Recently we have determined that the exiting definitions for theoretical models, data definitions, general definitions and instance models are not entirely consistent. Moreover, the terminology, especially the terminology that combines “theory” and “model” is confusing.

Our new terminology will be based on the concept of different “levels” of theories. We currently have what we are calling context theories, background theories, theories and final theories. Context theories are the starting point for a given scientific model. These theories are not defined, but their implicit presence is necessary for completeness. Typical examples include theories for arithmetic operations, differentiation, integration, vector calculus, etc. Following the context theories we have background theories. Background theories are defined, but not derived. Typically they will be the general forms of the conservation equations, like conservation of thermal energy or momentum, and constitutive equations. Assumptions are often invoked by The level of detail used to define background theories can vary, since we do not always need the full theory; we sometimes just need to know that the theory exists. The background theories are refined into other theories by making assumptions, like plane stress, or linear elasticity, or isothermal material properties, or laminar flow, etc. These theories are combined and refined until the point where we have final theories. All theories are part of the documentation, but the final theories are the ones that will be transformed into code.

We also have data definitions. A data definition is a label for part of a theory. Assumptions will be maintained from the previous terminology.

Below is an attempt to clarify the new concept of different levels of theories by re-writing the relevant parts of the NoPCM model using the new conceptual model of theories.

1 Assumptions

rmal-Energy-Only: The only form of energy that is relevant for this problem is thermal energy. All other forms of energy, such as mechanical energy, are assumed to be negligible. (RefBy: BT:consThermE.)

er-Coeffs-Constant: All heat transfer coefficients are constant over time. (RefBy: BT:nwtnCooling.)

Temp-Across-Tank: The water in the tank is fully mixed, so the temperature of the water is the same throughout the entire tank. (RefBy: RT:rocTempSimp.)

stant-over-Volume: The density of water has no spatial variation; that is, it is constant over their entire volume. (RefBy: RT:rocTempSimp.)

stant-over-Volume: The specific heat capacity of water has no spatial variation; that is, it is constant over its entire volume. (RefBy: RT:rocTempSimp.)

Cooling-Coil-Water: Newton’s law of convective cooling applies between the heating coil and the water. (RefBy: RT:htFluxWaterFromCoil.)

onstant-over-Time: The temperature of the heating coil is constant over time. (RefBy: LC:Temperature-Coil-Variable-Over-Day and RT:htFluxWaterFromCoil.)

nstant-over-Length: The temperature of the heating coil does not vary along its length. (RefBy: LC:Temperature-Coil-Variable-Over-Length.)

o-Temp-Discharge: The model only accounts for charging the tank, not discharging. The temperature of the water can only increase, or remain constant; it cannot decrease. This implies that the initial temperature is less than (or equal to) the temperature of the heating coil. (RefBy: LC:Discharging-Tank.)

ter-Always-Liquid: The operating temperature range of the system is such that the material (water in this case) is always in liquid state. That is, the temperature will not drop below the melting point temperature of water, or rise above its boiling point temperature. (RefBy: UC:Water-Fixed-States, BT:sensHtE, FT:heatEInWtr, and FT:eBalanceOnWtr.)

ct-Insulation-Tank: The tank is perfectly insulated so that there is no heat loss from the tank. (RefBy: LC:Tank-Lose-Heat and FT:eBalanceOnWtr.)

neration-By-Water: No internal heat is generated by the water; therefore, the volumetric heat generation per unit volume is zero. (RefBy: UC:No-Internal-Heat-Generation and FT:eBalanceOnWtr.)

eric-Pressure-Tank: The pressure in the tank is atmospheric, so the melting point temperature and boiling point temperature of water are 0°C and 100°C, respectively. (RefBy: FT:heatEInWtr.)

me-Coil-Negligible: When considering the volume of water in the tank, the volume of the heating coil is assumed to be negligible. (RefBy: DD:waterVolume_nopcm.)

