} ($W/m^2.K$)	% $rel.P$	ΔT
12	25	65.71	506.51	102.21	664.39	0.06	13.36
4	***50***	***21.92***	***506.77***	***104.18***	***680.96***	***0.02***	***13.62***

Case 4, duct width of 50 mm is the preferred design consideration for the molten salt duct inlet and outlet ports on the shell side as a substantial drop in pressure drop is achieved with an unchanged heat transfer performance in comparison to the 25 mm ducts.

Tube bank wall and molten salt duct inlet temperatures

In all the below cases, the influence of varying tube wall temperature and duct inlet temperature is investigated for a fixed tube pattern of 420 number of tubes, tube diameter of 4 mm and molten salt mass flow rate of 5 kg/s.

Case #	He side wall T (K)	MS duct inlet T (K)	ΔP (Pa)	Outlet T (K)	% $rel.P$	ΔT
13	483.15	453.15	26.14	461.77	0.03	8.62
10	523.15	493.15	15.95	501.88	0.02	8.73
14	623.15	593.15	7.87	601.74	0.01	8.59

A few cases are simulated to determine the He gas and molten salt heat exchange characteristics at differing operational setpoints of the temperatures. The aim was to study a range of COP performances of the HTHP which typically decreases with increase in the source-sink temperatures and the temperature difference between the two. Lower operating temperatures favours a high COP for an efficient operation of the HP. However, the pressure drop is increased by 64% which substantially reduces by 51% (compared to the baseline) with the increase in operating temperature and is a clear consequence of the molten salt thermos-physical properties.

Thus, the above scenarios present the interdependencies between the geometric parameters analysed that are tube layout pattern, tube diameter and duct width. Additionally, flow characteristics are analysed by simulating various mass flow rates of the molten salt in the shell side and heat pump operating setpoints are varied to predict its effect on the molten salt heat exchange.

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3.3 Qualitative representation

To describe the CFD simulation results from Section 3.2 qualitatively, contour plots of an optimal thermal-hydraulic performance example case are illustrated in the following figures 3.1, 3.2 and 3.3. The figures are generated for case #10 as referred from Section 3.2 which represents a tube layout pattern of 420 with tube diameter of 4 mm at mass flow rate of 5 kg/s, an inlet temperature of 493.15 K and 50 mm duct width.

Figure 3-1 shows the velocity distribution of molten salt across the tube bank and a satisfactory distribution of flow is evident as a result of the turbulent Re = 3500 regime. As a result of an effective spread within the tube bank including the regions of shell periphery, the inclusion of baffles wasn't deemed a requirement for the preliminary analysis. As a result of the sharp corner effects of the outlet duct, maximum velocity is obtained towards the exit.

