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D5.6 Development of knowledge-based decision support rules

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Summary

This deliverable presents a comprehensive compilation of rules and logic designed to develop algorithms for decision-making related to various GeoSmart innovations. These innovations include the PCM module, Steam Accumulator (later abandoned), Water Thermocline, Scaling reduction system, and Adiabatic cooling system. The outlined rules and logic form the foundation for deliverables D5.7, which will report the GeoSmart Decision Support System developed under task 5.7. This report primarily focuses on developing algorithms using rules and logic to provide techno-economic and environmental solutions for GeoSmart innovations in the GeoSmart Decision Support System (DSS) developed in task 5.7.

Algorithms for the PCM module, steam accumulator, and water thermocline were developed by leveraging insights from previous deliverables (D2.1, D2.2, and D2.3), providing a robust understanding of Thermal Energy Storage (TES) principles. This knowledge guided the formulation of rules and logic to optimise the performance of the PCM module and the initially considered steam accumulator. A 1D model from the current literature informed the water thermocline module's design. Additionally, the scaling reduction system's development incorporated models from deliverables (D4.1, D4.2, D4.3, D4.4 and D4.5) by the University of Iceland, Gerosion, CEA, FPS and Spike Renewables, offering valuable insights into scaling reduction mechanisms crucial for designing efficient geothermal power plants. In the Insheim (VNI) power plant context, fundamental thermodynamic principles, precise ambient temperature and relative humidity data (weather data) were employed to design the adiabatic cooling system. Deliverables D1.9 and D3.3 by VNI have played a supportive role in developing these algorithms.

Objectives Met

Develop the GeoSmart system simulator suite, which combines a flow assurance simulator, knowledge-based engineering, and decision support systems to provide robust options for future design capability across diverse European geothermal sites, investment decision making and policy analysis.

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1. INTRODUCTION

Developing knowledge-based decision support rules involves creating a system that uses existing knowledge to provide recommendations or solutions for various problems or decisions.

In this deliverable, we present a comprehensive set of rules and logic to develop the algorithms for decision-making about various GeoSmart innovations, including the PCM module, Steam Accumulation (abandoned later), Water Thermocline, scaling reduction system, and adiabatic cooling system. These rules and logic are the foundations for task 5.7 and will be used as a backend algorithm of the Decision Support System (DSS) developed in task 5.7.

The primary objective of GeoSmart is to provide flexible and more efficient geothermal energy solutions by implementing innovative Thermal Energy Storage (TES), scaling reduction systems, and adiabatic cooling technologies. By utilising Phase Change Materials (PCMs), Steam Accumulators (later abandoned), and Water Thermocline, we aim to enhance the flexibility of existing geothermal power plants while ensuring a reliable and sustainable energy supply. Furthermore, the scaling reduction system and the adiabatic cooling system are technologies that enhance the efficiency of the plants. To develop the algorithms for the PCM module, steam accumulator, and water thermocline, we relied on the knowledge and insights gained from previous deliverables, specifically D2.1, D2.2, and D2.3. These deliverables provided a good understanding of TES operation principles and explored important theoretical aspects of the project. Leveraging this foundation, we devised rules and logic to develop algorithms that optimise the performance and functionalities of the PCM module and steam accumulator (abandoned later). The water thermocline module was developed based on a 1D model in the current literature [1]. The development of the scaling reduction system involved utilising rate equations and models obtained from deliverables D4.1, D4.2, D4.3, and D4.4 submitted by the University of Iceland and others. These deliverables contributed valuable insights into scaling reduction mechanisms, which are essential in designing efficient geothermal power plants.

We employed fundamental thermodynamic theories in the Insheim power plant context to create the adiabatic cooling system, specifically ambient temperature and relative humidity data (weather data). Considering these environmental factors, we aimed to enhance the power plant's overall efficiency while minimising its environmental impact.

The knowledge-based decision rules developed in this work serve as a crucial step towards implementing a robust Decision Support System in the subsequent deliverable, D5.7. By integrating these rules into the system, users can assess geothermal power plants' financial and environmental impacts with and without adopting the GeoSmart innovations. This integration will empower users to make informed decisions and identify the most suitable solutions for their plant requirements.

2. METHODS

This section presents the methodology employed to generate the knowledge-based decision rules for the Thermal Energy Storage (TES) solutions, namely PCM (Phase Change Material) storage, Steam Accumulator (later abandoned), and Water Thermocline. It also covers efficiency-enhancing solutions, including scaling reduction and adiabatic cooling systems. Additionally, we outline the optimisation process considering financial and environmental parameters and performances.

2.1 KB Rules Development

The following steps were undertaken to develop the knowledge-based rules (KB Rules) for the Knowledge-Based Decision Support System (KBDSS) tool:

- Knowledge Acquisition
- Knowledge Model or Knowledge Representation
- Knowledge Accuracy Check
- Transformation of Knowledge into Scalable Machine-Readable Format.

2.1.1 Knowledge Acquisition

Relevant knowledge about Flexibility and Efficiency Enhancement solutions was acquired to establish a solid foundation for the knowledge-based decision rules. This involved a comprehensive literature review consultations and communications with relevant partners.

Deliverables D2.1, D2.2, and D2.3 provided valuable insights into the flexibility of TES solutions and provided an in-depth understanding of TES operation and important theoretical aspects. However, for the water thermocline, an existing 1D model from the current literature was utilised as a reference [1]. Additionally, collaborative discussions with the CEA (Commissariat à l'énergie atomique et aux énergies alternatives) enriched the knowledge acquisition process for the TES modules.

In the case of the efficiency-enhancing solutions, the scaling reduction system was thoroughly investigated. Deliverables D4.1, D4.2, D4.3, D4.4, and D4.5 were extensively studied to acquire the necessary knowledge for this system. Specifically, deliverable D4.1, which focuses on the reaction kinematics of silica scaling, played a crucial role in obtaining the rate of reactions. Furthermore, clear communication and knowledge exchange with the relevant partners, the University of Iceland and Spike Renewables, further enhanced our understanding and insights into the scaling reduction system. For the adiabatic cooling system, thermodynamics theories were fundamental to acquiring knowledge. Deliverable D3.3 was supported by providing supplementary information and further contextualisation to enhance the understanding of thermodynamic concepts in relation to the adiabatic cooling system.

Through a comprehensive knowledge acquisition process, incorporating deliverables, literature reviews, and collaborative discussions, a diverse range of expertise and perspectives were incorporated into developing the knowledge-based decision rules for both the TES and Efficiency Enhancement solutions.

