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## ESFuelCell2012-91319

### COMPUTATIONAL EVALUATION OF LATENT HEAT ENERGY STORAGE USING A HIGH TEMPERATURE PHASE CHANGE MATERIAL

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#### ABSTRACT

Latent heat energy storage systems have higher energy density than their sensible heat counterparts and have the added benefit of constant temperature operation. This work computationally evaluates a thermal energy storage system using molten silicon as a phase change material. A cylindrical receiver, absorber, converter system was evaluated using the heat transfer in solids with surface-to surface radiation physics module of the commercially available COMSOL Multiphysics simulation software. The progression of the solidification and melting fronts through the phase change material was modeled for two different methods of concentrated solar irradiation delivery. Heating the core of the PCM rather than the top of the PCM decreased the required solar input by 17%, decreasing the solar collector area required as well as lowering overall system weight.

#### INTRODUCTION

In order to use solar energy as a constant source of power, an energy storage system must be employed. Thermal energy storage (TES) allows heat energy to be gathered and stored when available, and utilized, directly or converted to another form, when the source is no longer available. Historically, thermal energy has been stored as sensible heat in either water or economical solids, such as rock or concrete (1, 2). Hasnain (2) explains that a sensible heat system must either increase the range of operating temperatures or increase the mass to store more energy, thereby limiting its use in a small system. By comparison, phase change materials (PCMs) utilize the significant heat of fusion required to change the state of a material (typically solid to liquid); this allows higher energy storage density as well as energy storage within a smaller

temperature range. In 2005, the International Energy Agency (IEA) published an inventory of phase change materials appropriate for various applications including energy storage (3).

The use of PCM in low temperature energy storage for promoting cost effectiveness and energy efficiency in buildings has been evaluated (1, 2, 4). However, PCM use has had limited application to such power systems due to materials with an appropriate phase-change temperature (typically hydrated salts) offering a low power density and a low thermal conductivity, leading to a limited rate of charging and discharging (4). A focus on developing techniques to improve PCM conductivity has resulted. Imbedding honeycomb structures in the PCM, macro-encapsulation, and microencapsulation with conductive materials (1, 2, 3) have all been evaluated, but currently the technology requires large upfront costs for small increases in efficiency (4).

One field with perhaps the greatest potential for successful application of PCM technology, however, is concentrated solar power. Pistocchini (5) investigated the use of PCM storage in the field of concentrated solar power plants. In this terrestrial-based application, energy can be stored during the day and exhausted at night, capitalizing on a large desert diurnal temperature difference. Similarly, extraterrestrial concentrated solar power is another application area with the potential for significant success. For small satellites in low earth orbit, where solar exposure is followed by a period in eclipse, the energy density of a storage system is paramount for launch weight (and therefore cost) reduction. The capabilities of solar thermal energy storage in the form of a PCM with high melting temperatures and large heats of fusion, such as silicon, could meet these needs (6). The heat of fusion and thermal

conductivity of silicon are one and two orders of magnitude, respectively, greater than those of hydrated salts and paraffin waxes. In addition, silicon is an element and therefore may avoid the material degradation experienced with other phase change materials. The material properties of silicon indicate great potential as a PCM, warranting a more detailed numerical investigation.

In numerically modeling a phase-changing system, calculating the rate of movement of the boundary between the melted and solid portion of a material undergoing phase change is referred to as the Stefan problem. Many numerical techniques have been applied to various applications of the Stefan problem, including the relatively simple and accurate heat balance integral (HBIM) (7) and enthalpy methods (8). These two techniques were applied to the inward and outward cylindrical solidification case by Caldwell and Chan (9) and shown to be consistent. Ogoh and Groulx presented a one-dimensional (10) and a cylindrical finned (11) model of the phase change process in the commercially available software COMSOL. To simulate phase change they used the heat capacity method. Their one-dimensional results compared well to an analytical evaluation.

The computational work described here simulates a PCM-based thermal storage system using silicon in low earth orbit. An altitude of 1900 km was selected to represent the most demanding case of the low earth orbit with the longest time spent in eclipse. At this altitude 4500 seconds are spent in daylight and 3000 seconds in eclipse. The progression of the solidification and melting fronts through the phase change material was modeled to determine the amount of latent heat energy remaining in the core and subsequently the required energy input.