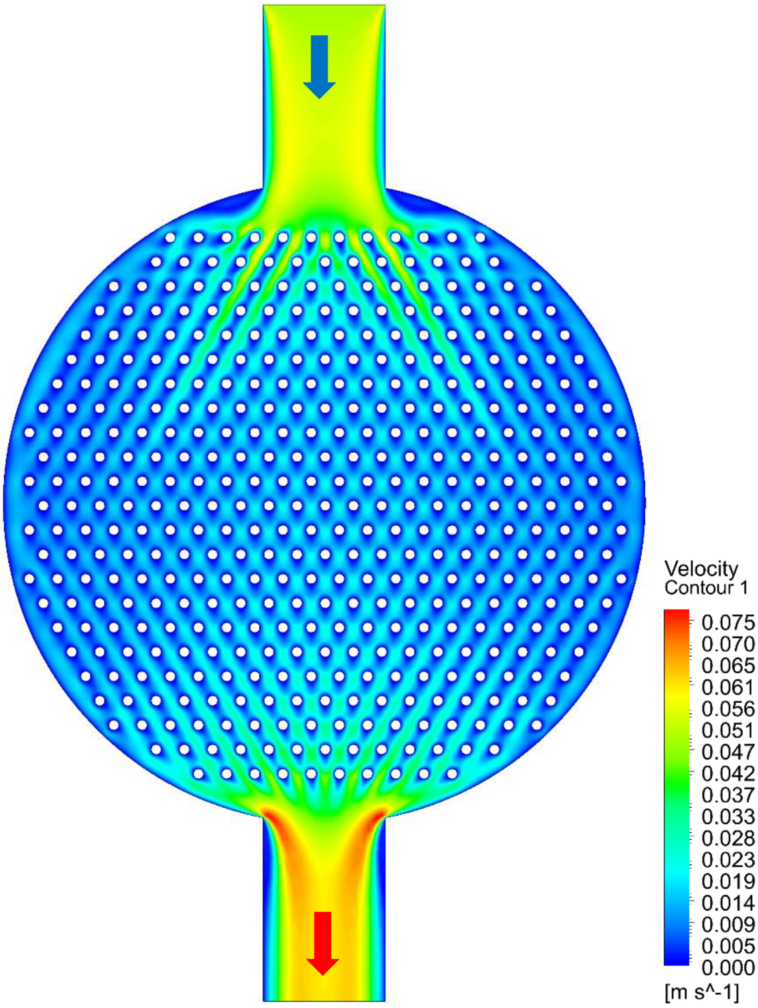

Figure 3-1: Molten salt velocity distribution at a mass flow rate of 5 kg/s for 420 tubes layout pattern and tube diameter of 4 mm, case #10.

The pressure distribution from Figure 3-2 shows the high magnitudes of pressure close to the entrance regions of the molten salt interacting the tube bank as a result of the turbulent fluid

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velocities of molten salt at a mass flow rate of 5 kg/s. To mitigate this pressure rise, prior to simulation extra rows of tubes are eliminated in the vicinity close to the inlet and outlet ducts. An average pressure drop of 15.95 Pa is calculated and is one of the lowest compared to the other simulation cases, thus leading to a high hydraulic performance.

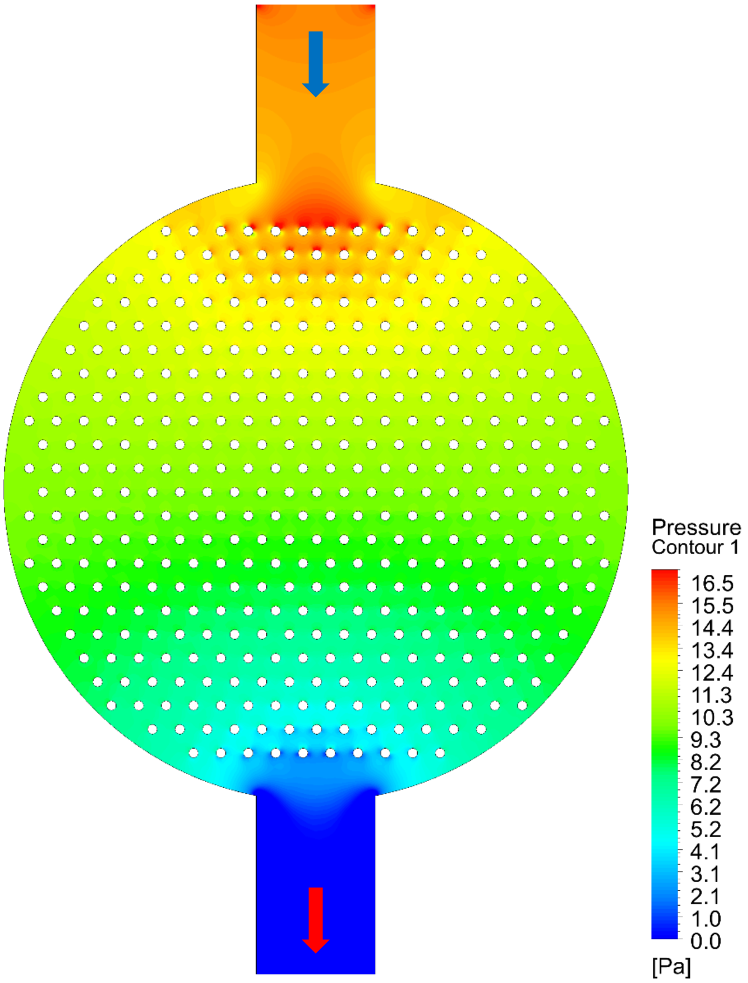

Figure 3-2: Molten salt pressure distribution for a mass flow rate of 5 kg/s with 420 tubes layout pattern and tube diameter of 4 mm, case #10.