2.1.2 Knowledge Models or Representations

In this step, the acquired knowledge is transformed into knowledge models or representations for each module within the GeoSmart project. These models serve as mathematical equations and formulas that capture the essential characteristics and behaviours of the respective solutions. The knowledge models are instrumental in developing a comprehensive understanding of the systems and formulating knowledge-based decision rules.

For the Thermal Energy Storage (TES) solutions, including PCM, Steam Accumulator (although later abandoned), and Water Thermocline, mathematical models were developed to describe their operations. These models consider factors such as charging time, charging and discharging temperatures, flow rates, and the power plant's maximum storage capacity. By incorporating these parameters, the knowledge models enable the calculation of variables such as Capacity and dimensions of the TES solutions, allowing users to select suitable options based on their specific requirements.

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Similarly, mathematical models were derived for the Efficiency Enhancement solutions, namely the Scaling Reduction and Adiabatic Cooling systems. These models consider inputs such as primary and secondary fluid conditions, pH levels, ambient temperature, relative humidity, and the number of fans. By leveraging these inputs, the knowledge models provide insights into the systems' performance, including reduced silica concentration, temperature reduction capability, and water consumption.

Developing these knowledge models or representations is crucial in transforming the acquired knowledge into practical and scalable machine-readable formats or algorithms.

2.1.3 Knowledge Accuracy Check

After developing the knowledge models and representations, a crucial step was undertaken to ensure the accuracy and reliability of the obtained results. In this step, the developed models were subjected to a knowledge accuracy check by collaborating with relevant partners and experts in the field.

For the Thermal Energy Storage (TES) solutions, the models, including those for PCM, Steam Accumulator (before its abandonment), and Water Thermocline, were shared with the CEA for verification. They played a crucial role in initially validating the accuracy and effectiveness of the TES models. Similarly, for the Scaling Reduction system, the knowledge model was adapted from deliverable D4.1 by the University of Iceland. The University of Iceland, known for its research and contributions to geothermal energy, collaborated to verify the accuracy and robustness of the scaling reduction system model.

Additionally, it is important to note that validating the developed models is an ongoing process within the GeoSmart project. While the knowledge accuracy check with relevant partners provided initial validation, further validation will be conducted during the project's demonstration phase. This validation process will occur when the TES modules, including PCM, Water Thermocline, and other components, as well as the Efficiency Enhancement solutions such as the Scaling Reduction system and Adiabatic Cooling system, are installed and operated in the KZD2 and VNI geothermal power plant settings.

The validation phase of the project is critical in ensuring the practical applicability and effectiveness of the developed knowledge-based decision rules. This validation process will enable the comparison of the model predictions with the actual outcomes observed during the operation of the systems. Any discrepancies or deviations will be carefully analysed, and if necessary, the knowledge models will be refined and adjusted to improve their accuracy and reliability. By aligning the model predictions with the real-world results, the project will provide valuable insights and enhance confidence in the decision support system's ability to guide users in making informed choices regarding implementing TES and Efficiency Enhancement solutions in geothermal power plants.

2.1.4 Transformation of Knowledge into Scalable Machine-Readable Format

The final step in developing knowledge-based decision rules within the GeoSmart project involves transforming the acquired, verified, and validated knowledge models into a scalable machine-readable format. This step facilitates the integration of the developed knowledge into a Knowledge-Based Decision Support System (KBDSS), enabling users to access and utilise the knowledge-based rules effectively.

The mathematical equations, formulas, and models obtained earlier are translated into code and algorithms during this step. This conversion process ensures that the knowledge-based rules are encoded in a format that

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computers can easily understand and process. The KBDSS tool can execute the rules and provide users with valuable insights and decision support by transforming the knowledge into a machine-readable format.

Users can access a user-friendly interface that facilitates decision-making processes by implementing the developed knowledge-based rules within the KBDSS tool. They can input their requirements, preferences, and constraints, and the tool will provide them with various options, cost estimates, environmental impact assessments, and other relevant information to aid in selecting the most suitable TES and Efficiency Enhancement solutions for their specific geothermal power plant.

2.2 Solution Optimisation

The GeoSmart project's optimisation process aims to identify the most suitable solutions for geothermal power plants based on financial parameters and environmental performance. This optimisation is facilitated by the integration of cost models and environmental performance models into the decision support system.

2.2.1 Cost Optimisation

The cost models consider key parameters, including capital expenditure, operational expenditure, and end-of-life costs, to evaluate the financial implications of each solution. By incorporating these parameters, the cost models generate important financial metrics, such as the levelised cost of energy (LCOE), net present value (NPV), internal rate of return (IRR), payback period, and return on investment (ROI).

The optimisation process utilises these financial metrics to identify the most economically viable solutions. Users can compare and analyse the cost-related indicators for each option, allowing them to select the solutions that align with their financial goals and constraints. The decision support system comprehensively presents cost-related information, enabling users to make informed decisions regarding the financial feasibility of different solutions.

2.2.2 Environmental Performance Optimisation

The environmental performance models estimate each solution's resource consumption, considering factors such as energy usage, water consumption, and emissions. Simapro, a software tool for life cycle assessment, calculates the solutions' environmental impact, including parameters like CO₂ emissions.

By assessing each solution's environmental consequences, users can evaluate its sustainability and environmental compatibility. The decision support system provides insights into the solutions' environmental performance, allowing users to identify alternatives that minimise resource consumption and environmental impact.

The methodology involved a systematic approach to knowledge acquisition, knowledge modelling, knowledge accuracy checks, and transformation into scalable machine-readable formats. The resulting knowledge-based decision rules (KB Rules) and the financial and environmental optimisation processes provided a robust framework for decision-making within the KBDSS tool.

3. RESULTS AND DISCUSSIONS

Knowledge-based (KB) rules are valuable tools for optimising various aspects of geothermal power plants, including flexibility solutions and efficiency enhancement systems. This section presents the developed rules in the form of models, equations, and theoretical foundations underlying each module within the Knowledge-

Based Decision Support System (KBDSS). These models were developed based on a comprehensive review of existing literature, consultations with relevant partners, and rigorous verification processes. By incorporating these knowledge-based rules, the KBDSS empowers geothermal power plant operators with insightful decision-making capabilities, enhancing operational flexibility, improving efficiency, and optimising cost and environmental performance.

To visually illustrate the interconnectedness of the various modules within the Geosmart KBDSS, we present a comprehensive flowchart in Fig. 1 that depicts the information flow and dependencies among the modules.

