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A Front Tracking Method Accelerated by Graphics Processing Units for Phase Change Modelling in Latent Heat Thermal Energy Storage: A Comparison with Interface Capturing Methods

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Latent heat thermal energy storage (LHTES) has recently evolved into a promising approach for energy savings and pollution reduction. Phase change materials (PCMs) and the latent heat accompanying the phase change can be utilized to accumulate, store, are release the energy. Computer simulation tools are usually applied in the optimal design of LHTES devices as the simulations are fast, relatively easy to perform and not expensive. The paper presents a performance and accuracy comparison between a front tracking algorithm and well-known interface capturing methods – the enthalpy and apparent heat capacity methods. Acceleration by means of graphics processing unit (GPU) is used to enhance the computational efficiency of the presented front tracking algorithm. A container filled with a commercial PCM, which has been utilized in a numerous LHTES applications, is considered in the comparison. Simulation results are also compared to experimental data. The evaluation of results shows that the front tracking algorithm allows for a significantly higher accuracy than in case of interface capturing methods. The higher accuracy of simulation tools then contributes to a more accurate design of LHTES devices and allows for their higher performance and efficiency.

1. Introduction

The minimization of the consumption of fossil fuels, their more efficient use as well as their gradual replacement with renewable and sustainable energy sources is an important strategy to reduce pollutants, CO_2 emissions, GHG content and the carbon footprint in the natural environment. An important approach in the efficient utilization of energy sources is the energy storage and, in particular, latent heat thermal energy storage (LHTES). Since experimental investigation is often expensive and time-consuming, many investigators aim at computer simulations. Computer modelling of LHTES is a heat transfer problem with phase changes and a number of studies have been published on this topic. Hansen and Kjellander (2016) investigated blast wages from boiling liquid expanding vapour explosions by means of CFD. They developed a 3D model for the investigation of pressure effects. Hübner et al. (2016) performed an analysis of the LHTES system coupled with the concentrated solar power plants. The design with finned tubes was investigated. Meddeb et al. (2009) performed a study into a heat exchanger for the processing of an industrial phosphoric acid. The authors investigated the overall heat transfer coefficient often applied as the boundary condition. In available studies, computer models of heat transfer are employed for the prediction of thermal behaviour. As accurate results are required, precise models and methods have to be used. From the numerical point of view, there are two categories of approaches: interface capturing and interface tracking methods, see (Liu et al., 2014). Interface capturing methods are very frequently utilized and these include the well-known enthalpy method and the apparent heat capacity method, see (Dutil et al., 2011). The principle of these methods is rather simple and the methods are easily implementable. The computation of models based on interface capturing is relatively fast and no additional

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treatment is required. A drawback of interface capturing methods is, however, their accuracy, especially in the vicinity of the phase interface (Liu et al., 2014). A lower accuracy means that computed values of the temperature can negatively be influenced by numerical errors. This may result in temperature fluctuations and perturbations, and therefore in inaccurate results. The second category consists of interface tracking methods. Such methods are, in comparison to interface capturing methods, much more demanding from both the mathematical and programming point of view due to the interface processing. Unlike to interface capturing where no care is paid to the phase interface, front tracking methods focus in detail to front elements, their location and movement, and balances between the phases. This is the reason why interface tracking is more precise in comparison to interface capturing but paid by higher computational costs. Li et al. (2003) reported a front tracking method which was validated by means of exact solutions available in the literature. The authors reported a high accuracy of their algorithm. Browne et al. (2004) carried out simulations of the grain growth during the solidification of an alloy. The authors reported an analysis of solidification in various grain zones. Seredynski et al. (2015) investigated the solidification of a semi-transparent material by a front tracking method. The authors reported that the solid fractions, which are often used for the identification distinct regions in a solidifying material, are not always constant. The survey of the published studies reveals that only very limited information is available about the computational demands and efficiency of front tracking methods. Numerical results of the authors indicate that front tracking methods can be very computationally demanding, especially in case of large domains and transient simulations. In the present paper, the front tracking algorithm based on algorithms presented by Udaykumar et al. (1996) and Li et al. (2003) is applied to the solution of the 2D Stefan problem. As mentioned, computational demands of front tracking method are reduced via the acceleration by means of graphics processing units and NVIDIA CUDA. Results obtained by the front tracking algorithm are compared to numerical results acquired with the use of the enthalpy and apparent heat capacity methods. Simulation results are also compared to experimentally gathered data. The exact solution to the 1D Stefan problem is utilized in the evaluation of computational accuracy. Results indicate that the GPU-accelerated front tracking algorithm represents an accurate and fast simulation method which can be used in numerical models of LHTES devices and systems.