Molten salt temperature distribution is presented in Figure 3-3 with a satisfactory spread overall despite the tightly packaged tube banks. Contours surrounding the tube bank show the heated tube bank which symbolises the He side at a fixed wall temperature of 523.15 K. As a result of turbulent flow velocities of molten salt the heat transfer exchange is appreciable and an averaged outlet temperature at the exit obtained is 501.8 K.

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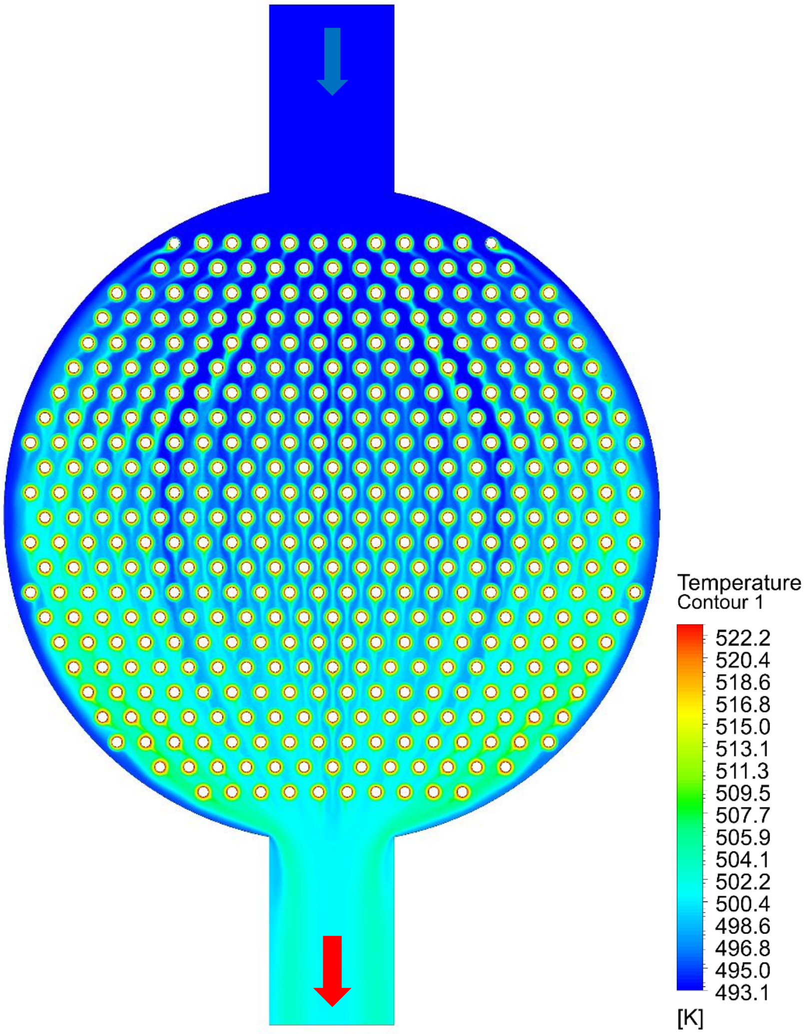

Figure 3-3: Molten salt temperature distribution at a mass flow rate of 5 kg/s for 420 tubes layout pattern and tube diameter of 4 mm, case #10.

3.4 Optimal scenarios and further steps

Based on a wide range of parameters investigated and their interdependencies, the optimal range of thermal-hydraulic performance can be identified.

- As typically a shell side turbulent flow is employed to promote effective circulation and heat exchange between the two media in a shell and tube exchanger, the molten salt mass flow rate of 5 kg/s or Re = 3500 is suggested in further works as it satisfies the pump operating range.
- Amongst the triangular layout tube bank patterns investigated, lower number of tubes i.e., 420, favoured higher hydraulic performance with a slight drop in the thermal performance, thus a tube layout pattern between a range of 400 – 550 nos is recommended for further design optimization.