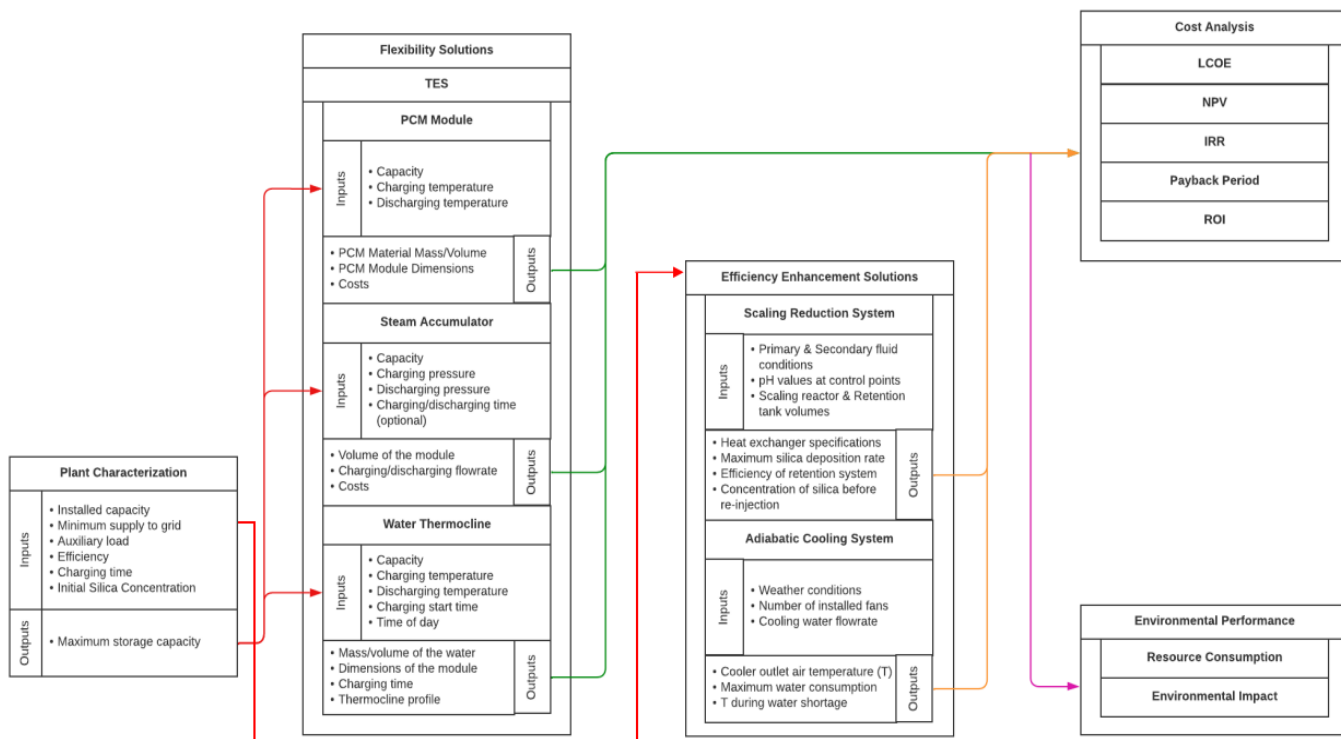


Figure 1. Flowchart of the information flow and connectivity between the GeoSmart KBDSS modules

Starting with the Plant Characterisation module, the flowchart showcases how outputs from this module serve as inputs to both the Flexibility Solutions (TES) and Efficiency Enhancement Solutions. The Flexibility of TES Solutions, including PCM, Steam Accumulator, and Water Thermocline, utilises the maximum storage capacity and other relevant parameters obtained from Plant Characterization. On the other hand, Efficiency Enhancement Solutions, such as the Scaling Reduction System and Adiabatic Cooling System, also benefit from the inputs derived from Plant Characterisation. The flowchart further highlights the connections between the cost analysis and environmental impact analysis modules, demonstrating the holistic approach of the Geosmart project. This flowchart provides a visual representation of the information flow and interdependencies among the Knowledge-Based Decision Support System modules, aiding in a comprehensive understanding of the system's functioning.

In the subsequent sections, we will delve into the details of each module, starting with the Plant Characterisation module. We will present the models, equations, and theories developed for the various modules, including TES solutions (PCM, Steam Accumulator, and Water Thermocline), the Scaling Reduction System, and the Adiabatic Cooling System.

3.1 Plant Characterisation Module

The Plant Characterization module serves as the foundation for our knowledge-based decision system. It encompasses characterising the power plant and gathering relevant parameters and data to inform subsequent modules. Through comprehensive analysis and calculations, this module enables us to determine crucial variables, such as the power plant's maximum storage capacity. Below, we describe the theories and equations that lay the module's foundation.

The main output of this module is the Maximum Storage Capacity for the Powerplant (C_{max}).

We use the following formula to find out the (C_{max}) –

$$(C_{max}) = \left[\frac{P_e - P_{grid, min} - P_{aux}}{\eta_{cycle}} - P_{t,min} \right] \times T_c \dots \dots \dots (1)$$

Where,

P_e = Plant capacity, MW_e

$P_{grid, min}$ = Minimum electric power to the grid, MW_e

P_{aux} = Auxiliary load, MW_e

η_{cycle} = Power plant efficiency, in a fraction

$P_{t, min}$ = Minimum thermal power to grid, MW_t

T_c = Maximum charging time, h

3.2 Flexibility or Thermal Energy Storage (TES) Solutions

The Flexibility Solutions, comprising Thermal Energy Storage (TES) modules, offer versatile and efficient energy management. Below, we will describe the models for all the TES modules: Phase Change Materials (PCM), Steam Accumulators, and Water Thermocline.

