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Project Acronym: I-UPS

D3.2 – Compact Heat Exchanger for High Temperature Heat Pump Optimized Design

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Executive summary

The deliverable, D3.2: Compact Heat Exchanger for High Temperature Heat Pump Optimized 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 optimized design geometry 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) Perform a parametric analysis of geometric dimensions to analyse the heat exchanger thermal-hydraulic performance;
2) Quantify the optimum design setup incorporating desired features for its additive manufacturing (metal 3D printing).

The methodology involves continuation of work carried from deliverable, D3.1 with a finalized heat exchanger geometry consisting of a comprehensive optimization of the piping dimensions, shell wall thicknesses and the shell side ducts. Iterative designs are built and developed via a CFD based study based on the key performance metrics: pressure drop, heat transfer rate and heat transfer coefficient. Based on the parametric results, an optimized design specification is identified, and the overall heat exchanger performance is quantified using CFD. Few geometric modifications are incorporated on the finalised version such that it can be adapted for additive manufacturing using SS316 L material. The manufactured component will be experimentally tested for structural, thermal conditions/loading and its performance comparison will be further described in D3.3 (WP3).

This work leads to the executive design and drawings of the heat exchanger to be manufactured and tested in the next steps of WP3 and finally fully integrated into the high temperature heat pump in WP4.

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1. Introduction

1.1 Scope

This deliverable describes the current state of work on the optimized design and simulation of a key component of the I-UPS system that is the heat exchanger (HX). With the continuation of work carried out in D3.1 (WP3) and outcomes from D3.2, the optimized 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 of an optimized HX is quantified and further considered for advanced manufacturing using metal 3D printing as the next steps within the tasks of WP3 and I-UPS as a whole.

1.2 Structure

The first section of the deliverable outlines the key geometrical design parameters and constraints taken into consideration for the compact heat exchanger optimization model. The design considerations in this deliverable are taken in accordance with the proposed specifications of the heat exchanger from D2.1 and D3.1 such that a full integrated heat pump system can be achieved. In section further, results from the optimized geometry are discussed characterising the thermal-hydraulic performance. Subsequently, the selected heat exchanger design incorporates special features to achieve maximum suitability and compatibility with the additive manufacturing as the preferred fabrication direction along with its material.

1.3 Relation to other deliverables

The outcomes from this deliverable are projected to aid into a development of an experimental test campaign to validate the 3D printed compact heat exchanger's feasibility and performance across various structural, flow and thermal loads that forms D3.3 in WP3. Crucially, the optimized geometric design includes significant inputs from the ongoing activities in WP2, T2.1, T2.2 and is a continuation of the work carried out in WP3, T3.1 such that the further to be manufactured compact heat exchanger will be retrofitted to the modified HX housing in the HTHP design to ensure a seamless integration of the HX within the system.

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2. Background

The shell and tube compact heat exchanger is to be retrofitted within the HTHP package – cylinder bank that forms the hot-side of the circuit as described in D2.1 for the scope of the pilot testing. The fully integrated heat pump is shown in Fig. 2.1 operating on a Stirling cycle with pressurised helium gas in a V3 configuration (3 – cylinder bank) with a 45° orientation.

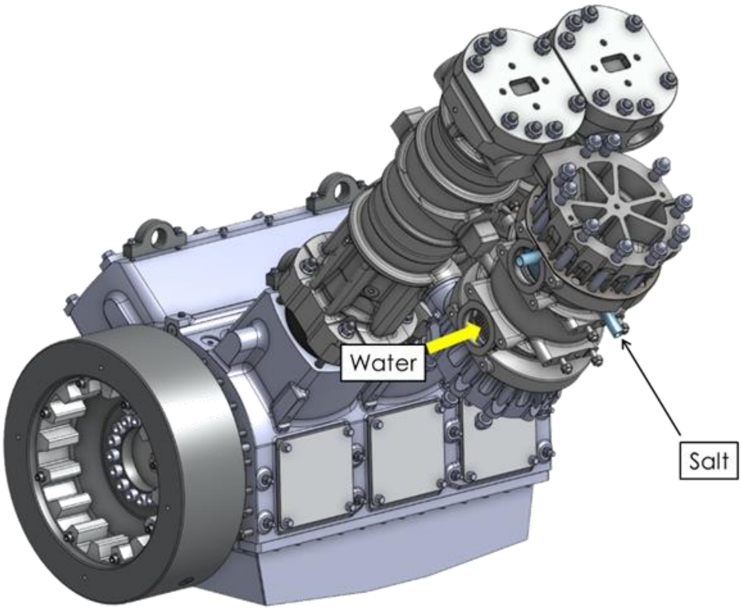

Figure 2-1: Heat exchanger location within the HTHP cylinder bank.

3. HX Geometry

This section describes the 3D CAD model of the HX design that is considered for geometric optimization. The design strategy follows an adoption of the existing pressurised gas to water heat exchanger developed by the project partner ENERIN for their HTHP as is continuation of design aspects described under D3.1. 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.

3.1 3D model overview

Based on the previously reported D2.1 and D3.1 design considerations for the heat exchanger geometry, the overall finalised geometric dimensions are as follows:

- Main HX diameter (D_{shell}) is 262 mm
- Length of the HX (L_{shell}) along the main axis in the range 163 mm
- Salt 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

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- Shell side ducts of 4” to 2” with concentric pipe reducers are preferred as standards from tubing supplier catalogues.

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

- Heating capacity target: ~40 kW delivered to molten salt
- Delta T for molten salt over the heat exchanger < 10K
    - 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 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/m^2K (KPI-9)
- Thermal power density ≥ 30 W/cm^3 (KPI-10),
- Specific power ≥ 20 kW/kg (KPI-11),
- Pressure drop ≤ 1% of the inlet working pressure (KPI-12)

3.2 Operating conditions

The shell and tube heat exchanger operates with pressurized helium gas flowing through the tubes from the heat pump while the molten salt from the thermal energy storage unit circulates around the shell driven by an external pump.
In a typical Stirling cycle heat pump, the piston-cylinder operates at high frequency, 20 – 100 Hz or 1200 – 6000 RPM (revolutions per minute) thus resulting in minimal temperature variation of the pressurized gas for the hot-side, thus it is practical to consider a constant temperature boundary condition for the tube side flow. Steady state simulations are performed with a fixed inner-tube wall temperature for the helium gas. In order to determine the working temperatures, a simulation variable is defined in the optimization model as further described in subsection 3.3.