2 Context Theories

Some theories do not have to be explicitly invoked. They are part of the context for the other theories, without having to be explicitly stated or defined. The context theories for this problem are as follows:

- arithmetic
- operations
- differentiation
- partial differentiation
- integration
- vector calculus (gradient operator, dot product)
- Gauss's divergence theorem [Should this be a separate theory? Possibly a theory that is in the background, but not actually printed in the SRS document? —SS]

3 Background Theories (BT)

Refname	**BT:consThermE**
Label	Conservation of thermal energy
Equation	$$-\nabla \cdot \mathbf{q} + g = \rho C \frac{\partial T}{\partial t}$$
Description	∇ is the gradient (Unitless) $\mathbf{q}$ is the thermal flux vector ($\frac{\mathrm{W}}{\mathrm{m}^2}$) g is the volumetric heat generation per unit volume ($\frac{\mathrm{W}}{\mathrm{m}^3}$) ρ is the density ($\frac{\mathrm{kg}}{\mathrm{m}^3}$) C is the specific heat capacity ($\frac{\mathrm{J}}{\mathrm{kg}^\circ\mathrm{C}}$) t is the time (s) T is the temperature ($^\circ$C)
Notes	The above equation gives the law of conservation of energy for transient heat transfer in a given material. For this equation to apply, other forms of energy, such as mechanical energy, are assumed to be negligible in the system (A:Thermal-Energy-Only). [Should we explicitly say that the above equation relies on vector calculus “theories”, or should we leave that implicit? —SS] Density (ρ) is defined in BT:density
Source	Fourier Law of Heat Conduction and Heat Equation
RefBy	RT:rocTempSimp

Refname	BT:sensHtE
Label	Sensible heat energy (no state change)
Equation	$$E = C^{\text{L}} m \Delta T$$
Description	E is the sensible heat (J) C^{L} is the specific heat capacity of a liquid ($\frac{\text{J}}{\text{kg}^{\circ}\text{C}}$) m is the mass (kg) ΔT is the change in temperature ($^{\circ}$C)
Notes	E occurs as long as the material does not reach a temperature where a phase change occurs, as assumed in A:Water-Always-Liquid. [This should actually be an assumption of no state change. This is a generic assumption that is necessary to use this theory. —SS]
Source	Definition of Sensible Heat
RefBy	FT:heatEInWtr

Refname	**BT:nwtnCooling**
Label	Newton's law of cooling
Equation	$$q(t) = h(T(t) - T_{\text{env}}(t))$$
Description	q is the heat flux ($\frac{\text{W}}{\text{m}^2}$) t is the time (s) h is the convective heat transfer coefficient ($\frac{\text{W}}{\text{m}^2{}^\circ\text{C}}$) T is the temperature of the body ($^\circ$C) T_{env} is the temperature of the environment surrounding the body ($^\circ$C)
Notes	Newton's law of cooling describes convective cooling from a surface. The law is stated as: the rate of heat loss from a body is proportional to the difference in temperatures between the body and its surroundings. h is assumed to be independent of T (from A:Heat-Transfer-Coeffs-Constant.
Source	[**incroperaEtAl2007**]
RefBy	RT:htFluxWaterFromCoil

Refname	BT:density
Label	Density
Equation	$$\rho = \frac{m}{V}$$
Description	ρ is the density of a material ($\frac{\mathrm{kg}}{\mathrm{m}^3}$) m is the mass of the body (kg) V is the volume of the body (m^3)
Notes	Density is the mass per unit volume.
Source	–
RefBy	BT:consThermE, RT:rocTempSimp, DD:waterMass

4 Refined Theories

This section collects the laws and equations that will be used to build the instance models.

