Software Requirements Specification for Solar Water Heating Systems Incorporating Phase Change Material

Thulasi Jegatheesan, Brooks MacLachlan, and Spencer Smith

April 20, 2018

Contents

1 Reference Material

This section records information for easy reference.

1.1 Table of Units

Throughout this document SI (Système International d'Unités) is employed as the unit system. In addition to the basic units, several derived units are used as described below. For each unit, the symbol is given followed by a description of the unit and the SI name.

symbol	unit	SI
m	length	metre
kg	mass	kilogram
s	time	second
°C	temperature	centigrade
J	energy	Joule
W	power	Watt ($\mathrm{W} = \mathrm{J\,s^{-1}}$)

1.2 Table of Symbols

The table that follows summarizes the symbols used in this document along with their units. The choice of symbols was made to be consistent with the heat transfer literature and with existing documentation for solar water heating systems. The symbols are listed in alphabetical order.

symbol	unit	description
A_C	$\mathrm{m^2}$	coil surface area
A_{in}	$\mathrm{m^2}$	surface area over which heat is transferred in
A_{out}	$\mathrm{m^2}$	surface area over which heat is transferred out
A_P	$\mathrm{m^2}$	phase change material surface area
C	$\mathrm{J/(kg\,°C)}$	specific heat capacity

C^L	J/(kg °C)	specific heat capacity of a liquid
C_P^L	J/(kg °C)	specific heat capacity of PCM as a liquid
C^S	J/(kg °C)	specific heat capacity of a solid
C_P^S	J/(kg °C)	specific heat capacity of PCM as a solid
C^V	J/(kg °C)	specific heat capacity of a vapour
C_W	J/(kg °C)	specific heat capacity of water
D	m	diameter of tank
E	J	sensible heat energy
$E_{P\text{melt}}^{\text{init}}$	J	heat energy in the PCM at the instant when melting begins
E_P	J	heat energy in the PCM
E_W	J	heat energy in the water
g	W/m^3	volumetric heat generation per unit volume
h	W/(m^2 °C)	convective heat transfer coefficient
h_C	W/(m^2 °C)	convective heat transfer coefficient between coil and water
H_f	J/kg	specific latent heat of fusion
h_P	W/(m^2 °C)	convective heat transfer coefficient between water and PCM
L	m	length of tank
m	kg	mass
m_P	kg	mass of phase change material
m_W	kg	mass of water
$\mathbf{\hat{n}}$	unitless	unit outward normal vector for a surface
q	W/m^2	heat flux
Q	J	latent heat energy
$\mathbf{q}$	W/m^2	thermal flux vector
q_C	W/m^2	heat flux from coil
q_{in}	W/m^2	heat flux in
q_{out}	W/m^2	heat flux out
q_P	W/m^2	heat flux into phase change material
Q_P	J	latent heat energy added to PCM
R	unitless	Aspect ratio (ratio of tank diameter (D) to tank length (L))
S	unitless	surface
t	s	time
T	°C	temperature
T_{boil}	°C	temperature at boiling point
T_C	°C	temperature of coil

T_{env}	°C	temperature of environment
t_{final}	s	final time
T_{init}	°C	initial temperature
T_{melt}	°C	temperature at melting point
$t_{\text{melt}}^{\text{init}}$	s	time at which melting of PCM begins
$t_{\text{melt}}^{\text{final}}$	s	time at which melting of PCM ends
T_{melt}^{P}	°C	temperature at melting point for PCM
T_P	°C	temperature of phase change material
T_W	°C	temperature of water
V	m^3	volume
V_P	m^3	volume of PCM
V_{tank}	m^3	volume of the cylindrical tank
V_W	m^3	volume of water
ΔT	°C	temperature difference
η	unitless	ODE parameter
ρ	kg/m^3	density, mass per unit volume
ρ_P	kg/m^3	density of PCM
ρ_W	kg/m^3	density of water
τ	s	dummy variable for integration over time
τ_P^L	s	ODE parameter for liquid PCM
τ_P^S	s	ODE parameter for solid PCM
τ_W	s	ODE parameter for water
ϕ	unitless	melt fraction

1.3 Abbreviations and Acronyms

symbol	description
A	Assumption
DD	Data Definition
GD	General Definition
GS	Goal Statement
IM	Instance Model
LC	Likely Change
ODE	Ordinary Differential Equation
PCM	Phase Change Material
PS	Physical System Description
R	Requirement
RHS	Right Hand Side
SRS	Software Requirements Specification
SWHS	Solar Water Heating System
T	Theoretical Model

2 Introduction

Due to the increasing cost, diminishing availability, and negative environmental impact of fossil fuels, there is a higher demand for renewable energy sources and energy storage technology. Solar water heating systems incorporating Phase Change Material (PCM) use a renewable energy source and provide a novel way of storing energy. Solar water heating systems with PCM improve over the traditional solar heating systems because of their smaller size. The smaller size is possible because of the ability of PCM to store thermal energy as latent heat, which allows higher thermal energy storage capacity per unit weight.

The following section provides an overview of the Software Requirements Specification (SRS) for a solar water heating system that incorporates PCM. The developed program will be referred to as Solar Water Heating System (SWHS). This section explains the purpose of this document, the scope of the system, the characteristics of the intended readers and the organization of the document.

2.1 Purpose of Document

The main purpose of this document is to describe the modelling of solar water heating systems incorporating PCM. The goals and theoretical models used in the SWHS code are provided, with an emphasis on explicitly identifying assumptions and unambiguous definitions. This

document is intended to be used as a reference to provide ad hoc access to all information necessary to understand and verify the model. The SRS is abstract because the contents say *what* problem is being solved, but do not say *how* to solve it.

This document will be used as a starting point for subsequent development phases, including writing the design specification and the software verification and validation plan. The design document will show how the requirements are to be realized, including decisions on the numerical algorithms and programming environment. The verification and validation plan will show the steps that will be used to increase confidence in the software documentation and the implementation. Although the SRS fits in a series of documents that follow the so-called waterfall model, the actual development process is not constrained in any way. Even when the process is not waterfall, as Parnas and Clements [5] point out, the most logical way to present the documentation is still to "fake" a rational design process.