## MODEL

The design of a system capable of receiving, absorbing, and converting solar energy, referred to as the RAC, was evaluated computationally. Describing the system from the center out radially, a 47 mm radius rod of phase change material with a height of 92 mm was housed in a cylindrical inner container with walls 5 mm thick. A 25 mm vacuum gap separated the outer walls of the inner container from two radiation shields, a 55 mm thick layer of insulation, and an outer container with 10 mm thick walls. A thermal to electric conversion (TEC) system were located above the inner container top surface. The TEC device would be a low bandwidth photovoltaic cell with a band gap of approximately 0.55eV, best simulated by an InGaAsSb cell. A top-down view of the system is shown in Figure 1 and a side view in Figure 3. The phase change material was silicon, the inner container silicon carbide, the radiation shields gold, the insulation carbon-bonded carbon fiber, and the outer casing graphite. The system was designed so radial energy losses were minimized.

A two-dimensional model, generated in the commercially available COMSOL Multiphysics, was used to evaluate the melting and solidification fronts in the phase change material and irradiation of the thermal to electric conversion system.

One-half of the test section cross-section was modeled and an axial symmetry condition applied to the centerline. A surface-to-surface radiation condition was applied to the outer circumference of the inner container of the system, all surfaces of both radiation shields, the bottom surface of the TEC, and the inner circumference of the insulation layer. A surface to ambient radiation condition was applied to the outer circumference of the outer container as well as its top and bottom and the top of the TEC. Incoming concentrated solar energy was modeled using two different methods, a constant flux was applied to the top of the inner container for Method I and a constant flux applied on the bottom of a narrow cylindrical extension of the container which extends into the center of the PCM for Method II. For all conditions, an ambient temperature of 300 K was assigned.

A combination of three different studies, one steady and two transient, all using the COMSOL heat transfer in solids physics module, were used to model the phase change process. A steady state model where a constant temperature condition was applied to the outer surface of the phase change material was evaluated to determine temperature profiles in the system after melting. These temperature profiles were used as an input to the transient study. In the transient study the constant surface temperature setting of the steady state evaluation was removed and the system was allowed to cool for the 3000 s associated with eclipse. The temperature profile after the completion of this phase was used as the initial condition for the heating period. The heat was applied as a constant heat flux, in one of the two methods described above, for the duration of the 4500 s daylight phase.

To mitigate the effects of beginning the orbit in the ideal case of the steady state solution of a perfectly melted core, a second orbit was simulated with the final profile from the heating cycle serving as the initial condition for the cooling phase and that fully cooled profile subsequently being used as the initial condition for a second heating phase. A direct PARDISO solver was used for all the components of the study.

The heat capacity method, where the specific heat of the liquid material,  $C_{p,l}$ , is increased by the latent heat of fusion,  $l_f$ , over a temperature range,  $\Delta T_m$ , centered on the phase change temperature was used to simulate phase change.

$$C_{p,m} = \frac{l_f}{\Delta T_m} + C_{p,l} \quad (1)$$

When the temperature of a particular element was within half  $\Delta T_m$  of the melting temperature a step discontinuity in the specific heat occurred. The increase in specific heat was modeled using a Heaviside smoothed step function over a 10 K temperature range.

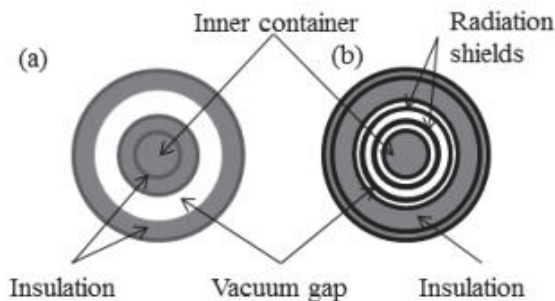
## VALIDATION

The steady state heat flux through different insulation and insulation/radiation shield configurations was evaluated in MATLAB and COMSOL for an initial validation of the

radiation modeling in COMSOL as well as to determine a design configuration that minimized thermal losses to the environment. The design described in the model section is the result of this preliminary validation.

