A MODELLING AND SIMULATION APPROACH FOR THERMAL ENERGY STORAGE DEVICES

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Abstract:
The energy efficiency simulation of building systems requires an accurate modelling of their individual components as well as a reliable representation of the dynamic interaction between them. We present in this paper, a modelling approach for an energy storage device, following an object-oriented paradigm based on the MODELICA modelling language. The model predicts 3D fluid motion in a thermally isolated cylindrical tank as well as the temperature profile variation, of the fluid within, in respond to variable tank volume, inlet and outlet conditions. The model integration in multi-component systems is straightforward via the simulation environment OpenModelica and does not require co-simulation as it was the practice in multi-domain simulations. A simulation test of the model shows its ability to achieve reliable results in a compromise manner between computationally light 1D models and computationally heavy CFD models. It also shows that in charging a 300L storage tank with cold water, a temperature uniformity in water layers inside the tank could not be achieved before 3h which is equivalent to half of the charging cycle period. This shows that the horizontal isothermal layer division used in the traditional 1D models, shall no longer be suitable for the future energy efficiency simulations of larger more complex multi-components systems integrating storage devices as the charge/discharge cycles becomes shorter and more interactive. Hence, a modelling and simulation approach such as the one described in this paper will be useful for the future energy efficiency studies related to thermal storage systems.

Keywords:
Object Oriented Modelling, MODELICA, Energy Efficiency, Thermal Energy Storage.

1. Context

In recent years, policies to promote improved energy efficiency have been established in response to European and International regulatory obligations. Thermal energy storage has proven to be a technology that can have positive effects on the energy efficiency of a building by contributing to an increased share of renewable energy and/or reduction in energy demand or peak loads for both heating and cooling [1]. For example, the integration of a thermal energy storage device in an air conditioning application can shift the power consumption from peak periods to off-peak periods which contributes significantly in reducing the energy consumption and increasing the overall efficiency of the chilled water plant. However, such component integration have created additional challenges to design and manage the resulting more complex system, where the storage device dynamic behavior plays a significant role between the energy supply and energy demand loops. To approach these challenges, an accurate modelling of the storage component dynamic behavior is required from one hand and from the other an easy and effective way to couple it with other components and simulate their interaction simultaneously is needed in order to evaluate the energy efficiency of the resulting multi-component system. Achieving these two requirements, simultaneously, was difficult to accomplish in traditional modelling and simulation practices. From one side, 3D-CFD (Computational Fluid Dynamics) tools are used for accurate modelling of the storage devices but the resulting models require large computational resources and computing time and are limited in terms of coupling with models from different simulation domains. From the opposite side, 1D-DAE (Differential Algebraic Equation) tools use simplified 1D models of
components with much less accuracy but are powerful in coupling and simulating the global multi-component system. It was possible to combine both modelling approaches through co-simulation [2]. However, co-simulation requires that the user has sufficient knowledge with at least three separate tools: the CFD tool, the DAE tool and the co-simulation environment tool which requires from the user, different skills level and training time.

Therefore, we present in this paper, a compromised modelling and simulation approach applied to a sensible heat storage device developed via the modelling language MODELICA with an open source tool OpenModelica v1.9.4.

2. Modelling efforts review

The effort to model sensible storage water tanks began in the early 1970s with the appearance of the hot water storage applications. The first mathematical models assumed that the entire liquid in the tank have a uniform temperature which changes with time as the result of net energy addition or withdrawal during the charge and discharge processes or due to the interaction with the surroundings [3]. When the natural separation between hot and cold water inside a single container was confirmed by [4], the modelling efforts turned towards a variety of multi-layer models where the liquid in the tank is divided into several isothermal layers that allowed a better description of the water temperature separation inside the tank (better known as the stratification phenomenon). Theses multi-layer models where classified into two categories depending on the inlet temperature condition. In the first category, where the inlet temperature is allowed to vary with time, [5,6] developed a multi-layer models assuming that the flow between layers seeks its temperature level without mixing along its path, while [7] developed a viscous entrainment model that accounts for heat loss to the surroundings and the mixing effects due to the entrainment of the tank fluid by the incoming stream. In the second category, where the inlet temperature is maintained constant, simpler and more accurate models have been developed and were based on solving the one-dimensional convection-diffusion equation. This equation can be derived using an energy balance on a control volume inside the tank which represents a fluid region of uniform temperature subject to heat loss to the ambient surroundings through the tank wall and insulation. The flow was assumed one-dimensional (the velocity is uniform over the tank cross section) and the problem of mixing introduced by the inflow has been treated in different ways: [8] did not include any mixing effect, [9] used an empirically derived mixing parameter, [10] quantified mixing by averaging the temperatures of a specified number of liquid elements, [11-13] introduced an effective diffusivity factor to model the mixing.