The TES solutions all have the input of minimum and maximum capacity. The maximum capacity is auto-filled with the Maximum Storage Capacity output from the Plant Characterization module discussed in section 3.1. Users can also input their values as the maximum capacity value for the specific TES module. Five capacity values are taken from the minimum to maximum range as follows:

$$\text{Capacity, } (C) = C_{min} + N \times \frac{C_{max} - C_{min}}{4} \dots \dots \dots (2) ; \text{ where } N = 0, 1, 2, 3, 4$$

Here,

C_{min} = Minimum Capacity input

C_{max} = Maximum Capacity input

3.2.1 PCM Storage Module

The total volume of PCM is under-estimated because there is some inert PCM (PCM that will not melt) in the region between the tubes bundle and the shell, this volume can represent 5 to 30% of the total amount of PCM, depending on the module size and geometry. We consider melting fraction (f) = 0.8, ensuring that the unused PCM is accounted for in the mass. This could be tweaked by the administrator/user based on the design. The density of HITEC (ρ_{hitec}), will vary depending on the temperature [1]. We created and used an equation that gives ρ_{hitec} as a function of the temperature. Maximum allowable charging temperature ($T_{c, max}$) = 400 °C, is an internal design variable considering Nitrate Content [2]. The sensible heat stored in the metallic parts will not be considered. It may be calculated after the solution, i.e., as an output. The sensible heat stored in the HTF will not be considered. It may also be calculated as the output. The PCM is considered to be isothermally heated

and melted. We consider a safety factor of 10% while calculating the volume of the PCM module. We also consider that the tubes (including the fin and profile) occupy about 20% of the total volume of the PCM module within the tube bundle. This value will be refined once all the values from the real system are available for validation. Another consideration is the top cap of the PCM module. We assume 15% of the volume is covered by the top caps at the top and bottom combined. The height of the tubes (L_t) will then be equal to the tube bundle height (height of the PCM module excluding top caps). The tubes' diameter, fin, and profile are internal design variables. The spacing between the tubes and the fins will also be considered constant and taken from the existing design of KZD2 to estimate the volume occupied by the tubes. The user may also be able to provide the maximum height/length of the module ($L_{mod_max, pcm}$) as an input if appropriate. The height/length (L) to diameter (D) ratio (L/D) should be within 3 – 4.5 for optimal performance of an STHX [3]. This value is approximately 3.6 for the KZD2 site PCM module. We may use this value $\frac{L_t}{D_{mod, pcm}} = 3.5$ (this value may be updated later) as the ratio. For convenience, we have used the length of the tube (L_t) instead of the height/length of the module ($L_{mod, pcm}$) in the ratio. Considering the top caps, tubes (including the fin and profile) occupy about $0.85 \times 0.2 = 15\%$ (approximately) of the total volume of the PCM module, $V_{mod, pcm}$. The tubes, along with the fins and the profile, are hexagonal (from the design of CEA). In other words, the tubes are arranged in a staggered configuration. The apothem of the hexagon is 70mm according to the manufactured design specification.

Algorithm or model description:

The mass of the PCM material M_{pcm} , in kg, will be calculated using the following formula:

$$M_{pcm} = \frac{C_{pcm} \times 3600 \times 1000}{[c_{ps}(t_m - t_i) + f\Delta q + f c_{pl}(t_f - t_m)]} \dots\dots\dots (3)$$

Here,

C_{pcm} = capacity of the PCM module, MWh

t_m = melting temperature, °C

t_i = discharging temperature, °C

t_f = charging temperature, °C

c_{ps} = average specific heat of the solid phase between t_i and t_m , kJ/kg

c_{pl} = average specific heat of the liquid phase between t_m and t_f , kJ/kg K

f = melt fraction = 0.8 (from Theory & Assumption)

Δq = latent heat of fusion, kJ/kg

Next, we figure out the density of the PCM material (HITEC), ρ_{hitec} in kg/m³, at charging temperature t_f in °C, using the following equation –

$$\rho_{hitec} = -0.7309 \times t_f + 2084.4$$

The density of the HITEC is considered at the melting temperature of the PCM, $t_f=142$.

The charging temperature is the highest temperature the PCM material may go through, and the minimum density is found using this temperature. Now to get the **maximum volume** occupied by the PCM material/HITEC V_{pcm} is as follows:

$$V_{pcm} = \frac{M_{pcm}}{\rho_{hitec}}$$

he **volume of the PCM Module** ($V_{mod, pcm}$) is determined as follows. First of all, we know that $V_{mod, pcm}$ will be the summation of V_{pcm} , V_{tubes} and V_{top_cover} –

$$V_{mod, pcm} = (V_{pcm} + V_{tubes} + V_{top_cover})$$

Now, considering that the tubes occupy around 20% and the top caps occupy 15% of the total volume of the module, we will get –

$$V_{mod, pcm} = \frac{V_{pcm}}{0.65}$$

Since we have taken the minimum density of PCM material at maximum temperature (Charging temperature), we will not consider the volume of gas sky on top of the PCM module. However, we will consider a safety factor of 10%.

$$V_{mod, pcm} = \frac{V_{pcm}}{0.65 \times 0.9}$$

This is the formula we will use to determine the volume of the PCM module. We use V_{pcm} from step 1.

Now, the **height/length of the tubes or the tube bundle** L_t will also be calculated. We can consider the volume of the PCM module as a cylinder (excluding the top caps). In that case, we can use the height of the tube bundle or **length of the tube** (L_t) in the formula of a cylinder volume –

$$0.85 \times V_{mod, pcm} = \frac{\pi \times D_{mod, pcm}^2 \times L_t}{4}$$

From the theory & assumption section,

$$D_{mod, pcm} = \frac{L_t}{3.5}$$

So, the finalised formula for L_t will be,

$$V_{mod, pcm} = \frac{\pi \times L_t^3}{42}$$

or

$$L_t = \sqrt[3]{\frac{42 \times V_{mod, pcm}}{\pi}} \quad \dots \dots \dots \quad (4)$$

Now, we will calculate the **height of the module** ($L_{mod,pcm}$) and **the diameter of the module** ($D_{mod,pcm}$) along with the **top cap dimensions**.

First, let's calculate the **diameter of the module** $D_{mod, pcm}$ –

$$D_{mod, pcm} = \frac{L_t}{3.5}$$

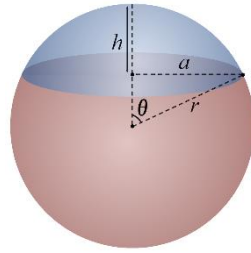
Now, we should work out the **dimensions of the top cap** to get to the **height of the module; the** $L_{mod,pcm}$. diameter of the top cap base will be the same as the diameter of the module –

$$D_{top_cap_base} = D_{mod, pcm}$$

Now, we also know the **volume of the top caps to be 20% of the PCM module volume**. For one of the top caps, it will be 10% –

$$V_{top_cap} = 0.1 \times V_{mod, pcm}$$

The formula for the volume of a spherical cap–



$$0.1 \times V_{mod, pcm} = \frac{\pi \times h \times (3a^2 + h^2)}{6}$$

Or, $3a^2\pi h + \pi h^3 - 0.6V_{mod, pcm} = 0$ (5)

Here, it a would be half of the top cap base diameter –

$$a = \frac{D_{top_cap_base}}{2}$$

After calculating h from equation (5), we will calculate the **height of the module, $L_{mod, pcm}$** –

$$L_{mod, pcm} = L_t + 2h$$

Important Note 1: Using the known values of a and $V_{mod, pcm}$ we will find out the values of h from equation (5). **Solving the equation will lead to 3 values of h .** We may use the logical values (i.e., not negative and non-imaginary). We may also use the following condition to find out the logical value(s) of h .

$$L_t + 2h < L_{mod_max, pcm}$$

If none of the values of h passes the condition, then we will use the **smallest non-negative value** of h .