2.2 Scope of Requirements

The scope of the requirements is limited to thermal analysis of a single solar water heating tank incorporating PCM. Given the appropriate inputs, the code for SWHS is intended to predict the temperature and energy histories for the water and the PCM. This entire document is written assuming that the substances inside the heating tank are water and PCM.

2.3 Characteristics of Intended Reader

Reviewers of this documentation should have a strong knowledge in heat transfer theory. A third or fourth year Mechanical Engineering course on this topic is recommended. The reviewers should also have an understanding of differential equations, as typically covered in first and second year Calculus courses. The users of SWHS can have a lower level of expertise, as explained in Section 3.2.

2.4 Organization of Document

The organization of this document follows the template for an SRS for scientific computing software proposed by [3] and [6]. The presentation follows the standard pattern of presenting goals, theories, definitions, and assumptions. For readers that would like a more bottom up approach, they can start reading the instance models in Section 4.2.5 and trace back to find any additional information they require. The instance models provide the Ordinary Differential Equations (ODEs) and algebraic equations that model the solar water heating system with PCM. SWHS solves these ODEs.

The goal statements are refined to the theoretical models, and theoretical models to the instance models. The instance models (Section 4.2.5) to be solved are referred to as IM1 to IM4.

3 General System Description

This section identifies the interfaces between the system and its environment, describes the user characteristics and lists the system constraints.

3.1 System Context

Figure 1 shows the system context. A circle represents an external entity outside the software, the user in this case. A rectangle represents the software system itself (SWHS). Arrows are used to show the data flow between the system and its environment.
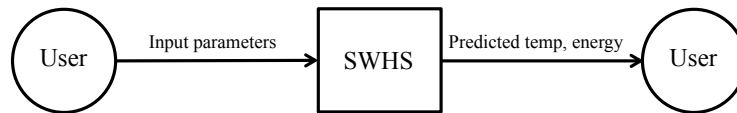

Figure 1: System Context

SWHS is mostly self-contained. The only external interaction is through the user interface. The responsibilities of the user and the system are as follows:

- User Responsibilities:

  - Provide the input data to the system, ensuring no errors in the data entry
  - Take care that consistent units are used for input variables

- SWHS Responsibilities:

  - Detect data type mismatch, such as a string of characters instead of a floating point number
  - Determine if the inputs satisfy the required physical and software constraints
  - Calculate the required outputs

3.2 User Characteristics

The end user of SWHS should have an understanding of undergraduate Level 1 Calculus and Physics.

3.3 System Constraints

There are no system constraints.

4 Specific System Description

This section first presents the problem description, which gives a high-level view of the problem to be solved. This is followed by the solution characteristics specification, which presents the assumptions, theories, definitions and finally the instance models (ODEs) that model the solar water heating tank with PCM.

4.1 Problem Description

SWHS is a computer program developed to investigate the effect of employing PCM within a solar water heating tank.

4.1.1 Terminology and Definitions

This subsection provides a list of terms that are used in the subsequent sections and their meaning, with the purpose of reducing ambiguity and making it easier to correctly understand the requirements:

- Heat Flux: The rate of heat energy transfer per unit area.

- Phase Change Material (PCM): A substance that uses phase changes (such as melting) to absorb or release large amounts of heat at a constant temperature.

- Specific Heat: heat capacity per unit mass.

- Thermal Conduction: the transfer of heat energy through a substance.

- Transient: Changing with time.

4.1.2 Physical System Description

The physical system of SWHS, as shown in Figure 2, includes the following elements:

PS1: Tank containing water.

PS2: Heating coil at bottom of tank. (q_C represents the heat flux from the coil into the water.)

PS3: PCM suspended in tank. (q_P represents the heat flux from the water into the PCM.)
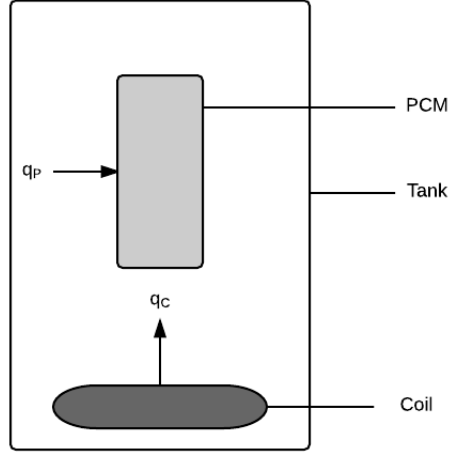
Figure 2: Solar water heating tank, with heat flux from coil and to the PCM of q_C and q_P, respectively

4.1.3 Goal Statements

Given the temperature of the coil, initial conditions for the temperature of the water and the PCM, and material properties, the goal statements are:

GS1: Predict the water temperature over time.

GS2: Predict the PCM temperature over time.

GS3: Predict the change in the energy of the water over time.

GS4: Predict the change in the energy of the PCM over time.

4.2 Solution Characteristics Specification

The instance models (ODEs) that govern SWHS are presented in Subsection 4.2.5. The information to understand the meaning of the instance models and their derivation is also presented, so that the instance models can be verified.

4.2.1 Assumptions

This section simplifies the original problem and helps in developing the theoretical model by filling in the missing information for the physical system. The numbers given in the square

9

brackets refer to the theoretical model [T], general definition [GD], data definition [DD], instance model [IM], or likely change [LC], in which the respective assumption is used.

A1: 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 [T1].

A2: All heat transfer coefficients are constant over time [GD1].

A3: The water in the tank is fully mixed, so the temperature is the same throughout the entire tank [GD2, DD2].

A4: The PCM has the same temperature throughout [GD2, DD2, LC1].

A5: Density of the water and PCM have no spatial variation; that is, they are each constant over their entire volume [GD2].

A6: Specific heat capacity of the water and PCM have no spatial variation; that is, they are each constant over their entire volume [GD2].

A7: Newton's law of convective cooling applies between the coil and the water [DD1].

A8: The temperature of the heating coil is constant over time [DD1, LC2].

A9: The temperature of the heating coil does not vary along its length [DD1, LC3].

A10: Newton's law of convective cooling applies between the water and the PCM [DD2].

A11: The model only accounts for charging of the tank, not discharging. The temperature of the water and PCM can only increase, or remain constant; they do not decrease. This implies that the initial temperature (A12) is less than (or equal) to the temperature of the coil [IM1, LC4].