For simplification of the optimization, the molten salt is defined with an atmospheric operating pressure of 101325 Pa with a fixed flowrate of 3 kg/s at 220 °C. The shell-side fluid is to be circulated using a high temperature capable Klaus Union pump available with the project partner KYOTO. The pump offers a flow rate in the range of 0.55 m^3/hr – 6.5 m^3/hr with an operational temperature rating at up to 450 °C. Based on the molten salt thermo-physical properties as indicated in D3.1, the working range of the pump effectively correlates to 0.2 kg/s – 3.6 kg/s. Hence for the optimization model, a flowrate of 3 kg/s is considered to suit the pilot project operational requirements.

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Taking into account the key specifications requirement of the heat pump a preliminary 3D CAD model of a shell and tube heat exchanger was developed to perform further design optimization. The pressurized Helium gas flows through a tube bank and the molten salt circulates within the shell side.

Figure 3-1 shows an overview of the heat exchanger model with the tubes and ducts.

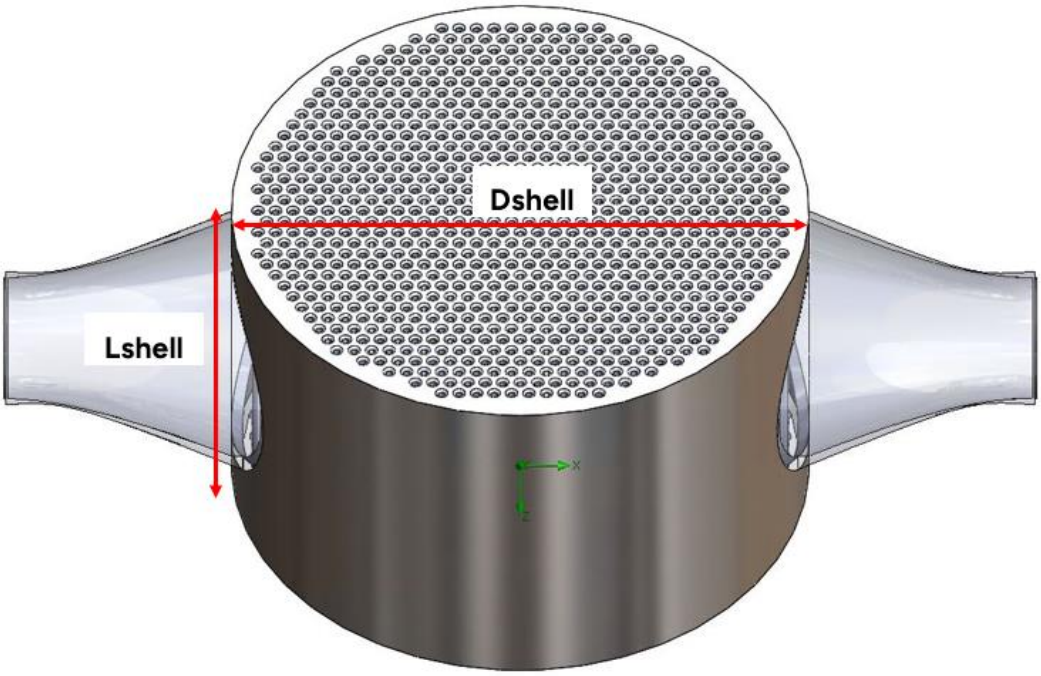

Figure 3-1: 3D CAD model of the compact shell and tube heat exchanger.

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

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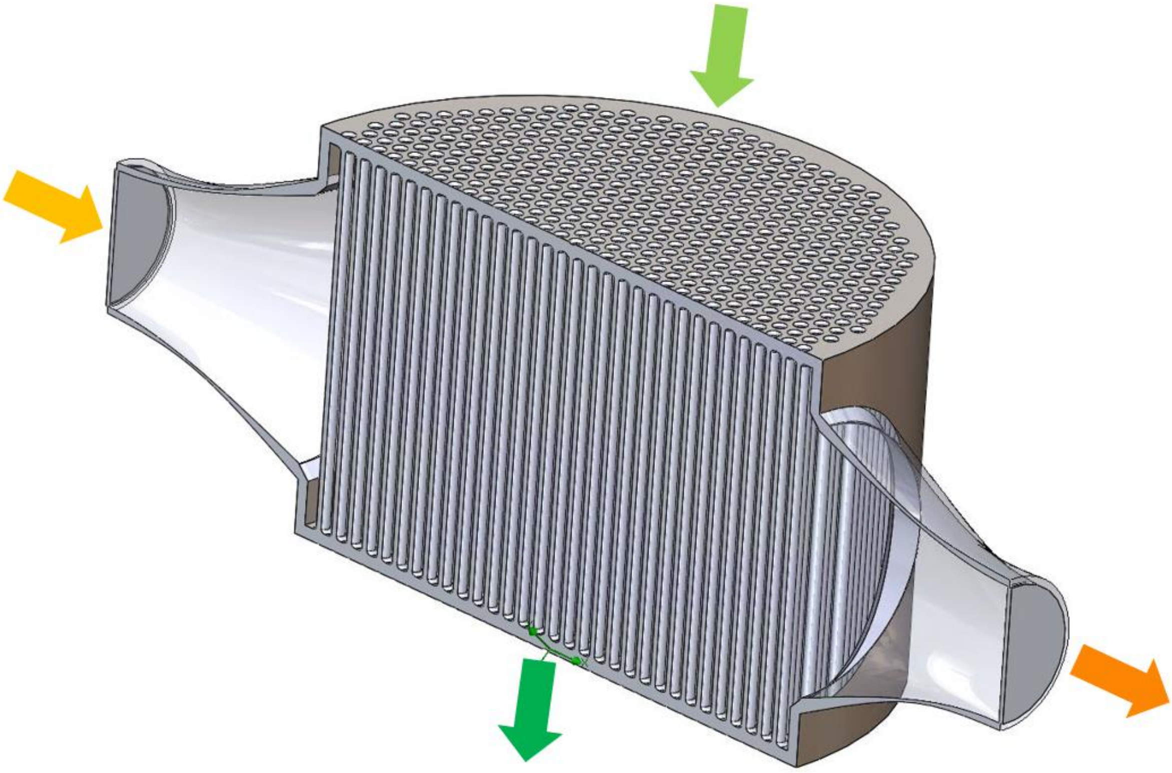