Refname	**RT:rocTempSimp**
Label	Simplified rate of change of temperature
Equation	$$mC\frac{dT}{dt} = q_{\text{in}}A_{\text{in}} - q_{\text{out}}A_{\text{out}} + gV$$
Description	m is the mass (kg) C is the specific heat capacity ($\frac{\text{J}}{\text{kg}^{\circ}\text{C}}$) t is the time (s) T is the temperature ($^{\circ}$C) q_{in} is the heat flux input ($\frac{\text{W}}{\text{m}^2}$) A_{in} is the surface area over which heat is transferred in (m^2) q_{out} is the heat flux output ($\frac{\text{W}}{\text{m}^2}$) A_{out} is the surface area over which heat is transferred out (m^2) g is the volumetric heat generation per unit volume ($\frac{\text{W}}{\text{m}^3}$) V is the volume (m^3)
Source	–
RefBy	RT:rocTempSimp and FT:eBalanceOnWtr

Detailed derivation of simplified rate of change of temperature: Integrating BT:consThermE over a volume (V), we have:

$$-\int_{V} \nabla \cdot \mathbf{q}\, dV + \int_{V} g\, dV = \int_{V} \rho C \frac{\partial T}{\partial t}\, dV$$

Applying Gauss's Divergence Theorem to the first term over the surface S of the volume, with $\mathbf{q}$ as the thermal flux vector for the surface and $\hat{\mathbf{n}}$ as a unit outward normal vector for a surface:

$$-\int_{S} \mathbf{q} \cdot \hat{\mathbf{n}}\, dS + \int_{V} g\, dV = \int_{V} \rho C \frac{\partial T}{\partial t}\, dV$$

We consider an arbitrary volume. The volumetric heat generation per unit volume is assumed constant. Then Equation (1) can be written as:

$$q_{\text{in}}A_{\text{in}} - q_{\text{out}}A_{\text{out}} + gV = \int_V \rho C \frac{\partial T}{\partial t}\, dV$$

Where q_{in}, q_{out}, A_{in}, and A_{out} are explained in RT:rocTempSimp. [Why is this RT referencing itself? This seems like something that could be removed. —SS] Assuming ρ, C, and T are constant over the volume, which is true in our case by A:Constant-Water-Temp-Across-Tank, A:Density-Water-Constant-over-Volume, and A:Specific-Heat-Energy-Constant-over-Volume, we have:

$$\rho C V \frac{dT}{dt} = q_{\text{in}}A_{\text{in}} - q_{\text{out}}A_{\text{out}} + gV$$

Using the fact that $\rho{=}m/V$ (BT:density), Equation (2) can be written as:

$$mC \frac{dT}{dt} = q_{\text{in}}A_{\text{in}} - q_{\text{out}}A_{\text{out}} + gV$$

Refname	RT:htFluxWaterFromCoil
Label	Heat flux into the water from the coil
Units	$\frac{\text{W}}{\text{m}^2}$
Equation	$$q_{\text{C}} = h_{\text{C}} \left(T_{\text{C}} - T_{\text{W}} \left(t\right)\right)$$
Description	q_{C} is the heat flux into the water from the coil ($\frac{\text{W}}{\text{m}^2}$) h_{C} is the convective heat transfer coefficient between coil and water ($\frac{\text{W}}{\text{m}^2{}^{\circ}\text{C}}$) T_{C} is the temperature of the heating coil (${}^{\circ}$C) T_{W} is the temperature of the water (${}^{\circ}$C) t is the time (s)
Notes	q_{C} is found by assuming that Newton's law of cooling applies (A:Newton-Law-Convective-Cooling-Coil-Water). This law (defined in BT:nwtnCooling) is used on the surface of the heating coil. A:Temp-Heating-Coil-Constant-over-Time
Source	[**koothoor2013**]
RefBy	FT:eBalanceOnWtr

5 Definitions

This section collects and defines all the data needed to build the instance models.