A12: The initial temperature of the water and the PCM is the same [IM1, IM2, LC5].

A13: The simulation will start with the PCM in solid form [IM2, IM4].

A14: The operating temperature range of the system is such that the water is always in liquid form. That is, the temperature will not drop below the melting point of water, or rise above its boiling point [IM1, IM3].

A15: The tank is perfectly insulated so that there is no heat loss from the tank [IM1, LC6].

A16: No internal heat is generated by either the water or the PCM; therefore, the volumetric heat generation is zero [IM1, IM2].

A17: The volume change of the PCM due to melting is negligible [IM2].

A18: The PCM is either in a liquid or solid state, but not a gas [IM2, IM4].

A19: The pressure in the tank is atmospheric, so the melting and boiling points of water are 0^oC and 100^oC, respectively [IM1, IM3].

A20: When considering the volume of water in the tank, the volume of the coil is assumed to be negligible [R2].

4.2.2   Theoretical Models

This section focuses on the general equations and laws that SWHS is based on.

Number	T1
Label	**Conservation of thermal energy**
Equation	$-\nabla \cdot \mathbf{q} + g = \rho C \frac{\partial T}{\partial t}$
Description	The above equation gives the conservation of energy for transient heat transfer in a material of specific heat capacity C ($\mathrm{J\,kg^{-1}\,{}^\circ C^{-1}}$) and density ρ ($\mathrm{kg\,m^{-3}}$), where $\mathbf{q}$ is the thermal flux vector ($\mathrm{W\,m^{-2}}$), g is the volumetric heat generation ($\mathrm{W\,m^{-3}}$), T is the temperature (°C), t is time (s), and ∇ is the gradient operator. For this equation to apply, other forms of energy, such as mechanical energy, are assumed to be negligible in the system (A1). In general, the material properties (ρ and C) depend on temperature.
Source	http://www.efunda.com/formulae/heat_transfer/conduction/overview_cond.cfm
Ref. By	GD2

Number	T2
Label	**Sensible heat energy**
Equation	$E = \begin{cases} C^S m \Delta T & \text{if } T < T_{\text{melt}} \\ C^L m \Delta T & \text{if } T_{\text{melt}} < T < T_{\text{boil}} \\ C^V m \Delta T & \text{if } T_{\text{boil}} < T \end{cases}$ See T3, Latent heat energy, if $T = T_{\text{boil}}$ or $T = T_{\text{melt}}$.
Description	E is the change in sensible heat energy (J). C^S, C^L, C^V are the specific heat capacities of a solid, liquid, and vapour, respectively ($\text{J kg}^{-1}\,{}^{\circ}\text{C}^{-1}$). m is the mass (kg). T is the temperature (°C), and ΔT is the change in temperature (°C). T_{melt} and T_{boil} are the melting and boiling points, respectively (°C). Sensible heating occurs as long as the material does not reach a temperature where a phase change occurs. A phase change occurs if $T = T_{\text{boil}}$ or $T = T_{\text{melt}}$. If this is the case, refer to T3, Latent heat energy.
Source	http://en.wikipedia.org/wiki/Sensible_heat
Ref. By	IM3, IM4

Number	T3
Label	**Latent heat energy**
Equation	$T = T_{\text{melt}}$ or $T = T_{\text{boil}}$, $Q(t) = \int_0^t \frac{dQ(\tau)}{d\tau} d\tau$, with $Q(0) = 0$
Description	Q is the change in thermal energy (J), latent heat energy. $\int_0^t \frac{dQ(\tau)}{d\tau} d\tau$ is the rate of change of Q with respect to time τ (s). t is the time (s) elapsed, as long as the phase change is not complete. The status of the phase change depends on the melt fraction DD4. T_{melt} and T_{boil} are the melting and boiling points, respectively (°C). Latent heating stops when all material has changed to the new phase.
Source	http://en.wikipedia.org/wiki/Latent_heat
Ref. By	T2, IM4

4.2.3 General Definitions

This section collects the laws and equations that will be used in deriving the data definitions, which in turn are used to build the instance models.

Number	GD1
Label	**Newton's law of cooling**
SI Units	$\mathrm{W\,m^{-2}}$
Equation	$q(t) = h\Delta T(t)$
Description	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.
	$q(t)$ is the thermal flux ($\mathrm{W\,m^{-2}}$).
	h is the heat transfer coefficient, assumed independent of T (A2) ($\mathrm{W\,m^{-2}\,{}^{\circ}C^{-1}}$).
	$\Delta T(t) = T(t) - T_{\mathrm{env}}(t)$ is the time-dependent thermal gradient between the environment and the object (°C).
Source	[2, p. 8]
Ref. By	DD1, DD2

Number	GD2
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	The basic equation governing the rate of change of temperature, for a given volume V, with time.
	m is the mass (kg).
	C is the specific heat capacity ($\text{J kg}^{-1}\,{}^{\circ}\text{C}^{-1}$).
	T is the temperature (${}^{\circ}\text{C}$) and t is the time (s).
	q_{in} and q_{out} are the in and out heat transfer rates, respectively (W m^{-2}).
	A_{in} and A_{out} are the surface areas over which the heat is being transferred in and out, respectively (m^2).
	g is the volumetric heat generated (W m^{-3}).
	V is the volume (m^3).
Ref. By	IM1, IM2

Detailed derivation of simplified rate of change of temperature

Integrating (T1) over a volume (V), we have

$$-\int_V \nabla \mathbf{q}\, dV + \int_V g\, dV = \int_V \rho C \frac{\partial T}{\partial t}\, dV.$$

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 for the surface,

$$-\int_S \mathbf{q} \cdot \hat{\mathbf{n}}\, dS + \int_V g\, dV = \int_V \rho C \frac{\partial T}{\partial t}\, dV. \tag{1}$$

We consider an arbitrary volume. The volumetric heat generation is assumed constant. Then (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 GD2. Assuming ρ, C and T are constant over the volume, which is true in our case by assumptions (A3), (A4), (A5), and (A6), we have

$$\rho C V \frac{dT}{dt} = q_{\text{in}}A_{\text{in}} - q_{\text{out}}A_{\text{out}} + gV. \tag{2}$$

Using the fact that $\rho = m/V$, (2) can be written as

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

4.2.4 Data Definitions

This section collects and defines all the data needed to build the instance models. The dimension of each quantity is also given.