2. Numerical solution of heat transfer with phase change – interface capturing and tracking

2.1 Interface capturing – enthalpy and apparent heat capacity methods

A feature of the interface capturing methods is that they do not track the phase interface explicitly. Their primary focus is on the temperature distribution determined from the solution of the heat transfer equation. The location of the phase interface is determined as a consequence of the temperature distribution. This feature also partially explains reasons for discrepancies, mainly in the vicinity of the phase interface. The governing heat transfer equation for phase change problems is (with the use of the Einstein notation):

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x_i}\left(k \frac{\partial T}{\partial x_i}\right) + S \tag{1}$$

where ρ is the density, c_p is the specific heat at a constant pressure, T is the temperature of the matter in the domain, t is the time of the process evolution, x_i are spatial coordinates, and k is the thermal conductivity. The internal source of heat S is a key term for interface capturing methods as it represents the latent heat. In case of the enthalpy method, the latent heat is incorporated into the source term via the thermodynamic function of volume enthalpy H which is defined as a function of the temperature as (Dutil et al., 2011):

$$H(T) = \int_{T_{ref}}^{T} \left(\rho c_p - \rho L_f \frac{\partial f_s}{\partial \omega}\right) d\omega \tag{2}$$

where T_{ref} is a reference temperature, L_f is the amount of the latent heat of the phase change, and f_s is the solid fraction which represents the ratio between the phases. The incorporation of the enthalpy defined in Eq(2) into the heat transfer Eq(1) leads to the enthalpy formulation of the heat transfer equation:

$$\frac{\partial H}{\partial t} = \frac{\partial}{\partial x_i}\left(k \frac{\partial T}{\partial x_i}\right) \tag{3}$$

which has to be solved in two steps: first for the enthalpy from which the temperature is determined in the second step. A typical enthalpy-temperature relationship for a material undergoing the phase change is shown in Figure 1. The apparent heat capacity method, often referred to as the effective heat capacity method, takes into account the latent heat of the phase change by means of an artificial increase of the physical heat capacity in the temperature range of the phase change. A function similar to the density of probability for the normal distribution is often assumed to the apparent heat capacity as shown in Figure 1, see e.g. (Dutil et al., 2011). The apparent heat capacity c_{app} is related to the enthalpy as $c_{app} = \partial H/\partial T$ and its substitution into the governing heat transfer Eq(1) leads to:

$$\rho c_{app}\frac{\partial T}{\partial t} = \frac{\partial}{\partial x_i}\left(k\frac{\partial T}{\partial x_i}\right) \qquad (4)$$

The solution of Eq(4) requires only the determination of the temperature which makes the use of the apparent heat capacity easier than in case of the enthalpy method. On the other hand, the apparent heat capacity method is rather sensitive to the size of the time step. Larger steps can lead to violation of the energy balance causing significant discrepancies in computational results as reported in the literature.

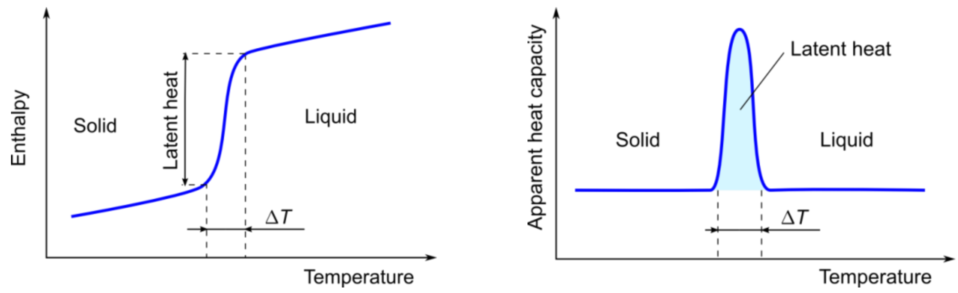


Figure 1: The schematic of the enthalpy (left) and apparent heat capacity (right) methods.