Important Note 2: However, after calculation, if $L_{mod, pcm} > L_{mod_max, pcm}$ (max height from user input), then we will do the following –

$$L_{mod, pcm} = L_{mod_max, pcm}$$

In this step, we will determine the **number of the tubes (N_t)**. Each tube will have a hexagonal shape as mentioned in the theory and assumption. As the apothem is 70mm, the area occupied by a tube (A_t) will be the following:

$$A_t = \frac{1}{2} \times \frac{6 \times 2 \times 0.07}{\sqrt{3}} \times 0.07$$

Or,

$$A_t = 2\sqrt{3} \times (0.07)^2$$

We have assumed that the 80% PCM material will be within the tube bundles and melt completely. If we consider the 80% of circular profile of the PCM module or area of the circle, we will consider 80% of the cylinder volume. Accordingly, we can find the **number of tubes (N_t)** from both areas–

$$2D \text{ area of the tube bundle} = \text{Number of tubes } (N_t) \times \text{Area of a single tube } (A_t)$$

Or,

$$0.8 \times \frac{\pi D_{mod, pcm}^2}{4} = N_t \times A_t$$

Finally,

$$N_t = \frac{\pi D_{mod, pcm}^2}{5 \times A_t} \quad \dots \dots \quad \dots \dots \quad (6)$$

Model limitations and recommendations:

In conclusion, the PCM Module is a valuable starting point in designing thermal energy storage systems. It offers a linear model based on geometry and simplified physics, providing initial insights into PCM storage. However, a comprehensive understanding of parameters such as melting fraction and charging time requires extensive analysis and simulation. Therefore, further investigation and detailed simulations are recommended to evaluate PCM-based thermal energy storage systems more accurately.

3.2.2 Steam Accumulator

The steam accumulator has been abandoned in the GeoSmart project. However, the GeoSmart KBDSS tool still features the option to choose steam accumulators as a storage option. For the steam accumulator model, we assume that the total steam entered during charging equals the total steam going out during discharging. We also consider that the charging & discharging time will vary according to the flow rate.

Algorithm or model description:

The **general algorithm** for the design of a steam accumulator **without non-condensable gases** is presented in this section. Knowing the **charging pressure (P_{charge})** and **discharging pressure (P_{discharge})**, the charging and discharging temperatures and vapour / liquid enthalpies will be taken from the **Steam Table**:

- T_{charge} = T_{sat} (P_{charge}) → h_{L, sat} (P_{charge}, T_{charge}),
- T_{discharge} = T_{sat} (P_{discharge}) → h_{L, sat} (P_{discharge}, T_{discharge})

- h_L is the liquid water enthalpy

m_{L, initial} is the **initial mass of liquid, in kg**, within the steam accumulator –

$$m_{L, initial} = \frac{C \times 1000 \times 3600}{(h_{L, sat}(P_{charge}) - h_{L, sat}(P_{discharge}))}$$

- C = capacity in (MWh)

The **liquid volume (V_{liquid})**, in m³, can then be calculated with the following equation –

$$V_{liquid} = \frac{m_{L, initial}}{\rho_{L, sat}(P_{discharge}, T_{discharge})}$$

- ρ_{L, sat} (P_{discharge}) = saturated water density at the discharge pressure

The **total volume of the Steam Accumulator module (V_{total})**, in m³, can then be calculated with the following equation –

$$V_{total} = \frac{V_{liquid}}{\% V_{liquid}}$$

Where, %Vliquid = 0.67

Quantifying the **Mass of the discharged steam** (M_{st}), in kg, done using the way shown –

$$M_{st} = \rho_{steam} (P_{charge}) \times 0.33 \times V_{total}$$

According to the assumptions, total mass of the charging steam is M_{st} as well.

To work out the **Charging flowrate** (\dot{m}_c), in t/h, we will be using the **Charging time** (t_c) values as done below –

$$\dot{m}_c = \frac{M_{st}}{t_c \times 1000} \quad \dots \quad \dots \quad (7)$$

We will compute the **Discharging flowrate** (\dot{m}_d), in t/h, using the **Discharging time** (t_d) value –

$$\dot{m}_d = \frac{M_{st}}{t_d \times 1000} \quad \dots \quad \dots \quad (8)$$

We may estimate the **Cost of the Steam Accumulator** ($Cost_{sa}$), in £, using a **cost model** from the manufacturer. However, currently, we do not possess such models. Email communications with the manufacturers are ongoing in this regard.

Model limitations and recommendations:

The steam accumulator module relies on the assumption that the initial liquid inside the accumulator is approximately 67% of the total module volume, a common value found in steam accumulator designs. However, deviations from this assumption may require adjustments to the model. Further analysis and validation are recommended to ensure accurate predictions and optimise the design of the steam accumulator module.

3.2.3 Water thermocline model

Algorithm or model description:

A 1D transient model describes the transient temperature inside the Water Thermocline (WT) module using the energy equation as follows [4]:

$$\rho c \frac{\partial T}{\partial t} + \rho c v \frac{\partial T}{\partial h} = \lambda \frac{\partial^2 T}{\partial h^2}$$

Here, h is the axial coordinate measured along the vertical axis of the tank (m); $v = \frac{m_f}{A}$ is the convection velocity, which represents the velocity of the downward movement of the thermocline ($m s^{-1}$); m_f is the water mass flow rate during charging ($kg s^{-1}$); A is the cross-sectional area of the TCST (m^2); T is the temperature of the working fluid (K), ρ is the working fluid density ($kg m^{-3}$); c is the specific heat capacity of the working fluid ($kJ kg^{-1} K^{-1}$); λ is the thermal conductivity ($W m^{-1} K^{-1}$).