Figure 3-2: Sectional view of the 3D CAD model showing the tube bank and the internal volume. Green arrows indicate the flow of pressurised He gas through the tube bank and orange arrows indicate the flow of molten salt across the shell periphery.

3.3 Optimization methodology

A multi-objective parametric design optimization is carried out to determine the influence of certain variables to achieve the desired compact heat exchanger performance.
Key design parameters of influence are varied such as:

- Tube Inner Diameter (T_{ID}) – $2 \leq T_{ID} \leq 5$ (mm)
- Tube Outer Diameter (T_{OD}) – $3 \leq T_{OD} \leq 6$ (mm)
- Inter Tube Spacing (S_{tube}) – $3 \leq S_{tube} \leq 10$ (mm)

Whereas the tube wall offset distance (S_{wall}) is maintained at 2 mm. Similarly, the other major dimensions of the heat exchanger such as the shell diameter (D_{shell}) and the overall length (L_{shell}) are kept a constant at 262 and 163 mm respectively.

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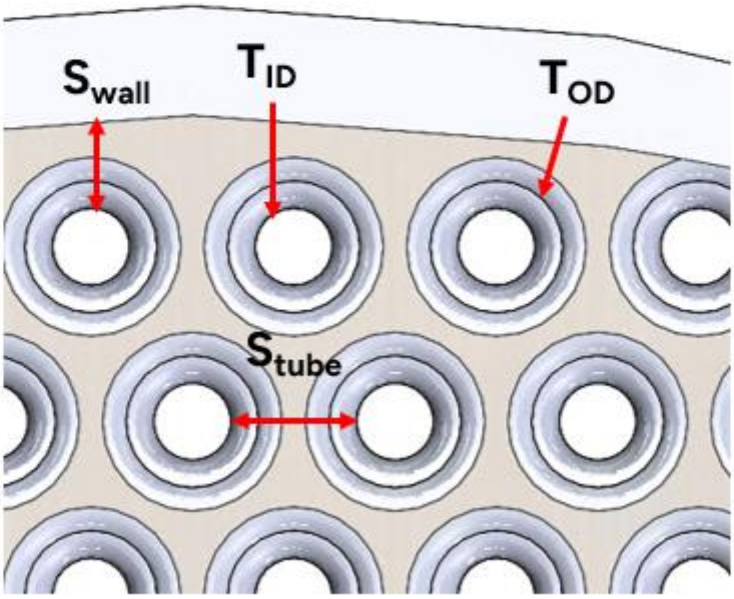

Figure 3-3: A close-up view of the key dimensional parameters for design optimization.

Another control variable of tube-side wall temperature (T_{wall}) is introduced to determine the operational working temperature of the pressured gas to achieve desired temperature of MS ($T_{out, salt}$). T_{wall} is varied between the range of 220 – 250 °C.

The molten-salt side operating conditions of mass flow rate at 3 kg/s and inlet temperature of 220°C are kept constant for the optimization study. An operating pressure of 101325 Pa (equivalent to atmospheric pressure of 1bar) is considered as typically the salts are not pressurized for pumping application.

Over 50 discrete simulations are generated as design of experiments (DOE) based on the software-controlled pairings of the variables across the above-mentioned range of the geometric and operational parameters.

The performance metrics to track the convergence of these simulations focused on the salt-side thermal-hydraulic estimations are as follows:

- Pressure difference (ΔP, Pa)
- Heat transfer coefficient (HTC, W/m^{2}K)
- Average outlet temperature ($T_{out, salt}$ °C)
- Heat transfer rate (Q, kW)

Based on the outcomes, the desired specification of the heat exchanger is decided on controlling the objective functions of performance criterion such as:

- $\Delta P \leq 1\%$ Pa (1000 Pa)
- $30 \leq Q \leq 45$ kW
- $HTC \geq 1100$ W/m^{2}K

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3.4 Optimization solutions

Results for key parameters of assessment such as pressure drop, heat transfer rate and heat transfer coefficient for the heat exchanger performance are presented below in terms of inter tube spacing and diameter ratio (Tube ID/Tube OD) which are considered as the dominating characteristics for the classifications.

Pressure drop:

Lower magnitudes of pressure drop are observed at higher diameter ratio and larger tube spacing. As a result of closer diameter ratios, i.e. thinner walls, more open channels are formed, and the pressure drop is reduced.