2.2 Interface tracking methods

In front tracking methods, the focus is on the explicit interface tracking. The temperature distribution is solved in the second step and according to the already-tracked front. Such approach is therefore opposite to interface capturing. This explicit approach of the interface tracking allows for higher accuracy, mainly in the vicinity of the interface. On the other hand, interface tracking algorithms are computationally more demanding. The front is tracked by means of mass-less points, so-called markers, which lie on the front and move in the domain. A suitable connection of markers forms the front. In the paper, a front tracking method is considered on the fixed grid. Basic principles of the method proposed by Udaykumar et al. (1996) and its effective modifications described by Li et al. (2003) were adopted. The method consists of three main steps: (A) advection of the markers within the domain and their reconstruction, (B) determination of velocities of the markers and (C) solution of the temperature distribution by means of the heat transfer equation. The schematic of the front tracking method is illustrated in Figure 2 where the solid-liquid phase transition is considered.

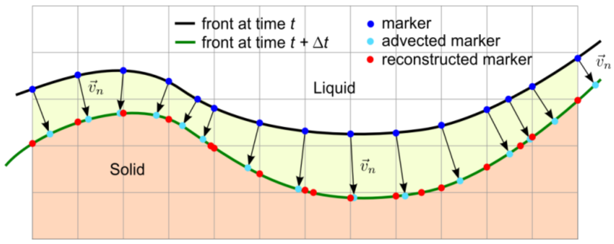


Figure 2: The schematic of the front tracking.

The velocity v_n of markers and therefore the movement of the front are driven according to the Stefan condition (Hahn and Ozisik, 2012) which expresses the energy balance at the interface as

$$k_{solid}\frac{\partial T_{solid}}{\partial n} - k_{liquid}\frac{\partial T_{liquid}}{\partial n} = \rho L_f v_n \qquad (5)$$

Once the steps (A) and (B) are completed and the new location of the front is determined, the calculation procedure of particular time iteration is finished by (C) the solution of the governing heat transfer equation given in Eq(1) with the zero-source term $S = 0$ as the latent heat is taken into account via Eq(5).

2.3 Parallel GPU acceleration of the interface tracking algorithm

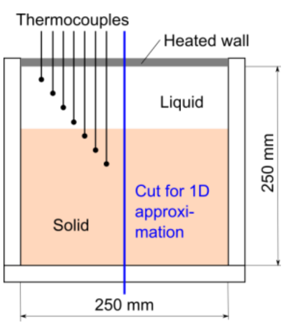
As mentioned the front tracking is computationally more demanding than interface capturing. This is caused by numerous operations required by the explicit front tracking. In particular, markers have to be handled separately, their movement and location need to be treated in cooperation with neighbouring markers and according to the temperature distribution. Some special treatment is also deserved to the front reconstruction. The solution of governing equations – the last step of the front tracking algorithm – is the only main step in interface capturing methods and it explains their relatively low computational requirements. An effort therefore was to accelerate the algorithm which would make it more applicable and efficient. Since a number of operations are independent to other entities, their concurrent processing in parallel manner is applicable. In recent years, parallel computing with the use of graphics processing units (GPUs) has been offering a huge computational performance (Owens et al., 2007). A GPU, which consists of a large number of computational units (thousands of units), is designed for massively parallel computing. NVIDIA, as one of main manufacturers of GPUs, provides the CUDA – the programming platform for the control of GPUs. A GPU performs an identical code on its computational units but with different data. The code which is designed for parallel processing is implemented in so-called kernels. The applicability of the GPU computing in heat transfer problems has already been verified; see Klimeš and Štětina (2013). The described approach of the GPU computing can thus be utilized for acceleration of the front tracking method. The following independent parts of the front tracking algorithm were implemented into kernels written in the C/CUDA language:

- identification of markers translated in the domain within one time step, determination of reconstructed markers, reconstruction of front,
- solution of the Stefan condition and determination of the velocity for individual markers,
- identification of phases in individual domain volumes, and
- solution of the governing equations in individual domain volumes.