The analytical solution with the dimensionless variables is given in [1] as:

$$\theta(\xi, \tau) = \frac{1}{2} \operatorname{erfc} \left(\frac{\xi - u\tau}{2\sqrt{\tau}} \right)$$

Here, θ is the dimensionless temperature along the vertical axis of the WT module, which is a function of the dimensionless vertical position (ξ) and time (τ). The dimensionless velocity scale is represented by u .

Now let's define these dimensionless parameters:

$$\theta = \frac{T - T_h}{T_h - T_c}$$

Here, T is the temperature at any particular vertical position, T_h is the inlet or charging temperature, and T_c is the initial colder water temperature (also assumed to be the same as the discharging outlet temperature).

$$\xi = \frac{h}{H}$$

Here, H is the tank height.

$$\tau = Fo = \frac{ta}{H^2}$$

Here, Fo is the Fourier number for the time scale, t is charging time (s), a is the thermal diffusivity (m^2/s).

$$u = Pe = \frac{vH}{a}$$

Here, Pe is the Peclet number for the velocity scale.

Now, we will explain the erfc term in the equations. This term refers to a really interesting function called the error function, $\operatorname{erf}(x)$. The c at the end of ' erfc ' denotes that we should use the complementary error function, which is just $[1 - \operatorname{erf}(x)]$. It creates the typical thermocline profile. The error function looks like this:

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

We can find out the storage capacity of the thermocline as follows:

$$\int_0^Q dQ = \int \int \rho(T) c_p(T) dV dT$$

Now, we can find out the theoretical maximum storage capacity using the temperature difference (assuming temperature averaged ρ and C_p (determined at $\frac{T_h+T_c}{2}$):

$$Q_{max} = \rho c_p \frac{\pi D^2 H}{4} (T_h - T_c)$$

Assuming the tank height is five times the diameter (according to the available design data of the water thermocline storage tank from WP 3), i.e., $H = 5D$, we get:

$$Q_{max} = \rho c_p \frac{\pi H^3}{100} (T_h - T_c)$$

There is a factor called capacity ratio. It is defined by [5]:

$$\sigma = \frac{Q_{stored}}{Q_{max}}$$

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We can assume the value of the capacity ratio $\sigma = 0.5$, which is a reasonable assumption. However, we will keep sigma as it is now, and previous equation can be rewritten as:

$$\frac{Q_{stored}}{\sigma} = \rho c_p \frac{\pi H^3}{100} (T_h - T_c)$$

Solving for H , we get:

$$H = 3.1692 \sqrt[3]{\frac{Q_{stored}}{\sigma \rho C_p (T_h - T_c)}}$$

We can find the diameter of the water thermocline module as follows:

$$D = \frac{H}{5}$$

The cross-sectional area of the WT module would be:

$$A = \frac{\pi D^2}{4}$$

Similarly, the volume of the water thermocline module:

$$V = \frac{\pi D^2 H}{4}$$

The total mass of the water inside of the water thermocline would be:

$$M_{water} = \rho V$$

Given the flow rate, m_f , The convection velocity is found as below:

$$v = \frac{m_f}{A}$$

Now, the Peclet number (Pe) can also be found easily, considering thermal diffusivity (a) is determined at average temperature:

$$u = Pe = \frac{vH}{a}$$

The dimensionless charging time is defined as:

$$u\tau = Pe Fo$$

When $Pe Fo = 1$, it means the WT module is fully charged [without any threshold (explained in the following section)]. Similarly, a value of $Pe Fo \rightarrow 0$ ($Pe Fo \neq 0$) means the WT module is fully discharged (or the initial cold water condition). Let's see how a thermocline profile for a fully charged condition ($Pe Fo = 1$) looks like:

Graph of the thermocline profile at 100% charging time with $Q = 0.7t/h$.

Charging/Discharging time:

We can define two cut-off temperatures for charging and discharging as, so the thermocline is not lost within the tank. We can simply implement this as a threshold in the dimensionless charging time. We'll use a 10% threshold so the maximum and minimum values can be as follows:

$$PeFo_{max} = 0.9; \quad \text{charging ends}$$

$$PeFo_{min} = 0.1; \quad \text{discharging ends}$$

Now, the time required for charging or discharging, $t_{charge/discharge}$, in hours, can be found from the water flowrate, m_f , and the water mass, M , as shown below:

$$t_{charge/discharge} = t = \frac{0.9 M}{3600 m_f}$$

So, the number of charging and discharging cycles within a day, N_c , would be:

$$N_c = \frac{24}{2 t}$$

The charging/discharging cycle through a whole day would look like below (considering a continuous charging/discharging cycle):

$$t_{day} = t_{charge, 1st \ cycle} + t_{discharge, 1st \ cycle} + t_{charge, 2nd \ cycle} + t_{discharge, 2nd \ cycle} + \dots$$

If we are given a charging start time, $t_{charge, start}$, then we can figure out the condition of the WT module (charging or discharging thermocline profile) at any given time throughout the day:

$$t_{charge, 1st \ cycle \ time \ range} = t_{charge, start} \quad \text{to} \quad t_{charge, start} + 1 \cdot t$$

Similarly,

$$t_{discharge, 1st \ cycle \ time \ range} = t_{charge, start} + 1 \cdot t \quad \text{to} \quad t_{charge, start} + 2 \cdot t$$

Ultimately, a general form of these equations would be:

$$t_{charge, n^{th} \ cycle \ time \ range} = t_{charge, start} + (2n - 2) \cdot t \quad \text{to} \quad t_{charge, start} + (2n - 1) \cdot t$$

$$t_{discharge, n^{th} \ cycle \ time \ range} = t_{charge, start} + (2n - 1) \cdot t \quad \text{to} \quad t_{charge, start} + (2n) \cdot t$$

3.3 Efficiency Enhancement Solutions

The Efficiency Enhancement Solutions encompass innovative approaches to improve overall system performance. This section will delve into the models for the Scaling Reduction System and Adiabatic Cooling System. These solutions aim to enhance efficiency and mitigate operational challenges, providing valuable insights for optimised energy management.

3.3.1 Scaling Reduction System

The Scaling Reduction System comprises three key components: the Scaling Heat Exchanger, Scaling Reactor, and Retention Tank. Each component effectively mitigates scaling issues and maintains optimal system performance. The algorithm considers all these components, along with the silica scaling rate.