Number	DD1
Label	**Heat flux out of coil**
Symbol	q_C
SI Units	W m^{-2}
Equation	$q_C(t) = h_C(T_C - T_W(t))$, over area A_C
Description	T_C is the temperature of the coil (°C). T_W is the temperature of the water (°C). The heat flux out of the coil, q_C (W m^{-2}), is found by assuming that Newton's Law of Cooling applies (A7). This law (GD1) is used on the surface of the coil, which has area A_C (m^2) and heat transfer coefficient h_C ($\text{W m}^{-2}\,°\text{C}^{-1}$). This equation assumes that the temperature of the coil is constant over time (A8) and that it does not vary along the length of the coil (A9).
Sources	[4]
Ref. By	IM1

Number	DD2
Label	**Heat flux into PCM**
Symbol	q_P
SI Units	$\mathrm{W\,m^{-2}}$
Equation	$q_P(t) = h_P(T_W(t) - T_P(t))$, over area A_P
Description	T_W is the temperature of the water (°C). T_P is the temperature of the PCM (°C). The heat flux into the PCM, q_P ($\mathrm{W\,m^{-2}}$), is found by assuming that Newton's Law of Cooling applies (A10). This law (GD1) is used on the surface of the PCM, which has area A_P (m²) and heat transfer coefficient h_P ($\mathrm{W\,m^{-2}\,°C^{-1}}$). This equation assumes that the temperature of the PCM and water each have constant values over the surface area over which they interact (A3 and A4).
Sources	[4]
Ref. By	IM1, IM2, IM4

Number	DD3
Label	**Specific latent heat of fusion**
Symbol	H_f
SI Units	$\mathrm{J\,kg^{-1}}$
Equation	$H_f = \frac{Q}{m}$
Description	H_f is the amount of heat energy required to completely melt a unit mass of a substance ($\mathrm{J\,kg^{-1}}$). Q is the heat energy required for melting (J). m is the mass being melted (kg).
Sources	[1, p. 282]
Ref. By	DD4, IM4

Number	DD4
Label	**Melt fraction**
Symbol	ϕ
SI Units	dimensionless
Equation	$\phi = \frac{Q_P}{H_f m_P}, \, (0 \le \phi \le 1)$
Description	ϕ is the fraction of the PCM that is liquid (dimensionless).
	Q_P is the latent heat energy added to the PCM (J).
	H_f is the latent heat of fusion of the PCM ($\mathrm{J\,kg^{-1}}$) (DD3).
	m_P is the mass of the PCM (kg).
Sources	[4]
Ref. By	T3, IM2, IM4

4.2.5 Instance Models

This section transforms the problem defined in Section 4.1 into one which is expressed in mathematical terms. It uses concrete symbols defined in Section 4.2.4 to replace the abstract symbols in the models identified in Sections 4.2.2 and 4.2.3.

The goals GS1 to GS4 are solved by IM1 to IM4. The solutions for IM1 and IM2 are coupled since the solution for T_W and T_P depend on one another. IM3 can be solved once IM1 has been solved. The solution of IM2 and IM4 are also coupled, since the temperature and energy of the PCM depend on the phase change.

Number	IM1
Label	**Energy balance on water to find T_W**
Input	m_W, C_W, h_C, A_C, h_P, A_P, t_{final}, T_C, T_{init}, $T_P(t)$ from IM2
	The input is constrained so that $T_{\text{init}} \leq T_C$ (A11)
Output	$T_W(t)$, $0 \leq t \leq t_{\text{final}}$, such that
	$\frac{dT_W}{dt} = \frac{1}{\tau_W}[(T_C - T_W(t)) + \eta(T_P(t) - T_W(t))]$,
	$T_W(0) = T_P(0) = T_{\text{init}}$ (A12) and $T_P(t)$ from IM2
Description	T_W is the water temperature (°C).
	T_P is the PCM temperature (°C).
	T_C is the coil temperature (°C).
	$\tau_W = \frac{m_W C_W}{h_C A_C}$ is a constant (s).
	$\eta = \frac{h_P A_P}{h_C A_C}$ is a constant (dimensionless).
	The above equation applies as long as the water is in liquid form, $0 < T_W < 100^o$C, where 0^oC and 100^oC are the melting and boiling points of water, respectively (A14, A19).
Sources	[4]
Ref. By	IM2

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 coil as q_C and from the water into the PCM as q_p, over areas A_C and A_P, respectively. No heat transfer occurs to the outside of the tank, since it has been assumed to be perfectly insulated (A15). Assuming no internal heat is generated (A16), $g = 0$. Therefore, the equation for GD2 can be written as:

$$m_W C_W \frac{dT_W}{dt} = q_C A_C - q_P A_P.$$

Using DD1 and DD2 for q_C and q_P respectively, this can be written as

$$m_W C_W \frac{dT_W}{dt} = h_C A_C(T_C - T_W) - h_P A_P(T_W - T_P). \tag{3}$$

Dividing (3) by $m_W C_W$, we obtain

$$\frac{dT_W}{dt} = \frac{h_C A_C}{m_W C_W}(T_C - T_W) - \frac{h_P A_P}{m_W C_W}(T_W - T_P). \tag{4}$$

Factoring the negative sign out of the second term of the RHS of Equation (4) and multiplying it by $\frac{h_C A_C}{h_C A_C}$ yields,

$$\frac{dT_W}{dt} = \frac{h_C A_C}{m_W C_W}(T_C - T_W) + \frac{h_C A_C}{h_C A_C}\frac{h_P A_P}{m_W C_W}(T_P - T_W),$$

which simplifies to

$$\frac{dT_W}{dt} = \frac{h_C A_C}{m_W C_W}(T_C - T_W) + \frac{h_P A_P}{h_C A_C}\frac{h_C A_C}{m_W C_W}(T_P - T_W). \tag{5}$$

Setting $\tau_W = \frac{m_W C_W}{h_C A_C}$ and $\eta = \frac{h_P A_P}{h_C A_C}$, Equation (5) can be written as

$$\frac{dT_W}{dt} = \frac{1}{\tau_W}(T_C - T_W) + \frac{\eta}{\tau_W}(T_P - T_W).$$