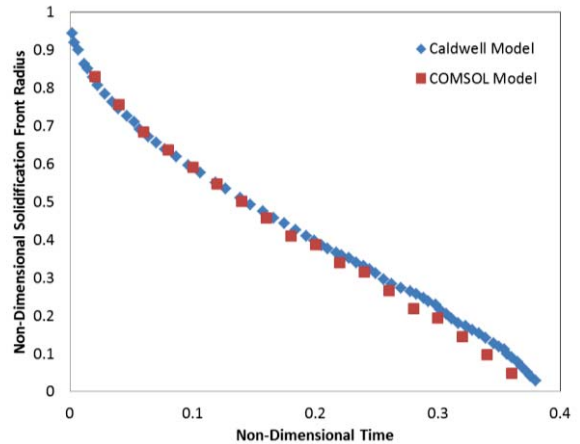
The system was modeled as concentric, one-dimensional cylinders. In all cases, the inner cylinder surface temperature was set to 1000 K and the outer surface radiated to an ambient temperature of 0 K. Emissivities and thermal conductivities were selected to model the design materials and available coatings. The outer surface temperature and heat flux were predicted. Several different configurations were evaluated.

The best results were obtained by insulating the hot side of the vacuum gap and utilizing polishing or coating to reduce radiative heat transfer, however, the high temperature of the container in this case made this configuration unusable. Not insulating the outer circumference of the inner container, and instead using radiation shielding between the container and the insulation, resulted in only slightly larger thermal losses. The results of this brief study lead to the combination of insulation on the outer casing to avoid exposure to peak temperatures and multiple radiation shields. Comparison of the analytical and computational predictions show good agreement with differences in temperature predictions less than 0.35% and in the predicted energy loss of 1.32%.



**FIGURE 1: Top down view of (a) best performing and (b) final design configurations.**

Once the steady state radiation model was validated, the phase change model employed in COMSOL was evaluated. The solidification of a cylinder of radius,  $r_0$ , exposed to a constant surface temperature was simulated in COMSOL. The location of the solidification front as a function of time was predicted and compared to the enthalpy model for inward cylindrical solidification published by Caldwell and Chen (9) which showed excellent agreement with the cylindrical HBIM model. The COMSOL results are compared with those of Caldwell and Chen in Figure 2. The COMSOL results agree well with the numerical values, validating the phase change portion of the model.



**FIGURE 2: Comparison of solidification front predicted by Caldwell (9) and COMSOL model.**

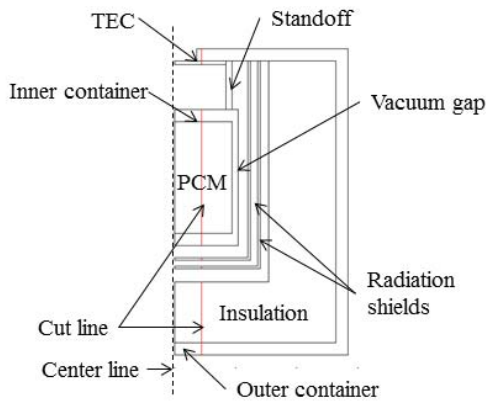
## RESULTS AND DISCUSSION

A receiver, absorber, converter system in low earth orbit was modeled. An altitude of 1900 km was selected, resulting in 4500 s spent in daylight and 3000 s in eclipse during each orbit. The progression of the solidification and melting fronts through the phase change material during orbit was modeled to track the amount of latent heat energy remaining in the core. The results from the cooling and heating cycles are presented for two different cases (1) top heating and (2) center heating. In the top heating case, Method I, a concentrated heat flux is applied to the top of the inner container. In the center heating case, Method II, a heat flux is applied to the center of the PCM.

### Method I: Top Heating

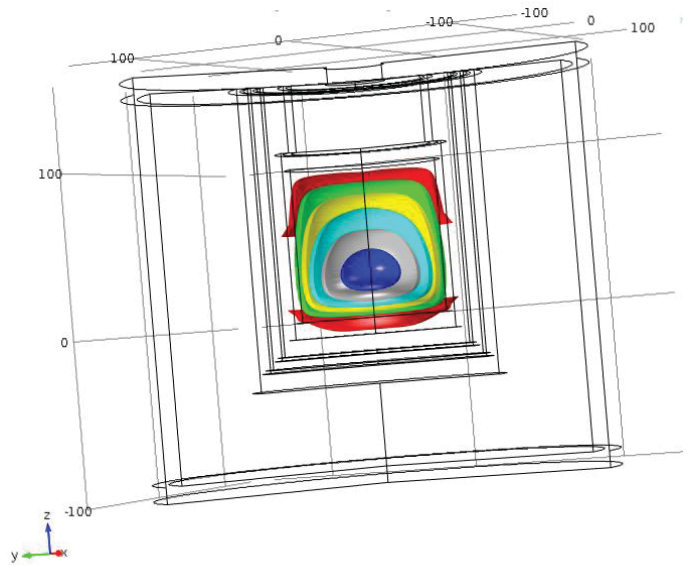
In the top heating study, the heat flux applied to the inner container top was varied until the PCM melted completely during the daylight phase and fully solidified during the eclipse phase. This corresponded to a constant surface heat transfer rate of 1800 W. The results presented are those found with the 1800 W input.