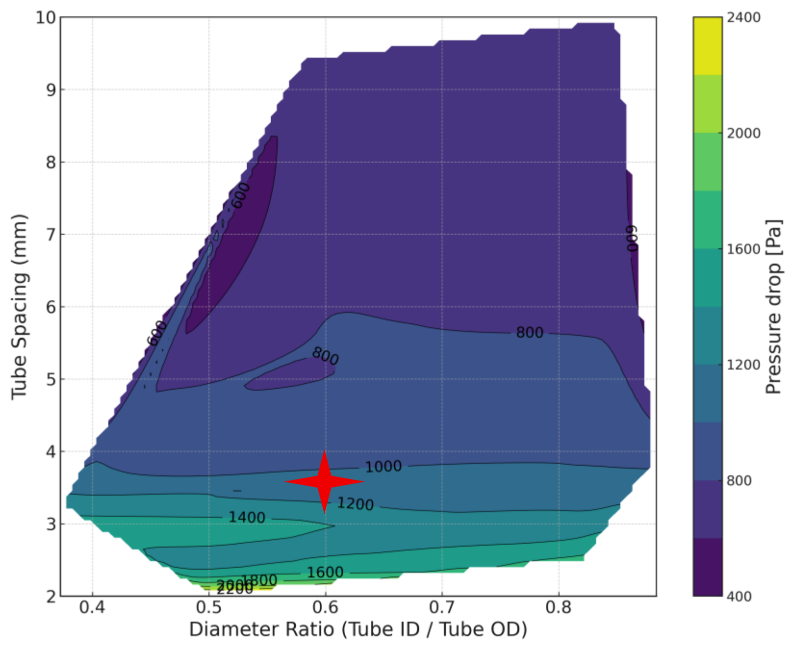

Figure 3-4: Contour plot of pressure drop for varying tube spacing and diameter ratio.

Heat transfer rate:

The desired heat transfer rate occurs for low-medium diameter ratio and moderate tube spacing. Thicker walls are favorable to facilitate an efficient heat exchange from the wall to fluid.

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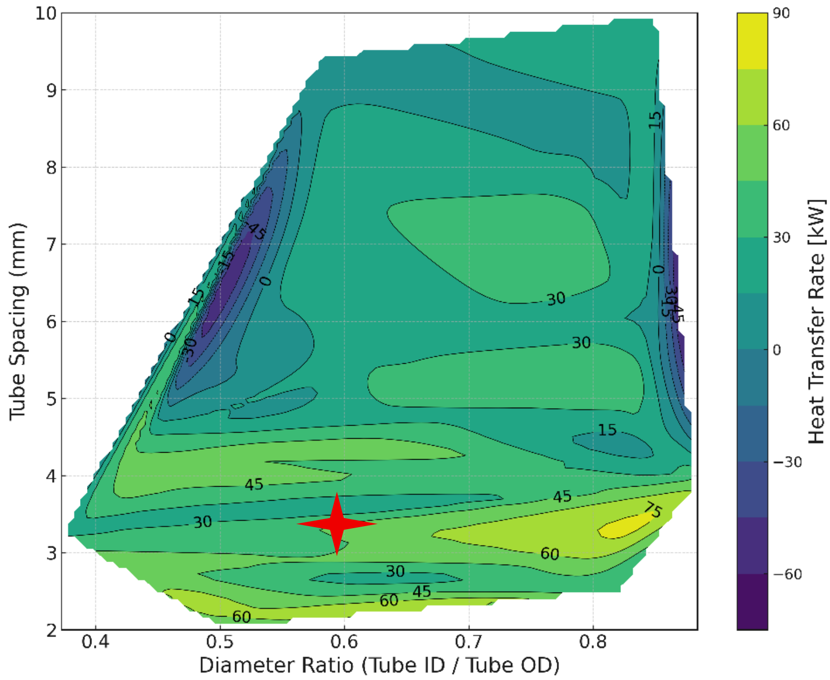

Figure 3-5: Contour plot of heat transfer rate for varying tube spacing and diameter ratio.

Heat transfer coefficient:

The desired heat transfer coefficient is attained at smaller tube spacing and moderate diameter ratios. Smaller tube spacing is favorable in promoting convection and results in adequate surface contact area for the fluid to exchange heat.

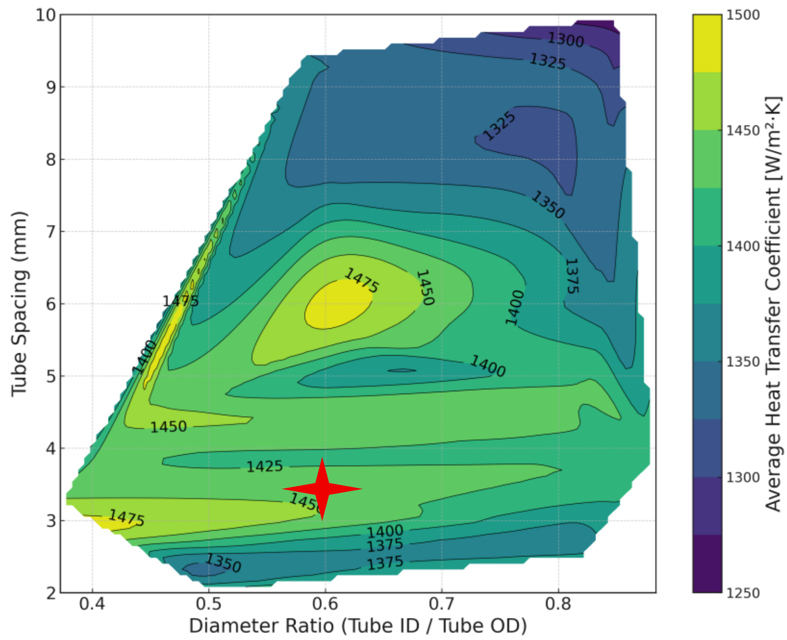

Figure 3-6: Contour plot of heat transfer coefficient for varying tube spacing and diameter ratio.

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3.5 Optimized Design

Based on the results generated from the multi-objective parametric design optimization, a composite scoring function is applied to determine the optimal design point based on the ranking of few key variables, as shown below in Eq 1.

$$Score = w_1 \cdot \left(\frac{Q - Q_{min}}{Q_{max} - Q_{min}}\right) + w_2 \cdot \left(\frac{HTC - HTC_{min}}{HTC_{max} - HTC_{min}}\right) - w_3 \cdot \left(\frac{\Delta P - 1000}{\Delta P_{max}}\right) \qquad (1)$$

Where w_1, w_2 and w_3 are the weights for thermal vs hydraulic performance. The pressure drop weight factor is considered sensitive in this study and thus carries the highest ranking while a balanced ranking for heat transfer rate and heat transfer coefficient is maintained.