Refname	**DD:waterMass**
Label	Mass of water
Symbol	m_{W}
Units	kg
Equation	$$m_{\text{W}} = V_{\text{W}} \rho_{\text{W}}$$
Description	m_{W} is the mass of water (kg) V_{W} is the volume of water (m^3) ρ_{W} is the density of water ($\frac{\text{kg}}{\text{m}^3}$)
Notes	Density (ρ) is defined in BT:density
Source	–
RefBy	FR:Find-Mass

Refname	DD:waterVolume.nopcm
Label	Volume of water
Symbol	V_{W}
Units	m^3
Equation	$$V_{\text{W}} = V_{\text{tank}}$$
Description	V_{W} is the volume of water (m^3) V_{tank} is the volume of the cylindrical tank (m^3)
Notes	Based on A:Volume-Coil-Negligible. V_{tank} is defined in DD:tankVolume.
Source	–
RefBy	FR:Find-Mass

Refname	**DD:tankVolume**
Label	Volume of the cylindrical tank
Symbol	V_{tank}
Units	m^3
Equation	$$V_{\text{tank}} = \pi \left(\frac{D}{2} \right)^2 L$$
Description	V_{tank} is the volume of the cylindrical tank (m^3) π is the ratio of circumference to diameter for any circle (Unitless) D is the diameter of tank (m) L is the length of tank (m)
Source	–
RefBy	DD:waterVolume_nopcm and FR:Find-Mass

Refname	DD:balanceDecayRate
Label	ODE parameter for water related to decay time
Symbol	τ_{W}
Units	s
Equation	$$\tau_{\text{W}} = \frac{m_{\text{W}} C_{\text{W}}}{h_{\text{C}} A_{\text{C}}}$$
Description	τ_{W} is the ODE parameter for water related to decay time (s) m_{W} is the mass of water (kg) C_{W} is the specific heat capacity of water ($\frac{\text{J}}{\text{kg}^{\circ}\text{C}}$) h_{C} is the convective heat transfer coefficient between coil and water ($\frac{\text{W}}{\text{m}^{2}{}^{\circ}\text{C}}$) A_{C} is the heating coil surface area (m^2)
Source	[**koothoor2013**]
RefBy	FR:Output-Input-Derived-Values and FT:eBalanceOnWtr

6 Final Theories

This section transforms the problem defined in the problem description into one which is expressed in mathematical terms. It uses concrete symbols defined in the data definitions to replace the abstract symbols in the models identified in theoretical models and general definitions.

The goal GS:Predict-Water-Temperature is met by FT:eBalanceOnWtr and the goal GS:Predict-Water-Energy is met by FT:heatEInWtr.

Refname	**FT:eBalanceOnWtr**
Label	Energy balance on water to find the temperature of the water
Input	T_{C}, T_{init}, t_{final}, A_{C}, h_{C}, C_{W}, m_{W}
Output	T_{W}
Input Constraints	$$T_{\text{C}} \geq T_{\text{init}}$$
Output Constraints	
Equation	$$\frac{dT_{\text{W}}}{dt} = \frac{1}{\tau_{\text{W}}} \left(T_{\text{C}} - T_{\text{W}}\left(t\right)\right)$$
Description	t is the time (s) T_{W} is the temperature of the water (°C) τ_{W} is the ODE parameter for water related to decay time (s) T_{C} is the temperature of the heating coil (°C)
Notes	τ_{W} is calculated from DD:balanceDecayRate. The above equation applies as long as the water is in liquid form, $0 < T_{\text{W}} < 100$ (°C) where 0 (°C) and 100 (°C) are the melting and boiling point temperatures of water, respectively (A:Water-Always-Liquid).
Source	[**koothoor2013**]
RefBy	UC:No-Internal-Heat-Generation, FR:Find-Mass, and FR:Calculate-Temperature-Water-Over-Time

Detailed derivation of the energy balance on water: To find the rate of change of T_{W}, we look at the energy balance on water. The volume being considered is the volume of water in the tank V_{W}, which has mass m_{W} and specific heat capacity, C_{W}. Heat transfer occurs in the water from the heating coil as q_{C} (RT:htFluxWaterFromCoil), over area A_{C}. No heat transfer occurs to the outside of the tank, since it has been assumed to be perfectly insulated (A:Perfect-Insulation-Tank). Since the assumption is made that no internal heat is generated (A:No-Internal-Heat-Generation-By-Water), $g = 0$. Therefore, the equation for RT:rocTempSimp can be written as:

$$m_{\text{W}} C_{\text{W}} \frac{dT_{\text{W}}}{dt} = q_{\text{C}} A_{\text{C}}$$