Previous models were designed as single independent components and a connection with other components was not possible. Therefore, in order to achieve a global system dynamic energy simulation, the TRNSYS tool written in FORTRAN programing language [14] was used to allow the storage tank models integration and connection to other components to construct a general multi-component system. [15] used a numerical one-dimensional model to show how stratified chilled water behaved in thermal storage tanks. A similar one-dimensional model was derived by [16] and developed in TRNSYS as a multinode model (Type 4) to represent a residential stratified hot water storage tank. A more detailed model (Type 60) was developed by [17] to incorporate internal heat exchangers, non-uniform cross-sections and net mass flow into and out of the tank. A plug-flow tank that models a stratified storage tank with a different approach from Type 4 and 60 was developed based on [18]. It uses variable segments of fluid which allows the model to simulate a particular zone of the tank using small segments without requiring a large total number of nodes or small time steps. [16] carried out a performance study of the TRNSYS tank models with experimental data and showed that the fully mixed tank model significantly under predicts the experimentally measured energy quantities whereas the plug flow model over predicts the energy quantities so as for the multinode models. It also showed that the plug flow model is computationnally more efficient. [19] carried out an analysis to verify the ability of the TRNSYS models to reproduce the temperature field in the storage tank, so as to use one the these types in a
large solar system. The results highlighted the limits of the stratified fluid models with the multinode approach used in TRNSYS.

Furthermore, the dynamic energy simulation programs, such as TRNSYS, are procedural programs where procedures call other procedures, thereby transferring the locus of control (an executing sequence of instructions) from one procedure to another. Inside these procedures are imperative statements for algebraic equations, differential equations, difference equations and numerical solution algorithms. This syntax for formulating physical phenomena was motivated by the programming languages that were available decades ago. However, the syntax is far removed from how a physicist would describe the laws that relate physical quantities to each other. Physical systems are more conveniently modeled by (i) defining an object, (ii) exposing its boundary conditions and (iii) encapsulating inside the object mathematical constraints between the boundary conditions, the state variables and their derivatives [20]. This modeling paradigm is used in tools like Dymola [21] and OpenModelica based on the Modelica programming language and allows a better model reusability and higher abstraction levels which reduce software cost and development time. A multinode storage tank model based on that modeling paradigm was implemented in an open-source library with dynamic simulation models for building energy and control systems [22].

Many theoretical and experimental studies have been performed along these modeling practices in order to understand the transient phenomena during the charging and discharging modes in the stratified tanks, and to identify the fundamental mechanisms of stratified tank operation. For more details on these experimental studies the interested reader may refer to [23]. These studies showed that, the design of thermal energy storage systems requires the knowledge of hydrodynamic and thermal behaviour of the fluid inside the tank and that the degradation and destruction of the stratification is attributed mainly to the mixing factors such as natural convection between hot and cold layers, recirculating flow caused by vertical wall conduction, and forced convection flow in charge and discharge cycles. The effect of the first and second factors can be minimized by including insulation, while the effect of last one is not easy to control and to evaluate since one-dimensional (1D) models cannot describe the flow structure in detail within the tank. This is mainly due to: higher flow rate, complex tank structure conditions, backflow generated from mixing and propulsion, which will destroy the relatively regular stratification that cannot be adequately treated by one-dimensional computations.