The considerations made for the weighing factors is with w_1 and w_2 as 1, whilst a higher priority towards maintaining the pressure drop ≤ 1000 Pa with a w_3 as 3, thus enabling a pressure sensitive design choice. Given the internal shell area and the tube dimensions, the heat transfer targets could be satisfactorily met in the majority of cases as is evident from the results described in Section 3.4.

The final optimized design from the set of geometric and operational parameters is identified based on the above shortlisting criteria to achieve the desired thermal-hydraulic performance of the heat exchanger.

The geometric specifications are:

- T_{ID} – 3.05 mm
- T_{OD} – 5.05 mm
- Number of tubes – 673
- S_{tube} – 3.42 mm
- Pitch layout pattern – 60° triangular

A few key qualitative contour plots are shown in Figure 3-7Figure 3-8 andFigure 3-9 to present the near uniform molten salt flow distributions across the tube bank and the heat exchange between the tube walls and salt fluid. The shell wall-to-tube clearance of 2 mm is maintained across all the simulations such that the core fluid is dispersed across the central regions of the tube bank that favours the occurrence of maximum heat exchange.

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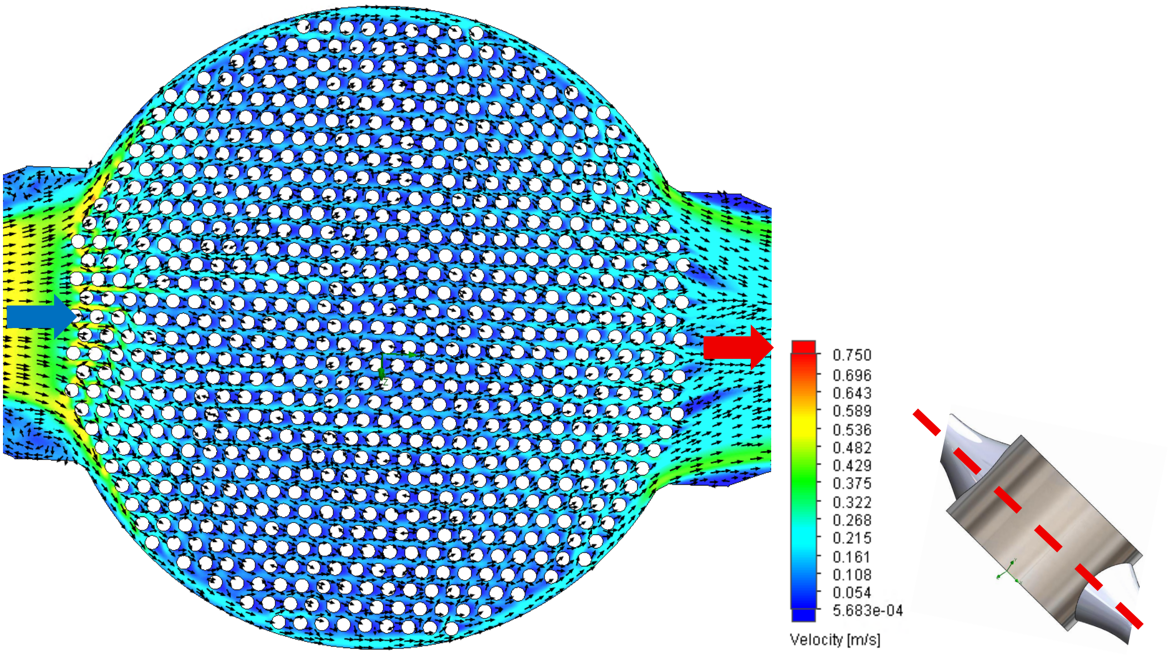

Figure 3-7: Contour and vector plot of the MS velocity distribution across the shell mid-plane for the optimized heat exchanger geometry.

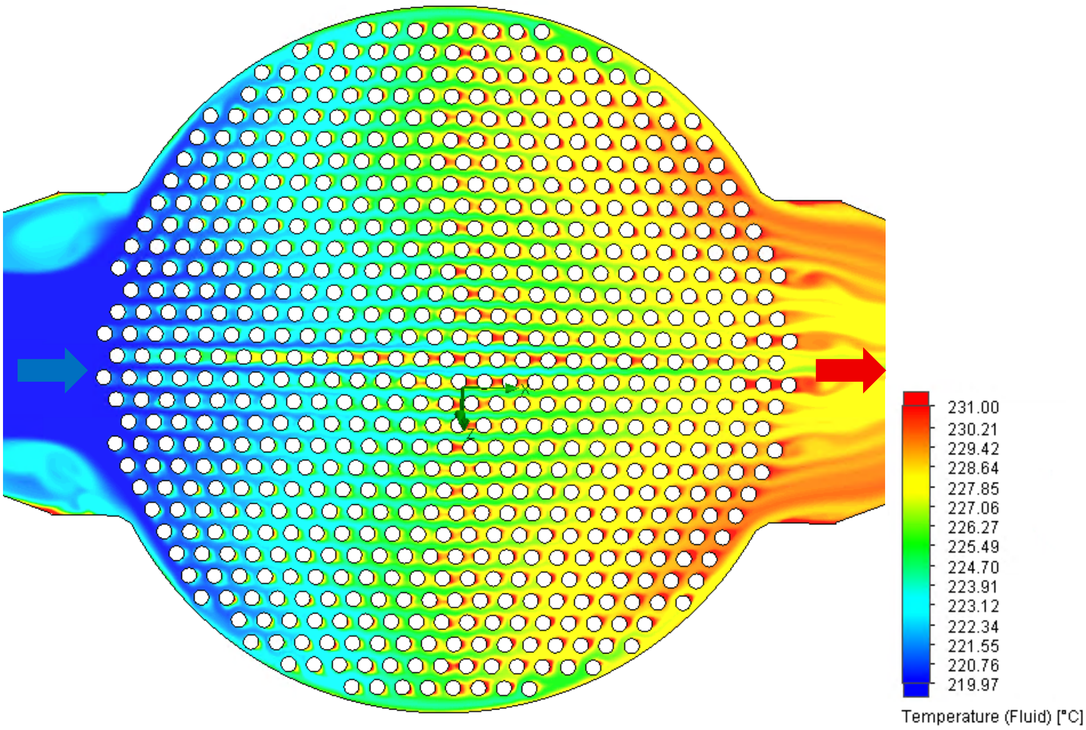

Figure 3-8: Contour plot of the MS temperature distribution across the shell mid-plane for the optimized heat exchanger geometry.