The temperature profile along the cutline, shown in Figure 3, associated with solidification during eclipse is shown in Figure 4 as a function of time. Energy is lost from the inner container circumference, top, and bottom through radiation and minor conduction through the standoffs by which the core is suspended. Because the system is heated from the top, as solidification begins, the top of the system is significantly warmer. The temperature of the center of the silicon core reaches the phase change temperature in less than 300 s but requires the remainder of the 3000 s phase to completely solidify.

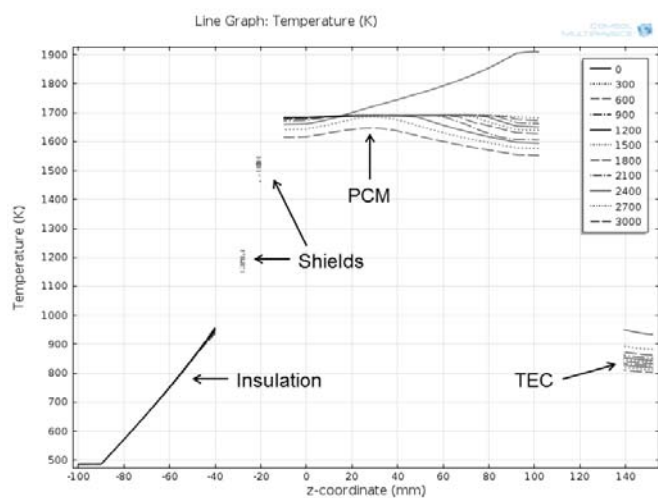


**FIGURE 3: Side view of RAC system with cut line used for data collection identified.**

The progression of the solidification front from the center out is shown in Figure 5. The different shades show an isotherm associated with 1687 K at different instances of time. The solidification front progresses more quickly from the top because the placement of the TEC prevents the installation of insulation and radiation shielding at the top of the container.



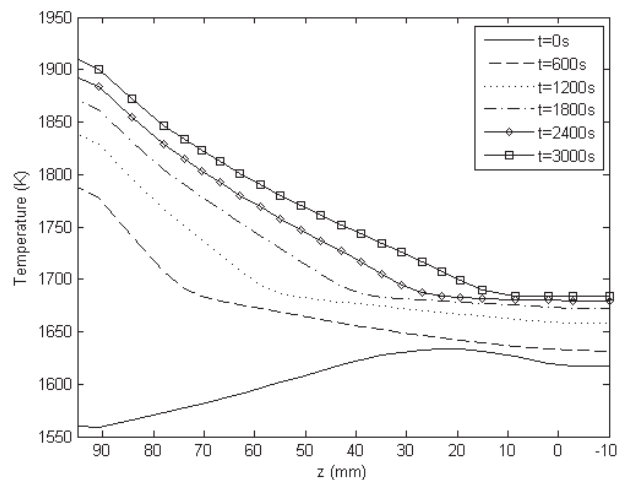
**FIGURE 5: Progression of solidification front with time.**



**FIGURE 4: Temperature profile along the cut line identified in Figure 3 at different times during solidification.**

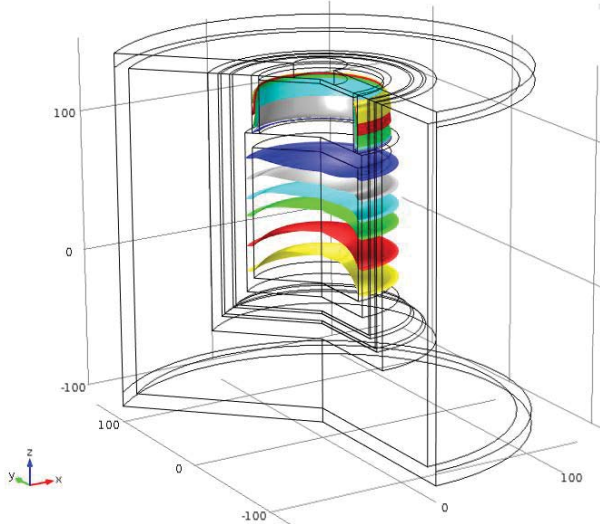
The solidification and sensible heat loss from the system result in the temperature profile shown in Figure 4 associated with time equal to 3000 s. This temperature profile serves as the initial condition for the daylight phase of the orbit. The temperature profile along the cutline through the PCM only, shown in Figure 6, shows the change in the temperature profile as the top surface of the inner container is subjected to a constant surface heat flux during the 4500 s of solar irradiation.