Using RT:htFluxWaterFromCoil for q_{C}, this can be written as:

$$m_{\text{W}} C_{\text{W}} \frac{dT_{\text{W}}}{dt} = h_{\text{C}} A_{\text{C}} \left(T_{\text{C}} - T_{\text{W}}\right)$$

Dividing Equation (2) by $m_{\text{W}} C_{\text{W}}$, we obtain:

$$\frac{dT_{\text{W}}}{dt} = \frac{h_{\text{C}} A_{\text{C}}}{m_{\text{W}} C_{\text{W}}} \left(T_{\text{C}} - T_{\text{W}}\right)$$

By substituting τ_{W} (from DD:balanceDecayRate), this can be written as:

$$\frac{dT_{\text{W}}}{dt} = \frac{1}{\tau_{\text{W}}} \left(T_{\text{C}} - T_{\text{W}}\right)$$

Refname	**FT:heatEInWtr**
Label	Heat energy in the water
Input	T_{init}, m_{W}, C_{W}, m_{W}
Output	E_{W}
Input Constraints	
Output Constraints	
Equation	$$E_{\text{W}}\left(t\right)=C_{\text{W}}m_{\text{W}}\left(T_{\text{W}}\left(t\right)-T_{\text{init}}\right)$$
Description	E_{W} is the change in heat energy in the water (J) t is the time (s) C_{W} is the specific heat capacity of water ($\frac{\text{J}}{\text{kg}^{\circ}\text{C}}$) m_{W} is the mass of water (kg) T_{W} is the temperature of the water (°C) T_{init} is the initial temperature (°C)
Notes	The above equation is derived using BT:sensHtE. The change in temperature is the difference between the temperature at time t (s), T_{W} and the initial temperature, T_{init} (°C). This equation applies as long as $0<T_{\text{W}}<100^{\circ}\text{C}$ (A:Water-Always-Liquid, A:Atmospheric-Pressure-Tank).
Source	[**koothoor2013**]
RefBy	FR:Calculate-Change-Heat_Energy-Water-Over-Time

6.0.1 Data Constraints

The Data Constraints Table shows the data constraints on the input variables. The column for physical constraints gives the physical limitations on the range of values that can be taken by the variable. The uncertainty column provides an estimate of the confidence with which the physical quantities can be measured. This information would be part of the input if one were performing an uncertainty quantification exercise. The constraints are conservative, to give the user of the model the flexibility to experiment with unusual situations. The column of typical values is intended to provide a feel for a common scenario. The column for software constraints restricts the range of inputs to reasonable values.

Var	Physical Constraints	Software Constraints	Typical Value	Uncert.
A_{C}	$A_{\text{C}} > 0$	$A_{\text{C}} \leq {A_{\text{C}}}^{\text{max}}$	0.12 m^2	10%
C_{W}	$C_{\text{W}} > 0$	${C_{\text{W}}}^{\text{min}} < C_{\text{W}} < {C_{\text{W}}}^{\text{max}}$	4186 $\frac{\text{J}}{\text{kg}^\circ\text{C}}$	10%
D	$D > 0$	$AR_{\text{min}} \leq D \leq AR_{\text{max}}$	0.412 m	10%
h_{C}	$h_{\text{C}} > 0$	${h_{\text{C}}}^{\text{min}} \leq h_{\text{C}} \leq {h_{\text{C}}}^{\text{max}}$	1000 $\frac{\text{W}}{\text{m}^2{}^\circ\text{C}}$	10%
L	$L > 0$	$L_{\text{min}} \leq L \leq L_{\text{max}}$	1.5 m	10%
T_{C}	$0 < T_{\text{C}} < 100$	–	50 °C	10%
T_{init}	$0 < T_{\text{init}} < 100$	–	40 °C	10%
t_{final}	$t_{\text{final}} > 0$	$t_{\text{final}} < {t_{\text{final}}}^{\text{max}}$	50000 s	10%
t_{step}	$0 < t_{\text{step}} < t_{\text{final}}$	–	0.01 s	10%
ρ_{W}	$\rho_{\text{W}} > 0$	${\rho_{\text{W}}}^{\text{min}} < \rho_{\text{W}} \leq {\rho_{\text{W}}}^{\text{max}}$	1000 $\frac{\text{kg}}{\text{m}^3}$	10%

Table 1: Input Data Constraints

6.0.2 Properties of a Correct Solution

The Data Constraints Table shows the data constraints on the output variables. The column for physical constraints gives the physical limitations on the range of values that can be taken by the variable.