Finally, factoring out $\frac{1}{\tau_W}$, we are left with the governing ODE for IM1:

$$\frac{dT_W}{dt} = \frac{1}{\tau_W}[(T_C - T_W) + \eta(T_P - T_W)].$$

Number	IM2
Label	**Energy balance on PCM to find T_P**
Input	m_P, C_P^S, C_P^L, h_P, A_P, t_{final}, T_{init}, T_{melt}^P, $T_W(t)$ from IM1
	The input is constrained so that $T_{\text{init}} < T_{\text{melt}}^P$ (A13)
Output	$T_P(t)$, $0 \leq t \leq t_{\text{final}}$, with initial conditions, $T_W(0) = T_P(0) = T_{\text{init}}$ (A12), and $T_W(t)$ from IM1, such that the following governing ODE is satisfied. The specific ODE depends on T_P as follows:
	$$\frac{dT_P}{dt} = \begin{cases} \frac{dT_P}{dt} = \frac{1}{\tau_P^S}(T_W(t) - T_P(t)) & \text{if } T_P < T_{\text{melt}}^P \\ \frac{dT_P}{dt} = \frac{1}{\tau_P^L}(T_W(t) - T_P(t)) & \text{if } T_P > T_{\text{melt}}^P \\ 0 & \text{if } T_P = T_{\text{melt}}^P \text{ and } 0 < \phi < 1 \end{cases}$$
	The temperature remains constant at T_{melt}^P, even with the heating (or cooling), until the phase change has occurred for all of the material; that is as long as $0 < \phi < 1$. ϕ (from DD4) is determined as part of the heat energy in the PCM, as given in IM4
	$t_{\text{melt}}^{\text{init}}$, the time at which melting begins.
	$t_{\text{melt}}^{\text{final}}$, the time at which melting ends.
Description	T_W is water temperature (°C).
	T_P is the PCM temperature (°C).
	$\tau_P^S = \frac{m_P C_P^S}{h_P A_P}$ is a constant (s).
	$\tau_P^L = \frac{m_P C_P^L}{h_P A_P}$ is a constant (s).
Sources	[4]
Ref. By	IM1, IM4

Detailed derivation of the energy balance on the PCM during sensible heating phase

To find the rate of change of T_P, we look at the energy balance on the PCM. The volume being considered is the volume of the PCM, V_P. The derivation that follows is initially for the solid PCM. The PCM in the tank has mass m_P and specific heat capacity C_P^S. Heat input from the water to the PCM is q_P over area A_P. There is no heat flux output. Assuming no internal heat generated (A16), $g = 0$, the equation for GD2 can be written as:

$$m_P C_P^S \frac{dT_P}{dt} = q_P A_P$$

Using DD2 for q_P, this equation can be written as

$$m_P C_P^S \frac{dT_P}{dt} = h_P A_P (T_W - T_P).$$

Dividing by $m_P C_P^S$ we obtain,

$$\frac{dT_P}{dt} = \frac{h_P A_P}{m_P C_P^S}(T_W - T_P).$$

Setting $\tau_P^S = \frac{m_P C_P^S}{h_P A_P}$, this can be written as

$$\frac{dT_P}{dt} = \frac{1}{\tau_P^S}(T_W - T_P). \tag{6}$$

Equation (6) applies for the solid PCM. In the case where all the PCM is melted, the same derivation applies, except that C_P^S is replaced by C_P^L, and thus τ_P^S is replaced by τ_P^L. Although a small change in surface area would be expected with melting, this is not included, since the volume change of the PCM with melting is assumed to be negligible (A17).

In the case where $T_P = T_{\text{melt}}^P$ and not all of the PCM is melted, the temperature does not change. Therefore, in this case $\frac{dT_P}{dt} = 0$.

This derivation does not consider the boiling of the PCM, as the PCM is assumed to either be in a solid or liquid state (A18).

Number	IM3
Label	**Heat energy in the water**
Input	C_W, m_W, T_{init}, $T_W(t)$ from IM1
Output	$E_W(t)$, $0 \le t \le t_{\text{final}}$, such that $E_W(t) = C_W m_W (T_W(t) - T_{\text{init}})$
Description	The above equation is derived using T2. E_W is the change in thermal energy of the liquid water relative to the energy at the initial temperature (T_{init}) (J). C_W is the specific heat capacity of liquid water ($\text{J kg}^{-1} \, {}^\circ\text{C}^{-1}$) and m_W is the mass of the water (kg). 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 $0 < T_W < 100^o\text{C}$ (A14, A19).
Sources	[4]
Ref. By	–

Number	IM4
Label	**Heat energy in the PCM**
Input	C_P^S, C_P^L, H_f, $T_P(t)$, T_{init}, m_P, T_{melt}^P, h_P, A_P, $t_{\text{melt}}^{\text{init}}$ (from IM2), t_{final} The input is constrained so that $T_{\text{init}} < T_{\text{melt}}^P$ (A13)
Output	$E_P(t)$, $0 \leq t \leq t_{\text{final}}$, such that $$E_P = \begin{cases} C_P^S m_P(T_P(t) - T_{\text{init}}) & \text{if } T_P < T_{\text{melt}}^P \\ E_{P\text{melt}}^{\text{init}} + H_f m_p + C_P^L m_P(T_P(t) - T_{\text{melt}}^P) & \text{if } T_P > T_{\text{melt}}^P \\ E_{P\text{melt}}^{\text{init}} + Q_P(t) & \text{if } T_P = T_{\text{melt}}^P, (0 < \phi < 1) \end{cases}$$ $$E_{P\text{melt}}^{\text{init}} = C_S^P m_p(T_{\text{melt}}^P - T_{\text{init}})$$ Here $Q_P(t)$ is found with the intial condition that $Q_P(t_{\text{melt}}^{\text{init}}) = 0$ and $$\frac{dQ_P(t)}{dt} = q_P(t)A_P = h_P A_P(T_W(t) - T_{\text{melt}}^P),$$ with the heat flux q_P from DD2, over area A_P, $\phi = \frac{Q_P}{H_f m_P}$ (DD4)
Description	The above equation is derived using T2 and T3. E_P is the change in thermal energy of the PCM relative to the energy at the initial temperature (T_{init}) (J). E_P for the solid PCM is found using T2 for sensible heating, with the specific heat capacity of the solid PCM, C_P^S ($\text{J kg}^{-1}\,{}^\circ\text{C}^{-1}$), and the change in the PCM temperature from the initial temperature (${}^\circ\text{C}$). E_P for the melted PCM ($T_P > T_{\text{melt}}^P$) is found using T2 for sensible heating of the liquid PCM, plus the energy when melting starts, plus the energy required to melt all of the PCM. The energy when melting starts is $E_{P\text{melt}}^{\text{init}}$ (J). The energy required to melt all of the PCM is $H_f m_p$ (J) (DD3). The specific heat capacity of the liquid PCM is C_P^L ($\text{J kg}^{-1}\,{}^\circ\text{C}^{-1}$) and the change in temperature is $T_p - T_{\text{melt}}^P$ (${}^\circ\text{C}$). E_P during melting of the PCM is found using the energy required at the instant melting of the PCM begins, $E_{P\text{melt}}^{\text{init}}$, plus the latent heat energy added to the PCM, Q_P (J), since the time when melting began ($t_{\text{melt}}^{\text{init}}$ (s)). The heat energy for boiling of the PCM is not detailed, since the PCM is assumed to either be in a solid or liquid state (A18).
Sources	[4]
Ref. By	IM2