The thermal resistance of silicon leads to a large temperature gradient between the top and bottom of the molten core. The temperature at the interface between the casing and the molten core is approaching the melting temperature of the casing, which threatens the structure of the device.



**FIGURE 6: Temperature profile along the cut line through the PCM identified in Figure 3 at different times during melt.**

The melting front is shown with isotherms associated with 1687 K in Figure 7. The phase change front moves from the inner container top vertically towards the bottom. As the melting front moves down, the front moves more quickly along the edges than along the centerline because the silicon carbide casing is approximately six times more conductive than the silicon core.



**FIGURE 7: Progression of solidification front with time.**

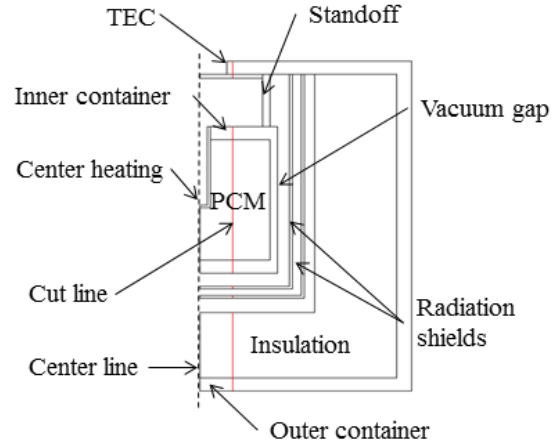
The heat added to the top surface of the container both conducts downward into the PCM but also through the standoff. In addition, the standoff is subjected to radiation from the top of the container. The combined conduction and radiation raises the standoff temperature well above the material melting point as is indicated by the shading in the standoffs in Figure 7. Because this analysis showed many of the system materials reaching their melting points, it was determined that a different heating method would be required, leading to the center heating study described below.

*Method II: Center Heating*

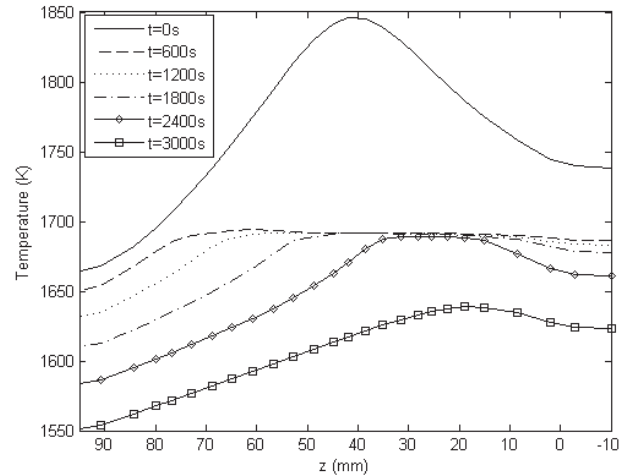
In the center heating study, the heat flux applied to the center of the system was varied until the PCM melted completely during the daylight phase and fully solidified during the eclipse phase. This corresponded to a constant surface heat transfer rate of 1500 W. The results presented are those found with the 1500 W input.

The center heating method concentrates the solar heat flux on the base of a vertical channel located in the center of the PCM. The temperature profile along the cutline in the PCM, shown in Figure 8, associated with solidification of the center heated PCM during eclipse is shown in Figure 9 as a function of time. The temperature profile at time equal to zero seconds is the final temperature profile associated with the previous melt phase. After approximately 300 s, the entire outline in the core is at the melt temperature and at each time step afterward, the solidification front moves downward. The temperatures are