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- Tube diameters of 4 mm and 5 mm resulted in high thermal-hydraulic performance over 6 mm where the pressure drop substantially increased. Thus, the optimal tube diameter range of 4 – 5 mm requires optimization to achieve the best case.
- Wider duct width presented the best hydraulic performance without compromising the thermal performance as was noted for the 50 mm over 25 mm. Thus, further optimization of wider ducts based on the standardised pumping hoses typically used for the molten salt circulation are to be considered.
- Further steps will involve a full-scale 3D CFD simulation model incorporating the 45° inclination of the proposed operation of the heat exchanger as represented in the CAD model in Section 2.
- Placement of the ducts will be a deciding factor in terms of implementation of baffles to enhance the molten salt circulation in the heat exchanger and for thermal-hydraulic performance quantification on a system level.
- The design will also require the need to incorporate a molten salt drainage port at the lowest point of the heat exchanger as proposed in D2.1.
- A further optimization strategy potentially using genetic algorithms is proposed which shall optimise the tube pattern arrangement, variable tube diameters and duct geometries to maximise the thermal-hydraulic performance of the heat exchanger.

4. Materials and manufacturing considerations

Advanced manufacturing techniques such as metal additive manufacturing has demonstrated a promising direction towards the fabrication of novel heat exchanger designs with complicated geometries that cannot be achieved using legacy manufacturing techniques. The potential of using different materials and novel geometries can help offset the trade-off between the pressure drop and heat transfer using design optimisation strategies.

- Recent works have employed Direct Metal Laser Sintering (DMLS) and Laser Powder-Bed Fusion (LPBF) as a preferred fabrication technique for intricate heat exchanger geometries.
    - DMLS : involves laser to selectively fuse metal powder particles layer by layer to create solid components. Sintering technique in particular.
        - Post processing may involve heat treatment, surface finishing for structural integrity.
        - High temperature materials of preference are: Stainless steel, titanium, cobalt-chromium and nickel alloys.
    - LPBF : It is a subset of DMLS, refers to process of melting or fusing powdered materials using laser to create complex geometries. Fusion technique in particular.
        - Surface finishing is likely required.
        - Form of metal powders suitable with titanium and other metal alloys.
- Material selection for the heat exchanger is a key consideration for several factors that account for:

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- high structural integrity to withstand the extreme pressurized He gas transients,
- corrosion resistance to molten salt and
- consistent high temperature operation.
- From the literature, Stainless Steel (austenitic grades 316L, 321, 347) alloys are a favourable material for corrosion resistance and high temperature strengths.
- Nickel alloy grades that are Inconel 600, 625 offer excellent high temperature strengths and oxidation resistance.
- Another high-performance alloy combining nickel + chromium + molybdenum + iron (Hastelloy) commonly graded as C-276, C-22 offers extreme temperature strength and outstanding resistance to oxidative, corrosive environments.

The above manufacturing techniques will be assessed also accounting for their specific costs and in comparison with more traditional manufacturing and welding/brazing procedure aiming at ensuring cost-effectiveness and safe operation

5. Conclusions

In this deliverable the current state of work on the preliminary sizing and design considerations of a pressurised He gas to molten salt heat exchanger that forms one of the key integral components of the I-UPS system is described. This deliverable summarises the work ongoing in WP3 with T3.1 and includes a crucial design direction from the specifications of D2.1 to facilitate for the heat exchangers integration within the HTHP. The preliminary work involves: 1) developing a 3D CAD model and to frame the objectives for simulations; 2) generating analytical estimations for determining the flow characteristics of the molten salts; 3) performing 2D planar CFD simulations to model various geometric and fluid parameters and study their interdependencies; 4) framing optimal scenarios and a favourable operating range of the heat exchanger. Across a wide range of parameters, superior thermal-hydraulic performance is obtained for the case involving 420 number of tubes, molten salt mass flow rate of 5 kg/s, tube diameter range of 4 – 5 mm and a 50 mm duct width. The heat transfer rate of about 100 kW is achieved at a minimal pressure drop penalty and the heat transfer coefficient of about 500 W/m^2.K is reached indicating favourable thermal performance and temperature distribution on the shell side.

This work forms the primary step towards a full-scale comprehensive heat exchanger design, optimisation and prototyping strategy which are the following tasks within the WP3 and in the full scope of I-UPS project.

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