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Natural convection characterization during melting of phase change materials: Development of a simplified front tracking method

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ABSTRACT

This study presents the development of a front tracking method for melting of phase change materials (PCMs) inside horizontal shell and tube heat exchangers. Two numerical models, i.e. pure conduction (PC) model as well as combined conduction and natural convection (CCNC) model, are used to develop the method. Governing equations are numerically solved by ANSYS Fluent v17.2. The PC model benefits from simplicity but its prediction is far from reality, whereas CCNC model's prediction is more realistic but its modeling is complicated. Generally, during the melting process, the upper half of the system is affected by the upward buoyancy-driven melted PCM motion. To consider this phenomenon, the front tracking method assumes that the upper and lower halves of the system have two separate melting fronts. Therefore, it is assumed that the natural convection contributes only to the upper half until the upper half liquid fraction value reaches unity. Meanwhile, the lower half melting front is assumed to be the same as that of the PC model. Once the upper half is totally melted, the method attributes the rest of the natural convection to the lower half of the system. Using three different PCMs and three different geometries, two correlations have been developed for each half based on two dimensionless numbers; i.e. the shell-to-tube radius ratio and PC model liquid fraction. The method is then verified using another PCM, which has not been included during the correlation development stage to guarantee the methods validity. These correlations provide results within ± 15% discrepancy range.

1. Introduction

Due to the inherent intermittency of renewable energy sources such as solar energy, thermal energy storage is required to tackle the time mismatch between energy supply and demand. Thermal energy storage can be generally classified as sensible and latent heat storages. In recent decades, latent heat storage in phase change materials (PCMs) received considerable attention (Nkwetta and Haghighat, 2014; Seddegh et al., 2017). This is due to their high latent heat capacity, which is essentially required for management of time mismatch between energy supply and demand (Mirzaei and Haghighat, 2012). Therefore, PCMs have found several applications, e.g. in ventilation systems (El-Sawi et al., 2014), refrigeration systems (Joybari et al., 2015), net zero energy buildings (Bastani and Haghighat, 2015), hot water tanks (Najafian et al., 2015), etc.

Shell and tube heat exchanges (STHXs) are used in several engineering applications particularly due to their manufacturing simplicity and economic feasibility (Seddegh et al., 2015). Agyenim et al. reviewed the materials, heat transfer and phase change problem formulation for latent heat thermal energy storage units (Agyenim et al., 2010). It was concluded that the most intensely studied unit was the shell and tube storage, accounting for about 70% of publications. Latent heat storage STHXs have found application in solar domestic hot water systems (Seddegh et al., 2015), solar thermal plants (Tehrani et al., 2016), solar collectors (Li et al., 2017), etc.

Basically, the design tools for heat exchangers could be classified in two major categories. The first category includes all the simplified methods including the well-known approaches of effectiveness-number of transfer units (ε-NTU) and logarithmic mean temperature difference (LMTD). These approaches normally oversimplify the process in PCMs and ignore some major phenomena such as natural convection. On the other hand, detailed CFD simulation of the process could lead to a design tool, which requires long computational time, is greatly complicated, and might be limited to the investigated case. However, between these two extremes, some "enhanced tools" can also be developed, which are almost as simple as the first category but provide

Abbreviations: CFD, computational fluid dynamics; *CCNC*, combined conduction and natural convection; *HTF*, heat transfer fluid; *NTU*, number of transfer units; *PC*, pure conduction; *PCM*, phase change material; *STHX*, shell and tube heat exchanger

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Nomenclature

a	correlation constant
b	correlation constant
c	correlation constant
C	mushy zone parameter (kg·m^{-3}·s^{-1})
C_p	specific heat (J·kg^{-1}·K^{-1})
D	diameter (m)
Fo	Fourier number (–)
g	gravity (m·s^{-2})
h	sensible specific enthalpy (J·kg^{-1})
H	total specific enthalpy (J·kg^{-1})
m	correlation exponent
n	correlation exponent
p	pressure (N·m^{-2})
Pr	Prandtl number (–)
r	radius (m)
R	shell-to-tube radius ratio (–)
Ra	Rayleigh number (–)
Ste	Stefan number (–)
t	time (s)
T	temperature (K)
U	dimensionless velocity (r-direction)
v	velocity (m·s^{-1})
V	dimensionless velocity (θ-direction)