With the computer science progress, powerful commercial computational fluid dynamics (CFD) packages [24,25] became available dealing with the complex 3D flows and mixing problems. Several 3D-CFD studies have recently been performed. They evaluate the effects of storage tank operating and geometrical parameters on the performance [19,26-31]. These CFD models have showed that they can accurately predict fluid motion and therefore are more adequate than 1D models, to evaluate the factors affecting the stratification. However, the accuracy of the CFD calculation results strongly depends on the assumptions, such as boundary conditions and simplification which are difficult to formulate in a modular manner. Therefore, the users should have good theoretical knowledge. Furthermore, CFD models require large computational resources and computing time (i.e. 24h of computing time to simulate 1h of real time [32]) and are limited in terms of coupling with models from different simulation domains such as electrical, mechanical, or thermo-hydraulic. Consequently, they are not applicable to evaluate the long-term thermal performance of storage tanks [33].

Hence, for a better energy efficiency evaluation of the storage systems, a need to narrow the gap between the 1D the 3D-CFD approaches revealed to be necessary [19]. In this context, some works have been done on the tank modelling itself by implementing a zonal modelling approach which consists of dividing the domain of study into zones in a compromise manner between a 1D mesh and 3D-CFD mesh [34-35]. Others work on a numerical coupling of a tank model from a CFD tool with other components from a 1D tool via co-simulation using three simulation tools simultaneously: CFD tool, 1D tool and co-simulation environment tool [36].
3. Theoretical foundation and modelling methodology

In a CFD modelling approach, the engineering applications that involve heat transfer and fluid motion, as it is the case of sensible storage applications, are described mathematically by a set of governing differential equations that represents the conservation of mass, momentum and energy. In the case of a Newtonian and incompressible fluid, these equations can be written in differential form as:

- **Conservation of mass (continuity equation):**

  \[ \nabla \cdot \mathbf{V} = 0 \]  

- **Conservation of momentum (Navier-Stokes equations):**

  \[ \frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{V} = -\frac{1}{\rho} \nabla P + \nu \nabla^2 \mathbf{V} + \mathbf{g} \beta (T - T_0) \]  

- **Conservation of energy:**

  \[ \frac{\partial T}{\partial t} + \mathbf{V} \cdot \nabla T = \frac{k}{\rho C_p} \nabla^2 T + \frac{S_r}{\rho C_p} \]  

The solution of these equations reports detailed information of the fluid-flow variables such as the velocity \( \mathbf{V} = \{ u, v, w \} \), the pressure \( P \) and the temperature \( T \). To solve the previous set of equations, a numerical method should be applied. Such method consists on discretizing the domain of study which replaces the continuous information contained in the exact solution of the differential equation, with discrete values at grid points inside that domain. By supplying appropriate boundary spatial and time conditions, we obtain a general model describing the fluid particle motion. The most redundant numerical resolution method is the Finite Volume Method (FVM) described in [37] and a methodology of resolution for the case of cylindrical coordinates can be found in [38]. In our development of the storage tank model, we focused on three essential points: a compromised way to divide the domain of study (mesh generation module), a compromised way to represent the velocity spatial components and finally, the use of a single Open source modelling and simulation tool. Therefore all the modelling work shall be developed in OpenModelica via the MODELICA language using an object-oriented paradigm to obtain a high level of abstraction and modularization [39]. The majority of the sensible storage applications use a vertical cylindrical tank. Therefore, we choose our standard domain to be a vertical cylinder specified by its height \( H \) and diameter \( D \). The cylindrical domain is divided into \( K \) layers (Fig. 1a), I circles (Fig. 1b) and J sectors (Fig. 1c) in the vertical, radial and angular directions respectively. Such division results in two types of node-centered control volumes (A and B) with different geometrical shape but with the same volume \( V_A = V_B \) and same vertical interface surface \( S_t(A, B) = S_b(A, B) \) (Fig. 1d). The nodes at the center of the control volumes form the main mesh grid.