Var	Physical Constraints
T_{W}	$T_{\text{init}} \leq T_{\text{W}} \leq T_{\text{C}}$
E_{W}	$E_{\text{W}} \geq 0$

Table 2: Output Data Constraints

7 Requirements

This section provides the functional requirements, the tasks and behaviours that the software is expected to complete, and the non-functional requirements, the qualities that the software is expected to exhibit.

7.1 Functional Requirements

This section provides the functional requirements, the tasks and behaviours that the software is expected to complete.

nput-Initial-Values: Input the following values described in the table for Required Inputs, which define the tank parameters, material properties, and initial conditions.

Find-Mass: Use the inputs in FR:Input-Initial-Values to find the mass needed for IM:eBalanceOnWtr, using DD:waterMass, DD:waterVolume_nopcm, and DD:tankVolume.

ysical_Constraints: Verify that the inputs satisfy the required physical constraints.

ut-Derived-Values: Output the input values and derived values in the following list: the values (from FR:Input-Initial-Values), the mass (from FR:Find-Mass), and τ_{W} (from DD:balanceDecayRate).

-Water-Over-Time: Calculate and output the temperature of the water ($T_{\mathrm{W}}(t)$) over the simulation time (from IM:eBalanceOnWtr).

-Water-Over-Time: Calculate and output the change in heat energy in the water ($E_{\mathrm{W}}(t)$) over the simulation time (from IM:heatEInWtr).

Symbol	**Description**	**Units**
A_{C}	Heating coil surface area	m^2
A_{tol}	Absolute tolerance	–
C_{W}	Specific heat capacity of water	$\frac{\mathrm{J}}{\mathrm{kg}^{\circ}\mathrm{C}}$
D	Diameter of tank	m
h_{C}	Convective heat transfer coefficient between coil and water	$\frac{\mathrm{W}}{\mathrm{m}^2{}^{\circ}\mathrm{C}}$
L	Length of tank	m
R_{tol}	Relative tolerance	–
T_{C}	Temperature of the heating coil	$^{\circ}\mathrm{C}$
T_{init}	Initial temperature	$^{\circ}\mathrm{C}$
t_{final}	Final time	s
t_{step}	Time step for simulation	s
ρ_{W}	Density of water	$\frac{\mathrm{kg}}{\mathrm{m}^3}$

Table 3: Required Inputs following FR:Input-Initial-Values

8 Likely Changes

This section lists the likely changes to be made to the software.

Variable-Over-Day: A:Temp-Heating-Coil-Constant-over-Time - The temperature of the heating coil will change over the course of the day, depending on the energy received from the sun.

iable-Over-Length: A:Temp-Heating-Coil-Constant-over-Length - The temperature of the heating coil will actually change along its length as the water within it cools.

Discharging-Tank: A:Charging-Tank-No-Temp-Discharge - The model currently only accounts for charging of the tank. That is, increasing the temperature of the water to match the temperature of the coil. A more complete model would also account for discharging of the tank.

Tank-Lose-Heat: A:Perfect-Insulation-Tank - Any real tank cannot be perfectly insulated and will lose heat.

9 Unlikely Changes

This section lists the unlikely changes to be made to the software.

Water-Fixed-States: A:Water-Always-Liquid - It is unlikely for the change of water from liquid to a solid, or from liquid to gas to be considered.

l-Heat-Generation: A:No-Internal-Heat-Generation-By-Water - Is used for the derivations of IM:eBalanceOnWtr.