Algorithm or model description:

Rate Calculation (k):

A mathematical function describing the rate of aqueous silica polymerisation at ~25-80°C, pH ~3-10, and ionic strength $I < 0.2$ molal (according to deliverable D4.1),

$$\frac{dm_{SiO_2(aq)}}{dt} = -k(m_{SiO_2(aq)} - m_{SiO_2(aq),eq})^4 \quad \dots \dots \dots \quad (9)$$

And,

$$k = A e^{\left(\frac{-E_a}{RT}\right)} \times a_{H_4SiO_4(aq)}^3 \times a_{H^+}^{-0.75}$$

Where k is the rate constant, $m_{SiO_2(aq)}$ and $m_{SiO_2(aq),eq}$ are aqueous monomeric silica in solution and AM silica equilibrium concentration, A is the pre-exponential factor of $(3.95 \pm 1.16) \times 10^6$, E_a is the activation energy with the value of 13.9 ± 9.8 kJ, T and R are temperature (in K) and the gas constant (J/mol-K), and $a_{H_4SiO_4(aq)}$ and a_{H^+} are the activities of aqueous $H_4SiO_4(aq)$ and H^+ species. The term a_{H^+} can be found by using this equation,

$$a_{H^+} = 10^{-pH}$$

The activity of $H_4SiO_4(aq)$ is,

$$a_{H_4SiO_4(aq)} = \frac{m_{H_4SiO_4(aq)} = \text{initial concn. of } SiO_2}{\left(\frac{1}{\gamma_{H_4SiO_4}} + \frac{K_1}{a_{H^+} \times \gamma_{H_3SiO_4}}\right)}$$

Here,

$$m_{SiO_2(aq)} = \text{Silica concentration in Geofluid (in } \frac{mol}{kg} \text{)}$$

$$m_{SiO_2(aq)} \left(\text{in } \frac{mol}{kg}\right) = \frac{m_{SiO_2(aq)} \text{ (in ppm)} \times 0.001}{60.08}$$

When $m_{SiO_2(aq)}$ (in ppm) is available.

$$\log K_1 = a + bT + \frac{c}{T} + \frac{d}{T^2} + eT^2 + f \log T$$

The values of the constants can be gathered from Equation 1 of Table 3 from the deliverable 4.1. And lastly,

$$\gamma = 10^{-0.5z^2 \left(\frac{\sqrt{I}}{1+\sqrt{I}} - 0.3I\right)}$$

Here, $z = 1$ (H_4SiO_4), $z = 2$ (H_3SiO_4), $z = 3$ (H_2SiO_4), $I = 0.01$ (assumed)

Now, to calculate $m_{SiO_2(aq)}$ in reaction for equation (4),

$$AM \text{ Silica Solubility (in } \frac{mol}{kg} \text{)} = K = \text{antilog} \left(a + bT + \frac{c}{T} + \frac{d}{T^2} + eT^2 + f \log T \right)$$

Amount of scaling calculation:

The equation to get the amount of scaling, we will find out the SiO₂ concentration in the fluid,

$$m_{SiO_2(aq)} = \frac{1}{\sqrt[3]{3k\Delta t + \frac{1}{(m_{SiO_2(aq)}^0 - m_{SiO_2(aq),eq})^3}}} + m_{SiO_2(aq),eq}$$

We can calculate the scaling rate, k , using the previous equations. Now, we need the equilibrium concentration of SiO₂, $m_{SiO_2(aq),eq}$.

$$m_{SiO_2(aq),eq} = m_{H_4SiO_4} + m_{H_3SiO_4} + m_{H_2SiO_4}$$

Now,

$$m_{H_4SiO_4} = K$$
$$m_{H_3SiO_4} = \frac{K_1 \times m_{H_4SiO_4} \times \gamma_{H_4SiO_4}}{a_{H^+} \times \gamma_{H_3SiO_4}}$$
$$m_{H_2SiO_4} = \frac{K_2 \times m_{H_4SiO_4} \times \gamma_{H_4SiO_4}}{a_{H^+} \times \gamma_{H_2SiO_4}}$$

K_1 and K_2 can be calculated from using same logarithmic equation and taking the constant values from table 3 of deliverable D4.1.

After finding out $m_{SiO_2(aq)}$ from equation (9), we get the silica scaling factor, SF –

$$SS = m_{SiO_2(aq)}^0 - m_{SiO_2(aq)}$$

$$\text{Silica Scaling Factor} = SF = SS \times \frac{60.08}{1000}$$

Scaling Heat Exchanger (SHX):

We can get the Log Mean Temperature Difference (LMTD) using the following formula

$$T_{LMTD} = \frac{(T_{hi} - T_{co}) - (T_{ho} - T_{ci})}{\ln\left(\frac{T_{hi} - T_{co}}{T_{ho} - T_{ci}}\right)}$$

Here,

The inlet temperature of the geofluid = T_{hi}

Outlet temperature of the geofluid = $T_{ho} = T_{shx, out}$

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The inlet temperature of the water = T_{ci}

Outlet temperature of the water = T_{co}

The initial concentration of silica in geofluid = $m_{SiO_2(aq)}^0$

The equation for Capacity/Thermal Power/Heat Load is as follows:

$$C_{shx} = \dot{m}_{shx, hot_{in}} \left(in \frac{kg}{s} \right) \times C_{ph} \times (T_{hi} - T_{ho})$$

Here,

Flowrate of the geofluid = $\dot{m}_{shx, hot_{in}}$

Geofluid specific heat capacity = $C_{ph} = 3000$

Water specific heat capacity = $C_{pw} = 4200$

Finally, the Heat Transfer Area would be:

$$A_{shx} = \frac{C_{shx}}{U \times T_{LMTD}}$$

Where,

Overall Heat Transfer Co-efficient = $U = 5000$ (design value)

Scaling Reactor (SR):

Here, some inputs will be taken from the user, such as the temperature of the geofluid at the inlet of the Scaling Reactor, $T_{sr, in}$ is,

$$T_{sr, in} = T_{shx, out}$$

And, pH of the geofluid at the inlet of Scaling Reactor = $pH_{sr, in}$ (**from input**)

Now, Flowrate of the geofluid at the inlet of Scaling Reactor is $\dot{m}_{sr, in}$ generally given in ton/h unit. We must convert it in m^3/s –

$$\dot{m}_{sr, in} \left(in \frac{m^3}{s} unit \right) = \frac{\dot{m}_{sr, in} \left(in \frac{ton}{h} unit \right) \times \frac{1}{3.6}}{\rho_{geofluid}}$$