![Fig. 1. Domain division: a) vertical, b) radial, c) angular, d) resulting control volumes](image_url)

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**Diagram Description:**
- **Vertical division**: Layers labeled from 1 to \( K \) with thickness \( \frac{H_{tank}}{K} \).
- **Radial division**: Showing radial cross-sections with radius \( R_i \) and radial thickness \( \frac{D_{tank}}{2} \).
- **Angular division**: Dividing the tank into \( J \) sectors with angular thickness \( \frac{360^\circ}{J} \).
- **Control Volumes**: Nodes at the center form the main mesh grid.
The module gives the user the possibility to work with a single vertical division as for the 1D case \{I=1, J=1\} or a fine scale mesh by modifying the \{I, J, K\} parameters. After elaborating the desired mesh, the model can calculate all the geometrical properties (Interfaces areas, distance between nodes, node heights, etc.). The fluid properties such as density, specific heat, heat transfer coefficient and others are integrated in a medium model where each property can be initialized as constant or variable depending on the desired case [39].

The calculation of the fluid temperature and the fluid flow velocities is done in another module. Discretizing the governing equations following the finite volume methodology of [37], leads to an algebraic system of equations for a single variable \(\phi\). These equations have a standard structure which can be implemented with the modelica language:

\[
a_p \phi_p = \sum_{nb} a_{nb} \phi_{nb} + \alpha^0_p \phi^0_p + S
\]  

The resolution of such a system can be obtained via the SIMPLE algorithm [37] and the coefficients can be evaluated as shown in Table 1.

For the energy equation, the variable \(\phi\) is the temperature which is evaluated at the center of the control volume where as for the momentum equations, the variable \(\phi\) is the radial\{u\}, angular\{v\} and vertical\{w\} velocity evaluated at the center of the corresponding control volume interfaces respectively.

To form the global model of the tank, all the modules are combined via hierarchical/inheritance mechanisms. In addition connector models that allow the fluid properties to be transferred from and into the tank model have been incorporated. This allows linking the model to other models with same connector configuration with a single line connection in the graphical interface of OpenModelica or via a code line.

Table 1. Coefficients of the algebraic equations

<table>
<thead>
<tr>
<th>Face (nb)</th>
<th>a</th>
<th>F</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>w (west)</td>
<td>max [F_w \left( D_n + \frac{F_w}{2} \right) ]</td>
<td>(\rho u )</td>
<td>(\frac{\Gamma_w}{\delta_{WP}} A_w)</td>
</tr>
<tr>
<td>s (south)</td>
<td>max [F_s \left( D_s + \frac{F_s}{2} \right) ]</td>
<td>(\rho u )</td>
<td>(\frac{\Gamma_s}{\delta_{SP}} A_s)</td>
</tr>
<tr>
<td>b (bottom)</td>
<td>max [-F_b \left( D_b + \frac{F_b}{2} \right) ]</td>
<td>(\rho u )</td>
<td>(\frac{\Gamma_b}{\delta_{BP}} A_b)</td>
</tr>
<tr>
<td>e (east)</td>
<td>max [-F_e \left( D_e + \frac{F_e}{2} \right) ]</td>
<td>(\rho u )</td>
<td>(\frac{\Gamma_e}{\delta_{PE}} A_e)</td>
</tr>
<tr>
<td>n (north)</td>
<td>max [-F_n \left( D_n + \frac{F_n}{2} \right) ]</td>
<td>(\rho u )</td>
<td>(\frac{\Gamma_n}{\delta_{PN}} A_n)</td>
</tr>
<tr>
<td>t (top)</td>
<td>max [-F_t \left( D_t + \frac{F_t}{2} \right) ]</td>
<td>(\rho u )</td>
<td>(\frac{\Gamma_t}{\delta_{PT}} A_t)</td>
</tr>
</tbody>
</table>

The \(a_p\) coefficient of the left term of (4) is evaluated as:

\[
a_p = \sum_{nb} a_{nb} + a^0_p + \Delta F - S_p
\]

Where:

\[
a^0_p = \frac{D^0_p \Delta V}{\Delta t}
\]

and

\[
\Delta F = F_e - F_w + F_n - F_s + F_t - F_b
\]
5. Simulation tests and results

To test the above described approach in OpenModelica, we study first a 1D case where the tank is divided into K layers. We consider the case of a cylindrical vertical tank (H=1.6 m x D=0.5m) divided into 4 horizontal layers with equivalent height and cross section area. The temperature of the fluid in the tank is initially at 40°C. A steady flow rate of 0.04 kg/s at 20°C is injected at the bottom layer (layer 1) and the same flow rate is extracted from the top layer (layer 4). The choice of the flow rate and temperature is made to be able to compare our results with those obtained in [35]. In addition, we are interested to investigate the capacity of the model to calculate the flow between the layers; we initiate the model with guessed flow values between the layers. These values are different from the injection flow value. We can evaluate the temperature of each layer by implementing the calculated velocity component of this flow in the algebraic form of (3).