Computational tests of the GPU-based parallel implementation of the front tracking algorithm were performed with the use of the GPU NVIDIA Tesla C2075. Benchmarking results have showed that the GPU acceleration allows for a significant reduction of the computational time: the parallel GPU algorithm is between 10-times to 30-times faster than the non-parallel algorithm (depends on configuration and other parameters). This makes the GPU-based front tracking algorithm computationally efficient and applicable in real-time use.

3. Computational accuracy – comparison of interface capturing and tracking

The accuracy of enthalpy and the apparent heat capacity methods was further compared to the front tracking method. Simulation results of a 2D problem were also compared to data acquired experimentally. However, the accuracy comparison of computational methods cannot be carried out by means of experimental data. The reason is that differences between simulated results are lower than the measurement error of quantities acquired experimentally. Due to this reason, an available 1D exact (analytical) solution was used in a proper location for the approximation and was utilized for the accuracy evaluation of computational methods. Figure 3 presents the schematic of the test case and the snapshot from the experimental investigation. The commercially available phase change material (PCM) Rubitherm RT28HC was used. Its nearly isothermal phase change temperature is 28 °C. The density is 880 kg·m^{-3} and 770 kg·m^{-3} in the solid and liquid phase, respectively, the heat capacity is 2 kJ·kg^{-1}·K^{-1} and the thermal conductivity is 0.2 W·m^{-1}·K^{-1} in both the phases. Initially, the PCM was located in a container made of the acrylic (translucent) glass at the solid state having the phase change temperature. The upper side of the container consisted of the aluminium heated wall and its temperature was maintained at the temperature of 50 °C. The ambient air was maintained at the phase change temperature providing adiabatic conditions on remaining walls. The thermocouples installed in the PCM were utilized for the measurement of temperatures and the front location was monitored by means of pictures taken by the digital camera and post-processed in the image analysis. A detailed description of the experimental setup and methods was presented by Charvát et al. (2016).



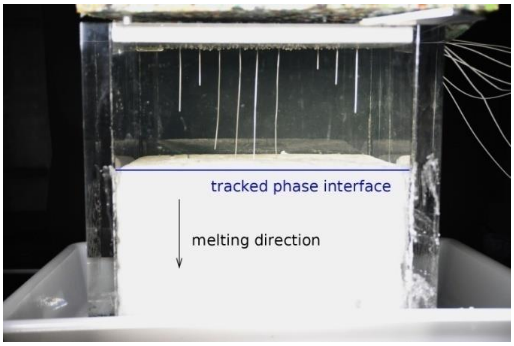


Figure 3: The investigated melting problem: the schematic (left) and the snapshot from the experiment (right).

The problem was solved by the enthalpy, apparent heat capacity and by the front tracking method. The time step of 0.1 s was applied with the explicit time discretization. The exact temperature distribution and front location in the cut shown in Figure 3 were determined by an exact 1D solution (Hahn and Ozisik, 2012). The exact temperature distribution in the liquid phase dependent on the distance from the surface x and of time is

$$T_l(x,t) = T_{boundary} + \frac{(T_{pch} - T_{boundary})}{\operatorname{erf}\lambda}\operatorname{erf}\left(\frac{x}{2\sqrt{\alpha_l t}}\right) \tag{6}$$

where λ and α_l are parameters dependent on material properties. The temperature in the solid phase remains T_{pch} and the exact location of the front is $s(t) = 2\lambda\sqrt{\alpha_l t}$. The detailed description of the exact solution and the determination of parameters λ and α_l were presented by Hahn and Ozisik (2012).
Figure 4 shows the simulated and experimental temperature distributions in the vertical cut of the PCM (see Figure 3). The front tracking and enthalpy methods provide very accurate results. The difference (the temperature error) between these two methods is undistinguishable in Figure 4. On the other hand, obvious discrepancies are seen in case of the apparent heat capacity method. One of reasons for such behaviour is its sensitivity to the dependence between the heat capacity and the temperature. The apparent heat capacity is not able to serve an isothermal phase transition and a very narrow temperature range needs to be used causing a violation of the energy conservation. Experimental temperatures measured by the thermocouple positioned in the distance of 15 mm from the heated surface are in a relatively good agreement with simulation and exact results. Discrepancies are mainly caused due to the non-constant temperature at the heated top wall; keeping the constant temperature there is rather difficult, mainly at the beginning of the experiment.