Here, $\rho_{geofluid}$ = Density of the geofluid in $kg/m^3 = 1000$ (assumed)

The time that geofluid stays within the scaling reactor, t_{sr} is,

$$t_{sr} = \frac{V_{sr}}{\dot{m}_{sr, in}}$$

Here, V_{sr} = Volume of the scaling reactor (**from input**) = $10 m^3$ (default)

To determine the amount of scaling within the Scaling Reactor, we will use the Scaling Factor SF in the first section. To find out the SF, we will need the following inputs –

Temperature, pH, Initial concentration of SiO₂ and time –

$$Temperature = T_{sr, in}$$

$$pH = pH_{sr, in}$$

$$Initial\ concentration\ of\ SiO_2 = m_{SiO_2(aq)}^0 \text{ (from SHX inputs)}$$

$$time = t_{sr}$$

We will calculate and show the output **Amount of Silica Scaling –**

$$Amount\ of\ Silica\ Scaling\ (in\ kg/h) = \frac{SF \times V_{sr} \times \rho_{geofluid}}{t_{sr}} \dots \dots (10)$$

And keep the value of the output $m_{SiO_2(aq), sr}$ from eq (9) stored in a variable –

$$m_{SiO_2(aq), sr} = m_{SiO_2(aq)}$$

Retention Tank (RT):

Similar to the Scaling Reactor (SR), we will take some inputs from the user here, such as: Temperature of the geofluid at the inlet of the Retention Tank, $T_{rt, in}$ will be taken from user,

$$T_{rt, in} = input; (default\ value = T_{sr, in})$$

Also, the pH of the geofluid in Retention tank, $pH_{rt, in}$ will be taken from user,

$$pH_{rt, in} = input; (default\ value = pH_{sr, in})$$

The flowrate of the geofluid at the inlet of Retention Tank in m³/s unit, $\dot{m}_{rt, in}$ (in $\frac{m^3}{s}$ unit) is,

$$\dot{m}_{rt, in} \left(in\ \frac{m^3}{s}\ unit \right) = \dot{m}_{sr, in} \left(in\ \frac{m^3}{s}\ unit \right)$$

The time that geofluid stays within the retention tank t_{rt} is,

$$t_{rt} = \frac{V_{rt}}{\dot{m}_{rt, in}}$$

Here, V_{rt} = Volume of the retention tank (**from input**) = 10 m³ (default)

Just as the Scaling Reactor (SR), the SF will be calculated here using the following inputs –

Temperature, pH, Initial concentration of SiO₂ and time –

$$Temperature = T_{sr, in}$$

$$pH = pH_{sr, in}$$

Initial concentration of $SiO_2 = m_{SiO_2(aq), sr}$ (from SR outputs)

$$time = t_{rt}$$

We will calculate and show the outputs **Amount of Silica Scaling** and $m_{SiO_2(aq)}$ using the above inputs.

$$\mathbf{Amount\ of\ Silica\ Scaling\ (in\ kg)} = SF \times V_{rt} \times \rho_{geofluid}$$

$m_{SiO_2(aq)} = m_{SiO_2(aq)_{final}}$ = Silica Concentration within the geofluid before reinjecting to the wells. (output) (It will be in mol/kg and should be converted to ppm).

We will find the efficiency of the Retention system η_{RS} , by using the following formula –

$$\eta_{RS} = \frac{SiO_{2in} - SiO_{2out}}{SiO_{2in} - SiO_{2eq}(50^\circ C)}$$

For the retention tank,

Where SiO_{2in} is the silica concentration of the mass flow in input and $SiO_{2eq}(50^\circ C)$ is the solubility at equilibrium of AM silica at $50^\circ C$.

$$SiO_{2in} = m_{SiO_2(aq), sr} \text{ (from SR outputs)}$$

$$SiO_{2out} = m_{SiO_2(aq)_{final}}$$

$$SiO_{2eq}(50^\circ C) = m_{SiO_2(aq),eq} \text{ (in SR function, use appropriate temp. instead of } 50^\circ C)$$

3.3.2 Adiabatic Cooling System

Adiabatic cooling involves using a fogging system that produces tiny water droplets near the condenser fans. These droplets evaporate and lower the temperature of the air passing through the condenser. Reducing the air temperature enhances cooling effectiveness and improves overall efficiency.

Algorithm or Model Description:

The model is based on the following assumptions:

- Overall effectiveness, ϵ of the fogging system is estimated.
- The cooling process is adiabatic, and water droplets evaporate entirely.
- There is negligible pressure drop across the system.

The dry bulb temperature, T_{in} and relative humidity are the primary inputs of the system. Real-time weather data can provide these values.

From the psychrometric chart, the wet bulb temperature, T_{WBT} and ambient air-specific humidity, ω_{in} , can be determined.

Now, the cooled air temperature, T_{out} can be determined by the following equation:

$$T_{out} = T_{in} - (T_{in} - T_{WBT})\epsilon$$

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The specific humidity of cooled air, ω_{out} can be found from the heat interaction between the ambient air and saturated air and presented as:

$$c_{p,air}(T_{in}-T_{out}) = (\omega_{out} - \omega_{in})h_{fg}$$

Where $c_{p,air}$ is the specific heat of air and h_{fg} is the enthalpy of water vaporisation.

The mass of air flowing through the adiabatic cooling system depends on the number of fans under which the fogging system is installed. Total air flowing through the cooling system

m_{air} = air flow rate of single fan × Number of fans active over the fogging system.

Then, the water consumption in the adiabatic cooling system can be determined using the following equation:

$$m_w = m_{air}(\omega_{out} - \omega_{in})$$

Finally, the model can also provide cooled air temperature in case of water shortage.

During water shortage, cooled air-specific humidity will be lower and can be determined using:

$$\omega_{out, new} = (m_w / m_{air}) + \omega_{in}$$

Now, the cooled air temperature will be higher and can be updated by:

$$T_{out, new} = T_{in} - ((\omega_{out} - \omega_{in}) h_{fg} / c_{p,air})$$

4. CONCLUSIONS

This deliverable establishes the foundation for the Decision Support System by presenting a comprehensive set of knowledge-based decision rules for the GeoSmart innovations: the PCM module, the Steam Accumulation (abandoned later), the Water Thermocline, the Scaling reduction system, and the adiabatic cooling system. The relational rule-based algorithm was developed based on theoretical insights and findings from previous deliverables and existing relevant literature, ensuring its practicality and relevance to the GeoSmart project.

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