4.2.6 Data Constraints

Tables 1 and 3 show the data constraints on the input and output variables, respectively. The column for physical constraints gives the physical limitations on the range of values that can be taken by the variable. The column for software constraints restricts the range of inputs to reasonable values. 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 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 specification parameters in Table 1 are listed in Table 2.

Table 1: Input Variables

Var	Physical Constraints	Software Constraints	Typical Value	Uncertainty
L	$L > 0$	$L_{\min} \le L \le L_{\max}$	1.5 m	10%
D	$D > 0$	$R_{\min} \le R \le R_{\max}$ where $R = \frac{D}{L}$	0.412 m	10%
V_P	$V_P > 0$ (*)	$V_P \ge \text{minfract} \cdot V_{\text{tank}}(D, L)$	0.05 m^3	10%
	$V_P < V_{\text{tank}}(D, L)$			
A_P	$A_P > 0$ (*)	$V_P \le A_P \le \frac{2}{h_{\min}} V_P$ (#)	1.2 m^2	10%
ρ_P	$\rho_P > 0$	$\rho_P^{\min} < \rho_P < \rho_P^{\max}$	1007 kg/m^3	10%
T_{melt}^P	$0 < T_{\text{melt}}^P < T_C$ (+)		44.2 °C	10%
C_P^S	$C_P^S > 0$	$C_{P\min}^S < C_P^S < C_{P\max}^S$	1760 J/(kg °C)	10%
C_P^L	$C_P^L > 0$	$C_{P\min}^L < C_P^S < C_{P\max}^L$	2270 J/(kg °C)	10%
H_f	$H_f > 0$	$H_f^{\min} < H_f < H_f^{\max}$	211600 J/kg	10%
A_C	$A_C > 0$ (*)	$A_C \le A_C^{\max}$	0.12 m^2	10%
T_C	$0 < T_C < 100$ (+)		50 °C	10%
ρ_W	$\rho_W > 0$	$\rho_W^{\min} < \rho_W \le \rho_W^{\max}$	1000 kg/m^3	10%
C_W	$C_W > 0$	$C_W^{\min} < C_W < C_W^{\max}$	4186 J/(kg °C)	10%
h_C	$h_C > 0$	$h_C^{\min} \le h_C \le h_C^{\max}$	1000 W/(m^2 °C)	10%
h_P	$h_P > 0$	$h_P^{\min} \le h_P \le h_P^{\max}$	1000 W/(m^2 °C)	10%
T_{init}	$0 < T_{\text{init}} < T_{\text{melt}}$ (+)		40 °C	10%
t_{final}	$t_{\text{final}} > 0$	$t_{\text{final}} < t_{\text{final}}^{\max}$ (**)	50000 s	10%

(*) These quantities cannot be equal to zero, or there will be a divide by zero in the model.

(+) These quantities cannot be zero, or there would be freezing (A14).

(#) The constraints on the surface area are calculated by considering the surface area to volume ratio. The assumption is that the lowest ratio is 1 and the highest possible is $2/h_{\min}$, where $h_{\min}$ is the thickness of a "sheet" of PCM. A thin sheet has the greatest surface area to volume ratio.

(**) The constraint on the maximum time at the end of the simulation is the total number of seconds in one day.

Table 2: Specification Parameter Values

Var	Value
$L_{\min}$	0.1 m
$L_{\max}$	50 m
$R_{\min}$	0.002
$R_{\max}$	200
minfrac	10^{-6}
$h_{\min}$	0.001 m
$\rho_P^{\min}$	500 kg m^{-3}
$\rho_P^{\max}$	20000 kg m^{-3}
$C_{P\min}^{S}$	100 J kg^{-1} °C^{-1}
$C_{P\max}^{S}$	4000 J kg^{-1} °C^{-1}
$C_{P\min}^{L}$	100 J kg^{-1} °C^{-1}
$C_{P\max}^{L}$	5000 J kg^{-1} °C^{-1}
$A_C^{\max}$	$\pi(\frac{D}{2})^2$ m^2
$\rho_W^{\min}$	950 kg m^{-3}
$\rho_W^{\max}$	1000 kg m^{-3}
$C_W^{\min}$	4170 J kg^{-1} °C^{-1}
$C_W^{\max}$	4210 J kg^{-1} °C^{-1}
$h_C^{\min}$	10 W m^{-2} °C^{-1}
$h_C^{\max}$	10000 W m^{-2} °C^{-1}
$h_P^{\min}$	10 W m^{-2} °C^{-1}
$h_P^{\max}$	10000 W m^{-2} °C^{-1}
$t_{\text{final}}^{\max}$	86400 s

Table 3: Output Variables

Var	Physical Constraints
T_W	$T_{\text{init}} \leq T_W \leq T_C$ (by A11)
T_P	$T_{\text{init}} \leq T_P \leq T_C$ (by A11)
E_W	$E_W \geq 0$
E_P	$E_P \geq 0$