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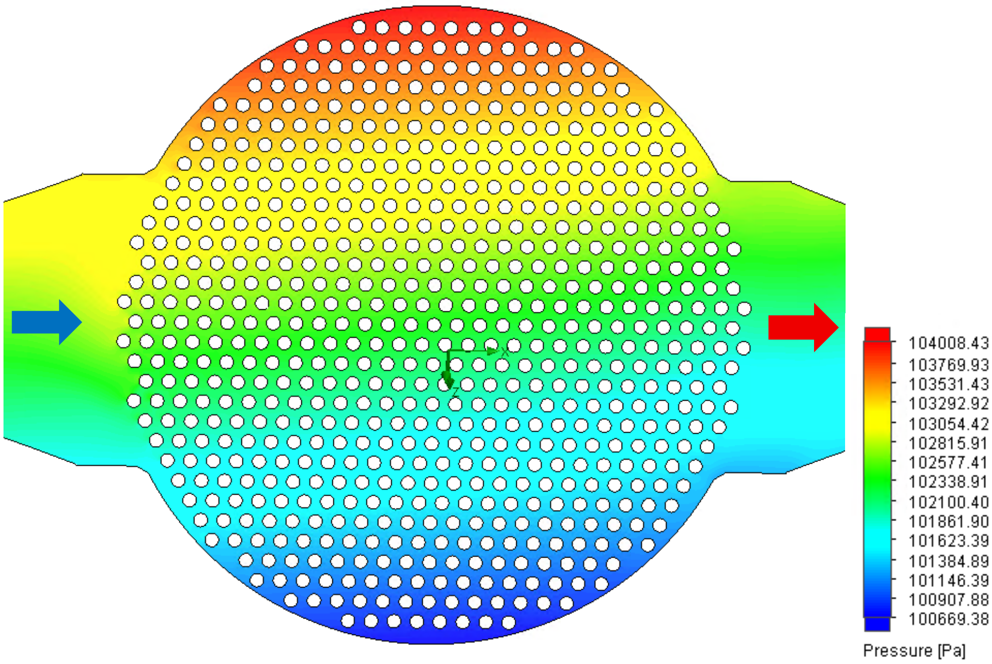
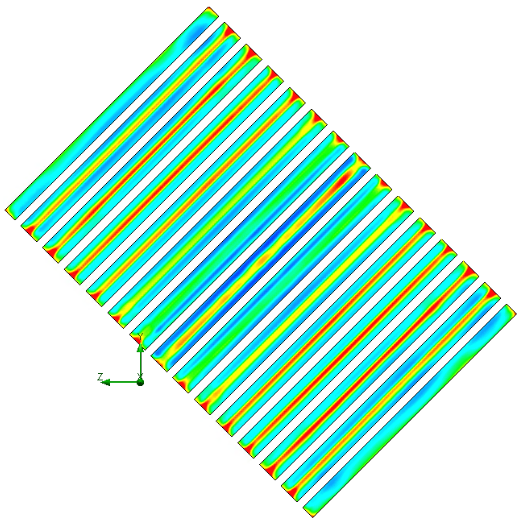
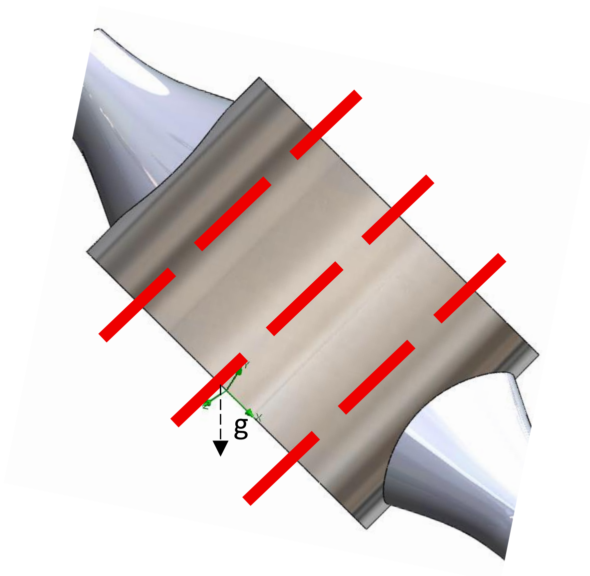


Figure 3-9: Contour plot of the MS pressure distribution across the shell mid-plane for the optimized heat exchanger geometry.

Additionally, the vertical sectional contour plots, as shown in Figure 3-10 of the molten salt fluid temperatures present the salt distributions in the axial direction of the heat exchanger, indicating a non-existence of dead velocity zones within the shell and tube heat exchanger.