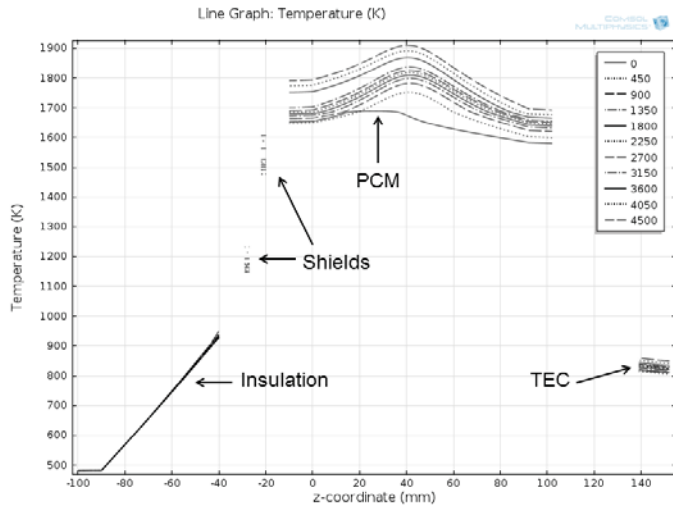
again lower on the top of the core than the bottom as the TEC system prevents the installation of insulation and allows for losses.



**FIGURE 8: Side view of RAC system with cut line used for data collection identified.**



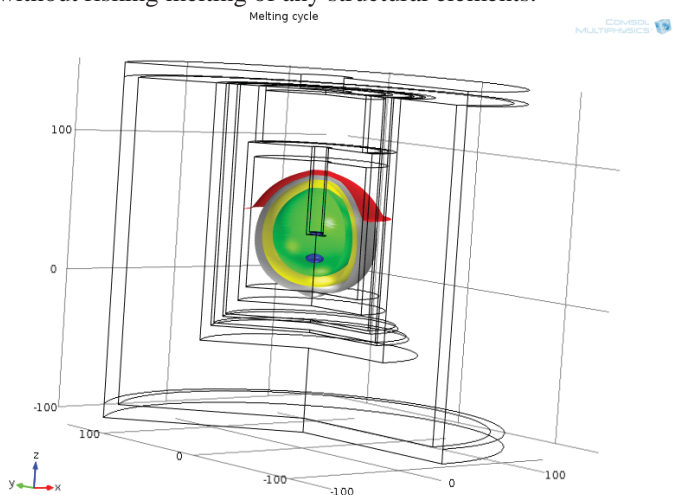
**FIGURE 9: Temperature profile along the cut line identified in Figure 8 at different times during solidification.**



**FIGURE 10: Temperature profile along the cut line identified in Figure 8 at different times during melt.**

The temperature profiles during the melt, as shown in Figure 10, increase symmetrically with the highest temperatures at the PCM center. Melting from the center out is beneficial as the solid silicon acts as insulation during the melting process and interfacial issues are eliminated. In addition, the required heat flux is reduced by about 17% which correspondingly decreases the required collector area and associated weight.

Figure 11 shows the expanding melting front during the center heating method. The different shades show a 1687 K isotherm at different times. Excessive temperatures do not reach the standoff, but the majority of the PCM completely melts and solidifies taking advantage of the latent heat storage without risking melting of any structural elements.



**FIGURE 11: Progression of melt front with time.**

The results for the center heated configuration predicts a container top temperature that oscillates between 1550K and 1650K during a single orbit. Therefore, the TEC surface

receives an average 2000 W of irradiation for this case, resulting in an approximate electric power output of 200 W based on a 50% spectral efficiency and a 20% TPV cell efficiency resulting in a conservative estimate of 10% electric conversion efficiency. In order to compare this system to a comparable design powered by a photovoltaic array and bank of batteries, a brief analysis was conducted to determine the required solar panel size and system weight. In the same orbit, a 3 m<sup>2</sup> array of photovoltaic cells would be required that in combination with battery storage would weigh approximately 20 kg. By comparison, the silicon design with a 70% solar concentration efficiency (12) would require 2.2 m<sup>2</sup> of collector area and a total weight of approximately 18 kg.

## CONCLUSION

A computational model of a thermal energy storage system using molten silicon as the phase change material was presented. The system was modeled in low earth orbit with 4500 s spent in daylight and 3000 s in eclipse. The progression of the solidification and melting fronts through the phase change material was modeled for two different methods of concentrated solar irradiation delivery. Heating the core of the PCM rather than the top of the PCM decreased the required solar input by 17% which would decrease the solar collector area required and lower overall system weight. This preliminary study will be expanded to include convection in the liquid phase as well as to investigate more suitable insulation materials.

## NOMENCLATURE

$C_p$	Specific heat (J/kg/K)
$L$	Latent heat (J/kg)
$T$	Temperature (K)
<i>Superscripts and Subscripts</i>	
$f$	Fusion
$l$	Liquid
$m$	Melt
<i>Greek Letters</i>	
$\Delta$	Change

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