4.2.7 Properties of a Correct Solution

A correct solution must exhibit the law of conservation of energy. This means that the energy change in the water should equal the difference between the total energy input from the coil and the energy output to the PCM. This can be shown as an equation by taking DD1 and DD2, multiplying each by their respective surface area of heat transfer, and integrating each over the simulation time, as follows:

$$E_W = \int_0^t h_C A_C (T_C - T_W(t)) dt - \int_0^t h_P A_P (T_W(t) - T_P(t)) dt \tag{7}$$

In addition, the energy change in the PCM should equal the energy input to the PCM from the water. This can be expressed as

$$E_P = \int_0^t h_P A_P (T_W(t) - T_P(t)) dt. \tag{8}$$

Equations (7) and (8) can be used as "sanity" checks to gain confindence in any solution computed by SWHS. The relative error between the results computed by SWHS and the results calculated from the right sides of these equations should be less than 0.001% (R9).

5 Requirements

This section provides the functional requirements, the business tasks that the software is expected to complete, and the nonfunctional requirements, the qualities that the software is expected to exhibit.

5.1 Functional Requirements

R1: Input the following quantities, which define the tank parameters, material properties and initial conditions:

symbol	unit	description
L	m	length of tank
D	m	diameter of tank
V_P	m^3	volume of PCM
A_P	m^2	phase change material surface area
ρ_P	kg/m^3	density of PCM
T_{melt}^P	°C	temperature at melting point for PCM
C_P^S	J/(kg °C)	specific heat capacity of PCM during sensible heating phase
C_P^L	J/(kg °C)	specific heat capacity of PCM during latent heating phase
H_f	J/kg	specific latent heat of fusion
A_C	m^2	coil surface area
T_C	°C	temperature of coil
ρ_W	kg/m^3	density of water
C_W	J/(kg °C)	specific heat capacity of water
h_C	W/(m^2 °C)	convective heat transfer coefficient between coil and water
h_P	W/(m^2 °C)	convective heat transfer coefficient between water and PCM
T_{init}	°C	initial temperature of water and PCM
t_{step}	s	time step for simulation
t_{final}	s	time at end of simulation
$AbsTol$	unitless	absolute tolerance
$RelTol$	unitless	relative tolerance
$ConsTol$	unitless	relative tolerance for law of conservation of energy

R2: Use the inputs in R1 to find the mass needed for IM1 to IM4, as follows:

$$m_W = V_W \rho_W = (V_{\text{tank}} - V_P)\rho_W = (\pi(D/2)^2 L - V_P)\rho_W$$
$$m_P = V_P \rho_P,$$

where V_W is the volume of water in the tank, V_{tank} is the volume inside of the cylindrical tank and V_P is the volume of the PCM. For this calculation the volume of the coil is assumed to be negligible (A20).

R3: Verify that the inputs satisfy the required physical constraints shown in Table 1.

R4: Output the input quantities and derived quantities in the following list: the quantities from R1, the masses from R2, τ_W (from IM1), η (from IM1), τ_P^S (from IM2) and τ_P^L (from IM2).

R5: Calculate and output the temperature of the water ($T_W(t)$) over the simulation time (from IM1). The algorithm selected for this calculation will use *AbsTol* and *RelTol* as inputs to control the absolute and relative tolerance of the solution.

R6: Calculate and output the temperature of the PCM ($T_P(t)$) over the simulation time (from IM2). The algorithm selected for this calculation will use *AbsTol* and *RelTol* as inputs to control the absolute and relative tolerance of the solution.

R7: Calculate and output the energy in the water ($E_W(t)$) over the simulation time (from IM3).

R8: Calculate and output the energy in the PCM ($E_P(t)$) over the simulation time (from IM4).

R9: Verify that the energy outputs ($E_W(t)$ and $E_P(t)$) follow the law of conservation of energy, as outlined in Section 4.2.7, with relative error no greater than 0.001%.

R10: Calculate and output the time at which the PCM begins to melt $t_{\text{melt}}^{\text{init}}$ (from IM2).

R11: Calculate and output the time at which the PCM stops melting $t_{\text{melt}}^{\text{final}}$ (from IM2).

5.2 Nonfunctional Requirements

Given the small size, and relative simplicity, of this problem, performance is not a priority. Any reasonable implementation will be very quick and use minimal storage. Rather than performance, the priority nonfunctional requirements are correctness, verifiability, understandability, reusability and maintainability.

6 Likely Changes

LC1: A4 - PCM is actually a poor thermal conductor, so the assumption of uniform PCM temperature is not likely.

LC2: A8 - The temperature of the heating coil will change over the course of the day, depending on the energy received from the sun.

LC3: A9 - The temperature of the water in the coil will actually change along its length as the water cools.

LC4: A11 - The model currently only accounts for charging of the tank. A more complete model would also account for discharging of the tank.

LC5: A12 - To add more flexibility to the simulation, the initial temperature of the water and the PCM could be allowed to have different values.

LC6: A15 - Any real tank cannot be perfectly insulated and will lose heat.

7 Traceability Matrices and Graphs

The purpose of the traceability matrices is to provide easy references on what has to be additionally modified if a certain component is changed. Every time a component is changed, the items in the column of that component that are marked with an "X" should be modified as well. Table 4 shows the dependencies of theoretical models, general definitions, data definitions, and instance models with each other. Table 5 shows the dependencies of instance models, requirements, and data constraints on each other. Table 6 shows the dependencies of theoretical models, general definitions, data definitions, instance models, and likely changes on the assumptions.

	T1	T2	T3	GD1	GD2	DD1	DD2	DD3	DD4	IM1	IM2	IM3	IM4
T1													
T2			X										
T3													
GD1													
GD2	X												
DD1			X										
DD2			X										
DD3													
DD4								X					
IM1				X	X	X					X		
IM2				X		X		X	X				X
IM3		X											
IM4		X	X				X	X	X		X		

Table 4: Traceability Matrix Showing the Connections Between Items of Different Sections

The purpose of the traceability graphs is also to provide easy references on what has to be additionally modified if a certain component is changed. The arrows in the graphs represent dependencies. The component at the tail of an arrow is depended on by the component at the head of that arrow. Therefore, if a component is changed, the components that it points to should also be changed. Figure 3 shows the dependencies of theoretical models, general definitions, data definitions, instance models, likely changes, and assumptions on each other. Figure 4 shows the dependencies of instance models, requirements, and data constraints on each other.