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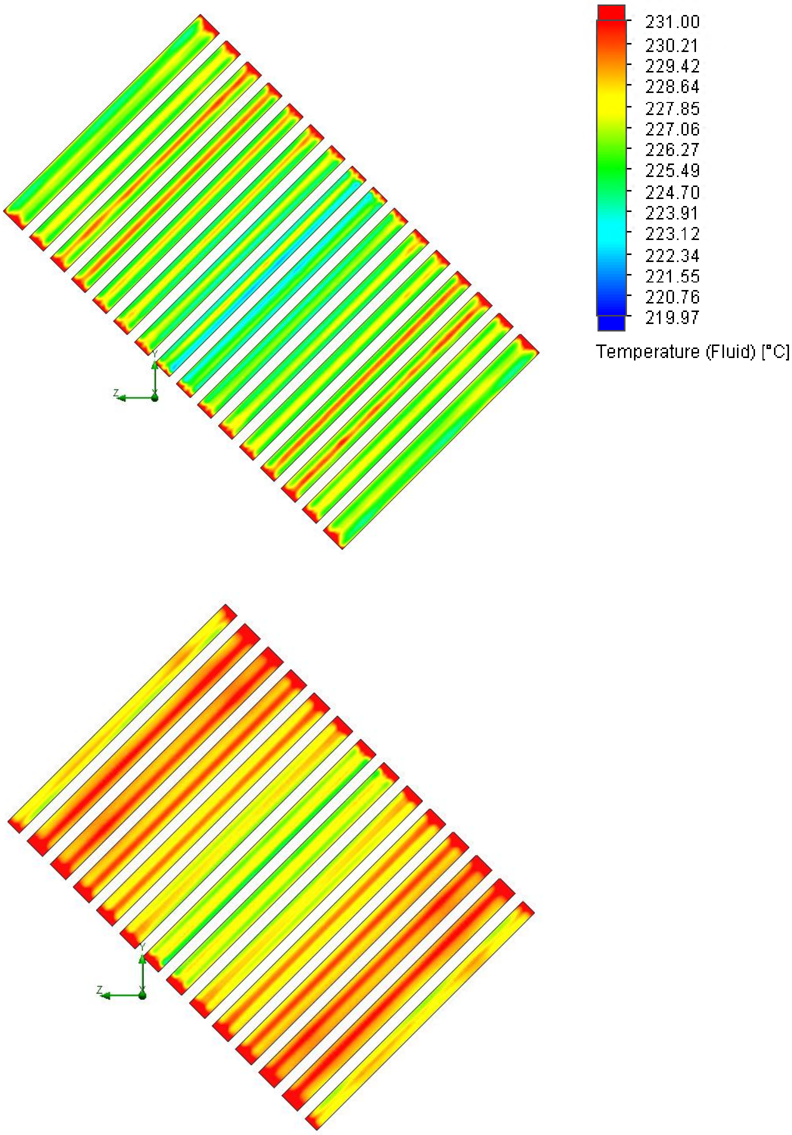

Figure 3-10: The spread of molten salt fluid temperatures across the axial direction of the shell and tube heat exchanger. The contour plots are shown in sequence with the sampling locations starting from near inlet, mid-plane and near outlet regions as also indicated in the reference schematic.

Key operational characteristics of the optimized heat exchanger geometry for given conditions of MS inlet at 3 kg/s and 220 °C results in the following thermal-hydraulic performance metrics:

- Desired He wall tube temperature of 240.5 °C
- Average MS outlet temperature of 9.2 °C
- Pressure drop in adjacent areas to the tube bank is 0.6 %
- Average heat transfer coefficient of 1445 W/m^{2}K
- Heat exchanger power rating of 42 kW

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3.6 Operational setpoints

An overview of the heat exchanger performance is undertaken by performing a sensitivity study on varying the He gas wall temperatures along with the corresponding MS inlet temperature conditions while maintaining a temperature difference between the two at 20.5 °C for consistency. Table 3-1 presents the effect of both operating fluid temperatures on the thermal-hydraulic performance of the heat exchanger. It can be noted that at elevated temperatures (300 °C and above), the molten salt performance is enhanced as the fluid viscosity decreases remarkably leading to an increase in the flow velocities and higher heat transfer capability with a reduction in the pressure drop. It is reflected with the rise in the molten salt delta T gains with corresponding increase in the power rating and heat transfer coefficients.

He wall T (°C)	MS inlet T (°C)	MS outlet T (°C)	MS delta T (°C)	delta P within tube bank (Pa)		Power rating (kW)	HTC (W/m²/K)
240.5	220	229.2	9.2	646	0.6%	42	1445
268.2	247.7	257.0	9.3	523	0.5%	42	1511
305.5	285	294.5	9.5	405	0.4%	43	1867
343.5	323	332.8	9.8	370	0.3%	44	1932
382.7	362.2	372.1	9.9	307	0.3%	45	2016

Table 3-1: Sensitivity study on a few key varying MS and He wall temperatures at a constant MS flowrate of 3 kg/s.

Table 3-2 presents the sensitivity study on MS flowrates for a fixed MS inlet temperature of 220 °C and a He wall temperature of 240.5 °C. It is noted that for increasing MS flowrate, the pressure drop increases substantially with a subsequent increase in the power rating and the heat transfer coefficient. This is as a result of the intensified turbulence characteristics of the fluid with heat transfer enhancement.

He wall T (°C)	MS inlet flowrate (kg/s)	MS inlet T (°C)	MS outlet T (°C)	MS delta T (°C)	delta P within tube bank (Pa)		Power rating (kW)	HTC (W/m²/K)
240.5	3	220	229.2	9.2	646	0.6%	42	1485
240.5	5	220	226.6	6.6	1302	1.3%	51	1772
240.5	7.5	220	224.9	4.9	2632	2.6%	57	2022
240.5	10	220	223.9	3.9	4187	4%	61	2181

Table 3-2: Sensitivity study on variable MS flowrate for a fixed MS inlet and He wall temperatures.

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4. Additive manufacturing considerations

The optimized shell and tube heat exchanger design is to be additively manufactured by leveraging the advanced manufacturing facilities and expertise of the project partners at Centre for Advanced Manufacturing Technologies (CAMT), Wrocław University.