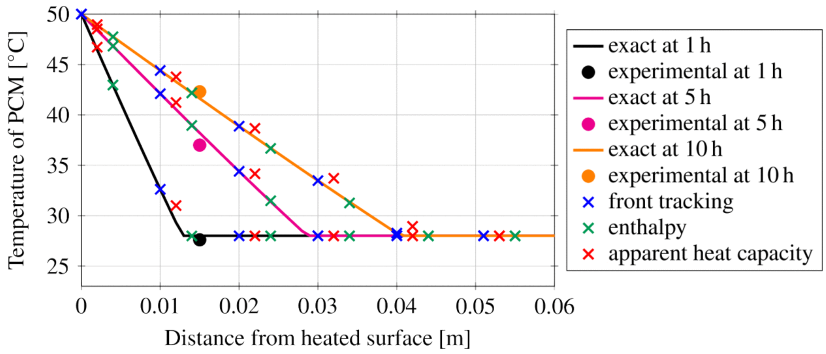


Figure 4: The simulated and experimental temperature distribution in the PCM in various time instances.

Figure 5 presents the simulated and experimentally determined front location in the vertical cut of the PCM as shown in Figure 3. Conclusions are similar to those applied to the temperature: the front tracking and enthalpy methods provide very good results indistinguishable from the exact solution. Discrepancies are evident in case of the apparent heat capacity method as well as from the experimental measurement as explained above.

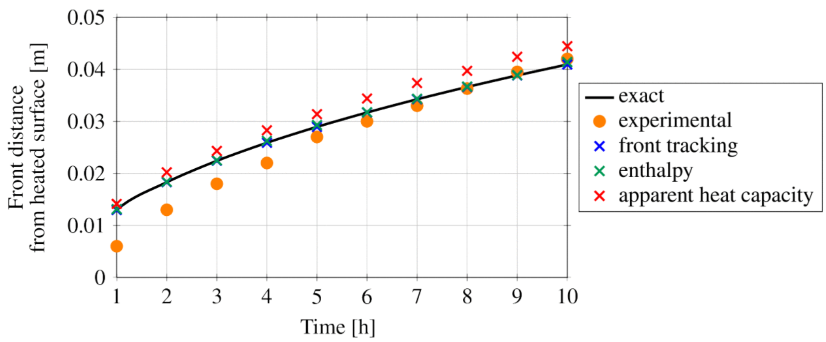


Figure 5: The simulated and experimental front location as a function of time.

Results of the accuracy analysis are presented in Table 1. As already discussed and visually observed in Figures 4 and 5, the front tracking and enthalpy methods provide very good results. However, values shown in Table 1 reveal that the front tracking method enables for about two-order higher accuracy in the determination of the temperature as well as in the determination of the front location. It is also evident from Table 1 that the apparent heat capacity method leads to significantly lower accuracy, and therefore it cannot be recommended for the solution of phase change problems with a nearly isothermal phase change temperature.

Table 1: The accuracy results and comparison of computational results with the exact solution.

	Front tracking method	Enthalpy method	Apparent heat capacity method
Mean absolute temperature error [°C]	0.00073	0.01828	0.26322
Maximum absolute temperature error [°C]	0.00895	0.29660	1.81850
Mean front location relative error [%]	0.026	0.696	8.980

4. Conclusions

The paper presents a comparison of computational methods for the solution of heat transfer problems with phase changes. A phase change material suitable for LHTES applications is considered and simulation results gained with the use of the front tracking method, enthalpy method, and the apparent heat capacity method are compared to experimental results and to an exact solution. Results show that the front tracking method, which is accelerated by means of the GPU computing approach, can provide results having higher order accuracy than the other two interface capturing methods. The GPU acceleration also allowed for a significant speed-up of the method and its real-time use. The reported benefits of the front tracking method can contribute to more efficient model-based design, operation and control of energy storage units, and thus to effective utilization of energy sources and reduction of negative impacts to natural environment.

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