NOTE: Building a tool to automatically generate the graphical representation of the matrix by scanning the labels and reference can be future work.

	IM1	IM2	IM3	IM4	4.2.6	R1	R2
IM1		X				X	X
IM2	X			X		X	X
IM3						X	X
IM4		X				X	X
R1							
R2						X	
R3					X		
R4	X	X				X	X
R5	X						
R6		X					
R7			X				
R8				X			
R9			X	X			
R10		X					
R11		X					

Table 5: Traceability Matrix Showing the Connections Between Requirements and Instance Models
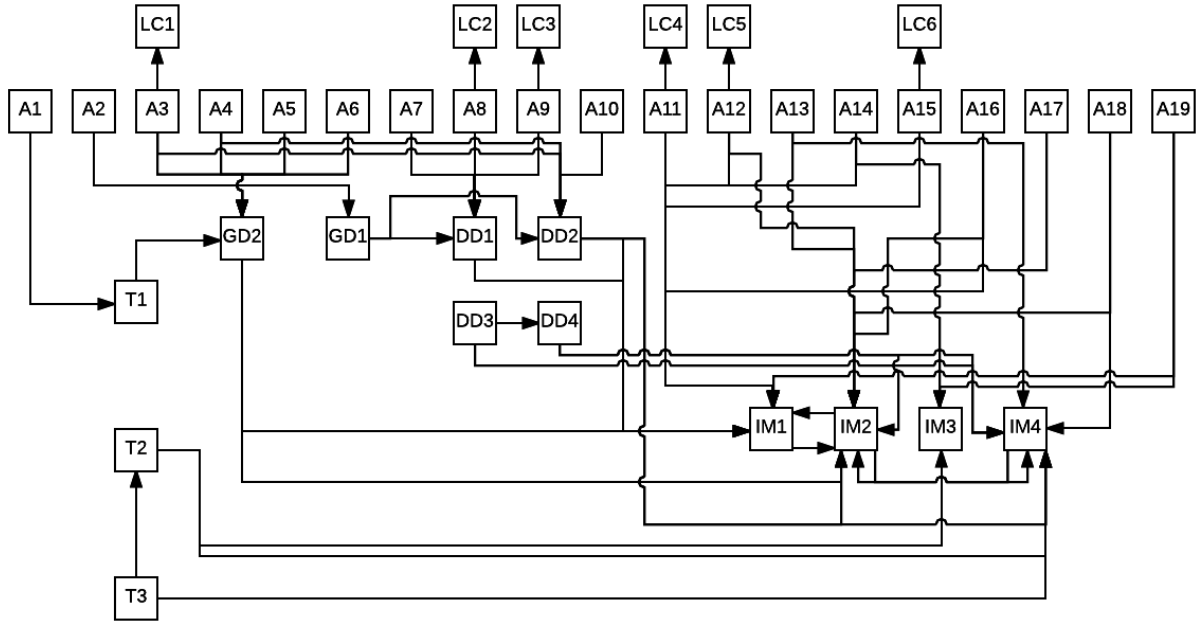
Figure 3: Traceability Matrix Showing the Connections Between Items of Different Sections
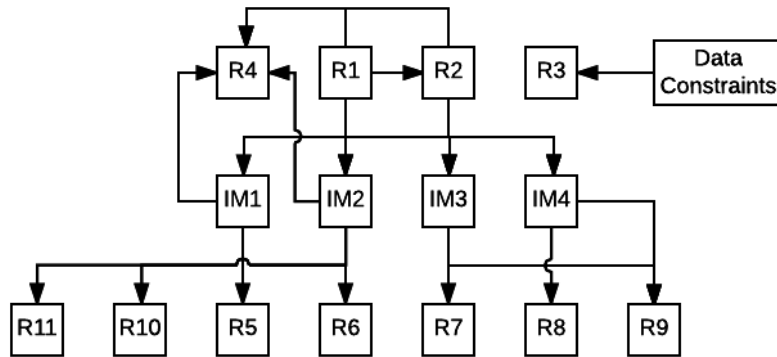

Figure 4:   Traceability Matrix Showing the Connections Between Requirements, Instance Models, and Data Constraints

	A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	A11	A12	A13	A14	A15	A16	A17	A18	A19
T1	X																		
T2																			
T3																			
GD1		X																	
GD2			X	X	X	X													
DD1							X	X	X										
DD2			X	X						X									
DD3																			
DD4																			
IM1											X	X		X	X	X			X
IM2												X	X			X	X	X	
IM3														X					X
IM4													X					X	
LC1				X															
LC2								X											
LC3									X										
LC4											X								
LC5													X						
LC6															X				

Table 6: Traceability Matrix Showing the Connections Between Assumptions and Other Items

References

[1] J. Frederick Bueche. *Introduction to Physics for Scientists*. McGraw Hill, United States, fourth edition edition, 1986.

[2] F. P. Incropera, D. P. Dewitt, T. L. Bergman, and A. S. Lavine. *Fundamentals of Heat and Mass Transfer*. John Wiley and Sons, United States, sixth edition edition, 2007.

[3] Nirmitha Koothoor. A document drive approach to certifying scientific computing software. Master's thesis, McMaster University, Hamilton, Ontario, Canada, 2013.

[4] Marilyn Lightstone. Derivation of tank/pcm model. Personal Notes, 2012.

[5] David L. Parnas and P.C. Clements. A rational design process: How and why to fake it. *IEEE Transactions on Software Engineering*, 12(2):251–257, February 1986.

[6] W. Spencer Smith and Lei Lai. A new requirements template for scientific computing. In J. Ralyté, P. Àgerfalk, and N. Kraiem, editors, *Proceedings of the First International Workshop on Situational Requirements Engineering Processes – Methods, Techniques and Tools to Support Situation-Specific Requirements Engineering Processes, SREP'05*, pages 107–121, Paris, France, 2005. In conjunction with 13th IEEE International Requirements Engineering Conference.