The heat exchanger core (shell body) will be 3D printed using SS316L material as a preference based on its superior compatibility with molten salt and for its several advantages as descried in D3.1. The stainless-steel alloy with a composition of Chromium, Nickel, Molybdenum results in good oxidative and corrosion resistance. The ternary nitrate molten salts used in the project are generally less aggressive to the stainless-steel and feature a stable material compatibility performance for salts at up to 550 °C. It offers moderate thermal expansion, thermal shock resistance and slightly higher than Ni-based alloys. However, thermal cycling can cause microcracking at the welds and thus stress-relieving treatments are recommended. SS316L is the most widely used AM powders specially in Laser Powder Bed Fusion (LBF) and Direct Energy Deposition (DED) systems. It is considered most cost-effective alloy material and widely available commercially.

Property	SS316	Inconel 625/718	Hastelloy N	Haynes 230	AISI 310	Carbon Steel	Ceramics
Max Temp (°C)	550–600	800–980	700–800	1050	~1050	~450	>1200
CTE (µm/m·°C)	~16.0	13–14	~12.5	~13.5	~15.9	~12.0	4–8
Corrosion (Nitrate)	Good	Excellent	Excellent	Excellent	Good	Poor	Excellent
Corrosion (Chloride)	Poor	Mod–Good	Moderate	Moderate	Poor	Very Poor	Excellent
Thermal Cycling	Moderate	Excellent	Good	Excellent	Good	Poor	Moderate
Creep Resistance	Fair	Excellent	Moderate	Excellent	Moderate	Very Poor	Excellent
AM Suitability	Excellent	Excellent	Limited	Limited	Moderate	Rare	Difficult
Cost ($/kg)	4–7	30–80	80–100	80–150	5–10	<2	High
Availability	Common	Wide	Specialty	Specialty	Common	Very Common	Custom

Table 4-1: Table showing material thermo-physical characteristics for high temperature applications include AM suitability.

The shell core of outer diameter of 262 mm, 163 mm overall length fits well within the print bed dimensions of 285 mm X 285 mm for the SLM (Selective Laser Melting) based 3D printer. Certain aspects of the design such as the shell wall thickness of 5 mm and the filleting of the contact regions of the tubes with the shell walls (top and bottom side) are adapted to suit the printing requirements, as shown in the Figure 4-1 below.

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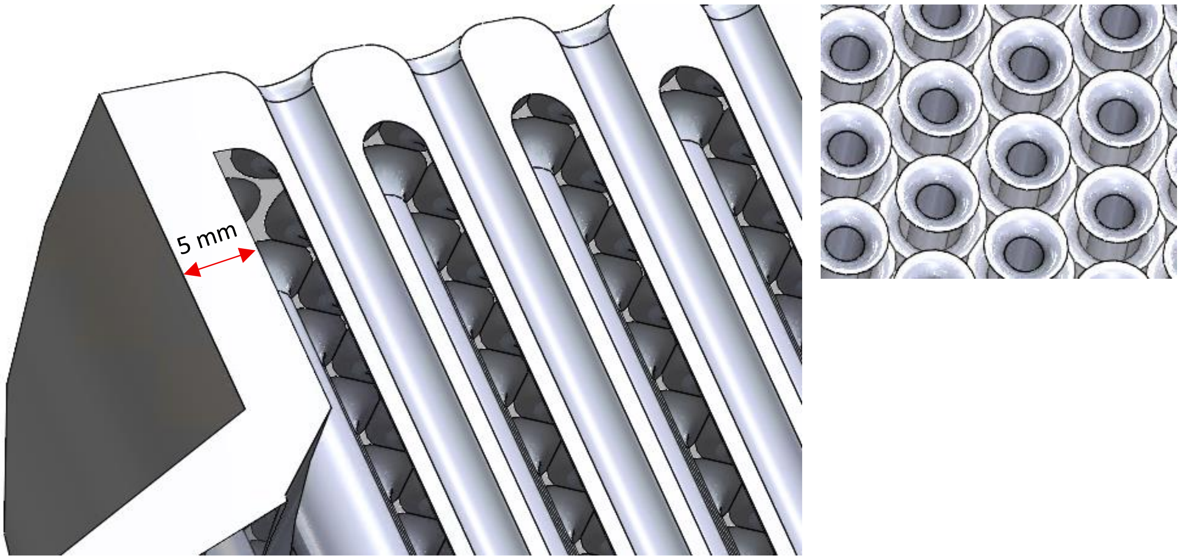

Figure 4-1: Close-up view of the fillet features added to the tube ends for preventing overhangs at the underside of inner shell walls.

The manufacturing shall be undertaken in iterative stages by printing several prototypes and samples to achieve a structurally and thermally stable component. Major consideration of additive manufacturing involves the post-processing of the printed components such as heat treatment and the sensitive clean-up of the powder residuals. Additionally, the surface roughness also is a crucial aspect in order for it to not negatively impact the heat exchanger performance.

The 2 shell-side MS ducts are to be commercially procured from the standard piping suppliers, and it shall be welded along the circumference to the 3D printed heat exchanger core. Figure 4-2 presents the outline of the heat exchanger core design readied for additive manufacturing.

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Figure 4-2: An overview of the optimized shell and tube geometry that is to be additively manufactured.

5. Conclusions

In this deliverable the current state of work on an optimized design geometry 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 T3.2 and includes a crucial design direction from the specifications of D2.1, D3.1 to facilitate for the heat exchangers integration within the HTHP. The optimized design work involves: 1) performing a multi-objective parametric design optimization of the 3D CAD model; 2) analyse and identify the optimal design setpoint model to achieve the desired thermal-hydraulic performance; 3) incorporate design features to maximise it compatibility with the SLM based additive manufacturing technique. An optimum design geometry with a tube ID of 3.05 mm, tube OD of 5.05 mm, 673 number of tubes is obtained with a tube wall temperature of 240.5 °C for an MS inlet of 3 kg/s at 220°C. The resulting desired heat exchanger performance for an optimized version is with a near-uniform flow distribution with 9.2 °C average MS outlet temperature, pressure drop of 0.6 % and a heat exchanger power rating of 42 kW.

This work leads to the executive design and drawings of the heat exchanger to be manufactured and tested in the next steps of WP3 and finally fully integrated into the high temperature heat pump in WP4.

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