![1D CFD model compared with 1D traditional model](image)

**Fig. 2. 1D CFD model compared with 1D traditional model [35]**

Fig. 2 shows a very good compatibility between our model and a traditional 1D model. Simulation results show that the model was able to correct the initial guessed values and converge them to the desired value which is the input flow value. This proves the feasibility of the CFD integration in the tool and thus, we proceed to apply the same procedure for a 3D tank division. In that case each layer contains several control volumes of type A and B. The fluid flow plays a major role in the energetic interaction between these control volumes. However, since the interface surfaces and distances between the grid points vary, the flow cannot be pre-defined and should be calculated. The calculation should also be able to adapt with the modification of the input and output location.

We first attempt to test a single layer in 2D. We choose a (I=2, J=3, K=1) grid and we define the flow injection and extraction points in radial directions.

![2D flow direction](image)

**Fig. 3. Schematic flow direction a) initial injection/extraction positions, b) flows after modification of an injection position c) flows after the modification of an extraction position**
Fig. 3a shows the flow direction at a time step obtained from the calculation of the velocity components in the momentum and continuity equations. Since we focus on presenting the flow adaptation and for the clarity of the image, the arrows are a schematic representation of the flow direction and their size does not reflect the value of the flow. We modify the injection point and the results show that the internal flows in Fig. 3b have adapted accordingly. The same goes for the flows in Fig. 3c that adapted with a modification of the extraction point. Fig 3 shows the capacity of the model to numerically adapt with the modification applied to the injection and extraction conditions. With the previous satisfactory results, a 3D case can now be tested. We consider a sensible cold water storage application with a cylindrical vertical tank (H=1.6 m x D=0.5m) with a volume of 300L. The tank is divided into a (I=2, J=3, K=4) mesh which is sufficient to represent a compromise flow motion between 3D particle motion scale used in CFD and uniform flow used in 1D. The temperature of the fluid in the tank is considered initially at 12°C. A steady flow rate of 0.04 kg/s at 6°C is injected at the bottom layer (layer 1) from the center of a radial interface of a control volume at the tank wall and the same flow rate is extracted from the equivalent control volume at the top layer (layer 4). Fig. 4a shows the center nodes of the mesh control volumes as well as the fluid flows schematic representation at the control volumes interfaces. The related temperature variation of each control volume as well as the average temperature of each layer is shown in Fig. 4b. The temperature difference between each control volume and the average temperature of the related layer is shown in Fig. 4c. For the chosen tank volume and operation conditions, Fig. 4c shows the disturbance caused by the injection flow on the average temperature evolution of the layer which leads to a major temperature difference between the regions of the same layer. It is significant at the injection layer with up to 3.4°C difference and tends to diminish for the rest of the layers. During the 6h cold fluid charging cycle, the injection layer took 3h to reach a uniform temperature, followed by 4.7h for the second layer and a longer time for the upper layers.

![Diagram](attachment:figure4.png)

*Fig. 4. a) Fluid flow between CV after 0.5h from the beginning of injection, b) CV and layer average temperature evolution, c) Temperature difference between the CV and the layer average temperature*
We move the injection position from the bottom layer (layer1) to the second layer (layer2) while maintaining the same extraction position (Fig. 5a). Fig. 5b shows that this injection/extraction scenario has raised the temperature gap between the CVs and their related layer. Also, Fig. 5c shows that the time to obtain a uniform temperature at the bottom layer (layer1) has increased from 3h to 4.3h and also from 4.7h to 5.3h for the layer above (layer 2). However, we notice that the time gap between the uniformity of the two first layers have decreased from 1.7 h (time difference between the dashed vertical line in Fig. 4c) for the first injection scenario to 0.9h (time difference between the dashed vertical line in Fig. 5c) for the second injection scenario.