Greek symbols

α	thermal diffusivity (m^2·s^{-1})
β	thermal expansion coefficient (K^{-1})
δ	small number to avoid division by zero, 0.001 (–)
γ	liquid fraction (–)
ΔH	latent specific enthalpy (J·kg^{-1})
λ	latent heat of fusion (J·kg^{-1})
μ	dynamic viscosity (kg·m^{-1}·s^{-1})
ρ	density (kg·m^{-3})
υ	kinematic viscosity (m^2·s^{-1})

Subscripts

$CCNC$	combined conduction and natural convection model
i	inner; initial; corresponding
l	liquidus
o	outer
PC	pure conduction model
ref	reference
s	solidus

Superscripts

f	final
L	lower half
mod	modified
U	upper half
$*$	dimensionless variable

acceptable results comparable to CFD.

The possible heat transfer mechanisms in PCMs are conduction, convection or a combination of both. Therefore, the simulation methods in the literature are based on the considered heat transfer mechanism: the pure conduction (PC) model and the combined conduction and natural convection (CCNC) model. Early research work considered only conduction as the dominant heat transfer mechanism during the melting and solidification processes (Seddegh et al., 2015). This is equivalent to a circular (or cylindrical in 3-D) PCM melting front shape around the heat transfer fluid (HTF) tube (Tay et al., 2012; Joybari and Haghighat, 2016). However, compared with experimental data, the PC model was reported to have very poor performance (Farid et al., 1989; Farid and Mohamed, 1987). This is due to the fact that as the PCM melts, the density changes create buoyancy forces resulting in an upward melted PCM motion (i.e. natural convection) affecting the upper half of the storage unit (Seddegh et al., 2016). Although the natural convection phenomenon has been widely reported (Al-Abidi et al., 2013; Sun et al., 2016), some simple approaches such as the well-known ε-NTU approach for heat exchanger design ignore its effect. Ignoring natural convection in the ε-NTU method resulted in the underestimation of effectiveness values during melting and solidification processes (Tay et al., 2012; Bruno, 2008; Tay et al., 2012a,b).

To account for the buoyancy effect during the melting process, effective thermal conductivity was introduced in order to have better accuracy in the ε-NTU method. Tay et al. compared the results of ε-NTU method (1-D) and CFD (3-D) with experimental data (Tay et al., 2012b). It was found that the 1-D ε-NTU could be utilized for PCM heat exchanger design instead of the complicated time-consuming 3-D CFD if the natural convection is accurately accounted by the effective thermal conductivity. It is common to develop power law effective thermal conductivity correlations as a function of Rayleigh number; i.e. $c(Ra)^n$ (Farid et al., 1989; Farid and Mohamed, 1987; Farid and Husian, 1990). Nevertheless, the main disadvantages of effective thermal conductivity are: (1) experimental data should be available *a priori* to evaluate the effective thermal conductivity; (2) derivation of effective thermal conductivity is a tedious task since several candidate thermal conductivity values should be examined to find the one that has similar heat transfer rate as that of the experimental process; (3) a constant value cannot be designated to the effective thermal conductivity of a fluid with varying temperature (Amin et al., 2014); and (4) despite all the complexity, it cannot provide information about the melting front location since it is essentially a conduction model.

During the phase change process, knowing the location of melting front is greatly important since it 1) shows what portion of the storage has gone through the phase change (also known as liquid fraction) and 2) indicates the speed of the front propagation. However, this knowledge has been proven to be hard to obtain, particularly experimentally. Calculation of liquid fraction from experimental data was formerly conducted by interruption of the process at various stages to remove the remaining solid part (Sparrow and Broadbent, 1982). However, in recent years, utilization of transparent tubes for direct visual observation (Liu and Groulx, 2014) or digital high resolution photography (Yang et al., 2016), which might include image processing (Jones et al., 2006), replaced the old technique. Due to such complexities, it is preferred to obtain liquid fraction values from numerical analysis.

In early numerical studies, front tracking was also a great challenge. The problem was the complexity of simultaneously solving the conventional energy equation for solid and liquid domains together with the energy balance at the melting front (i.e. a moving-boundary problem). However, introduction of enthalpy method significantly improved numerical studies by replacing the simultaneous solving with a single enthalpy-based energy equation for the whole domain (Voller and Prakash, 1987). Nevertheless, melting front tracking by enthalpy method is a two-step process, where first the enthalpy values are calculated and then the location of the melting front is determined from the respective temperature values (Li et al., 2003). Furthermore, as of today, the numerical analysis is still complicated and computationally intense and requires expertise to develop in-house codes or familiarity