From the above, we conclude that almost half of the transient operation time is not being really treated by the traditional 1D plug-flow models with their isothermal horizontal layer division. This didn’t have a major influence on the performance of the system since, in a traditional operation sequence, the discharge loop is turned off while the tank is being charged and therefore the energy evaluated was the energy available at the end of the charging cycle. However, with increased complexity and the new combination choices in the systems integrating thermal energy storage, a need to operate the charging and discharging cycles simultaneously reveal important and the evaluation of the energy efficiency of the system in that case requires to take into consideration the transient tank for shorter and more dynamic charging/discharging cycles. A better energy efficiency evaluation requires a reduction in the gap between the predicted and the real available energy in these operation cycles and thus, a need of a model such as the one developed in this work reveals to be a necessity.
6. Conclusion and perspective

A compromised modelling and simulation approach between 1D and CFD methods, applied to a storage device, was proposed. The developed model provided 3D flow profiles for the water inside the device in respect to the injection and extraction modified conditions. All the modelling and simulation effort was done via a single tool OpenModelica and did not require multiple tool implementations. The development of the model in the OpenModelica environment allows connecting it to other components available in Modelica Libraries via the use of a suitable connector. This allows the user to construct a global energetic system integrating a storage device and evaluate its energy performance without apprehending several tools in hand. A simulation for a 300L cold storage application showed the capacity of the proposed approach to integrate a CFD method into a system modelling tool which allows developing variable compromised models with different accuracy levels based on the user choice. It also shows that the 1D traditional models shall not be suitable for the future energy efficiency simulations as the layer isothermal division does not evaluate the transient energy behavior in almost half of the charging cycle. The effort to increase the energy efficiency of the recent systems integrating thermal storage devices, shall require a closer investigation on that transient energy behavior inside the storage device at a short charge/discharge cycles periods, hence the utility of the proposed modeling and simulation approach. In the future steps of this research, we are interested in building the same model with a commercially available CFD tool to be able to perform a full performance comparison, especially in terms of computational time on the same computer machine with the same simulation configurations.

Nomenclature

\(a\) convection-diffusion coefficient, kg/s
\(A\) area of the control volume interface, \(m^2\)
\(c_p\) specific heat, J/(kg K)
\(CV\) Control Volume
\(D\) diffusion coefficient, kg/s
\(F\) flow rate through the control volume face, kg/s
\(\tilde{g}\) gravitational force, N
\(P\) pressure, Pa
\(S\) general source term
\(T\) temperature, °C
\(\{u\}\) radial fluid flow velocity component, m/s
\(\{v\}\) angular fluid flow velocity component, m/s
\(\vec{V}\) fluid flow velocity vector
\(\{w\}\) vertical fluid flow velocity component, m/s

Greek symbols

\(\beta\) thermal volumetric expansion coefficient
\(\rho\) density, kg/m\(^3\)
\(\nu\) kinematic viscosity, m\(^2\)/s
\(k\) thermal conductivity, W/(m K)
\(\phi\) general dependant variable
\(\Delta t\) time step, s
\( \Delta V \)  Volume, m³
\( \Gamma \) general diffusion coefficient, kg/(m s)
\( \delta \) distance between nodes, m

**Subscripts**
- \( B \) neighbour at the bottom
- \( b \) control volume face between \( P \) and \( B \)
- \( BP \) between \( B \) and \( P \)
- \( E \) neighbour at the east side
- \( e \) control volume face between \( P \) and \( E \)
- \( N \) neighbour at the north side
- \( n \) control volume face between \( P \) and \( N \)
- \( nb \) general neighbour grid point
- \( P \) central grid point
- \( PE \) between \( P \) and \( E \)
- \( PN \) between \( P \) and \( N \)
- \( PT \) between \( P \) and \( T \)
- \( S \) neighbour at the south side
- \( s \) control volume face between \( P \) and \( S \)
- \( SP \) between \( S \) and \( P \)
- \( T \) neighbour at the top side
- \( t \) control volume face between \( P \) and \( T \)
- \( W \) neighbour at the west side
- \( w \) control volume face between \( P \) and \( W \)
- \( WP \) between \( W \) and \( P \)

** superscripts**
- \( 0 \) initial reference value

**References**


