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# Empirical equations for viscosity and specific heat capacity determination of paraffin PCM and fatty acid PCM

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**Abstract.** Phase change materials (PCM) used in thermal energy storage (TES) systems have been presented, over recent years, as one of the most effective options in energy storage. Paraffin and fatty acids are some of the most used PCM in TES systems, as they have high phase change enthalpy and in addition they do not present subcooling nor hysteresis and have proper cycling stability. The simulations and design of TES systems require the knowledge of the thermophysical properties of PCM. Thermal conductivity, viscosity, specific heat capacity (Cp) can be experimentally determined, but these are material and time consuming tasks. To avoid or to reduce them, and to have reliable data without the need of experimentation, thermal properties can be calculated by empirical equations. In this study, five different equations are given to calculate the viscosity and specific heat capacity of fatty acid PCM and paraffin PCM. Two of these equations concern, respectively, the empirical calculation of the viscosity and liquid Cp of the whole paraffin PCM family, while the other three equations presented are for the corresponding calculation of viscosity, solid Cp, liquid Cp of the whole fatty acid family of PCM. Therefore, this study summarize the work performed to obtain the main empirical equations to measure the above mentioned properties for whole fatty acid PCM family and whole paraffin PCM family. Moreover, empirical equations have been obtained to calculate these properties for other materials of these PCM groups and these empirical equations can be extrapolated for PCM with higher or lower phase change temperatures within a lower relative error 4%.

## 1. Introduction

Thermal energy storage (TES) systems use has been widely increased over recent years as a response to the energy efficiency improvement claimed by the governments [1,2]. TES systems have been applied in many fields to reach this energy efficiency enhancement: cold storage [3], domestic hot water [4], building comfort, solar power plants [5], etc. Phase change materials (PCM) are crucial to deploy the technology because the system requirements are easy to reach and the thermal performance of PCM are well known and well-controlled [6,7]. However, the properties of PCM are needed to be measured before the system design. Sometimes, during the design step these properties are difficult to measure or the designers have not access to equipment to proceed the properties evaluations. This study presents the main calculation to achieve empirical equation to predict the specific heat and viscosity of two of the most common PCM groups: fatty acids [8] and paraffin [9]. These empirical equations are useful not only to design TES systems as mention before but also to be used to calculate a number when simulation

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or modelling requires these properties. In summary, the main objective of this study is to present the main empirical equations calculated for $C_p$ and viscosity of paraffin-PCM and fatty-acid PCM.

## 2. Materials and methodology

The paraffin used in the study are RT21, RT27, and RT55, commercialized by Rubitherm, as well as n-octadecane Parafol 18–97, produced by Sasol Chemicals. Moreover, this study has used capric (decanoic acid, 98.5%, $C_{10}H_{20}O_2$), myristic (tetradecanoic acid, 98%, $C_{14}H_{28}O_2$), and stearic (octadecanoic acid, 98%, $C_{18}H_{36}O_2$) acids commercialized by Panreac, with respective melting points of 32 ºC, 54 ºC, and 66 ºC, to formulate the empirical equations presented. In addition, palmitic acid (hexadecanoic acid, 98%, $C_{16}H_{32}O_2$), with melting point of 62 ºC, was used to validate the equations.

**Viscosity analyses:** A Brookfield RST Controlled Stress rheometer was used to measure the viscosity of the materials [8]. The experimental conditions are as follows: 1 min isothermal stages, increasing the temperature 1 ºC with every isotherm. 1 ml samples were used and the measurements were performed with the RCT-50-1 cone spindle under a constant rotation speed of 1100 rpm.

**Specific heat capacity analyses:** A Mettler Toledo DSC 822e was used to perform the $C_p$ measurements. The experiments were conducted under 200 ml/min constant $N_2$ flow, using 40 ml aluminium crucibles and sample mass around 10 mg. DSC areas method was used to calculate the $C_p$ [10].

**Empirical equations development and evaluation:** The measured data have been numerically adjusted in order to find out empirical equations to calculate the viscosity and the $C_p$ at both solid and liquid states. The best fits were selected according to their R2, and to complement the statistical analysis done with the just mentioned parameters and select the best equation type, the relative errors between each equation and the measured data have also been calculated. The selected empirical equation was validated with the last PCM of each group mention at the beginning of this section. Moreover, in order to fit the best empirical equation for each PCM group, a correction factor was calculated as a function of the melting temperature.

## 3. Results

The calculated empirical equations are listed in Figure 1.a) which were used to present the graphical results. The measured values of $C_p$ and viscosity of the fatty acids under study are presented in Figure 1.b) [8]. Graphical results corroborate that the calculated values by using the empirical equation fit the measured values. Moreover, the same results are presented for the calculated empirical equation and $C_p$ and viscosity measurements for paraffin PCM in Figure 1.c) and Figure 1.d) [9].

Results show that, empirical equations have been obtained for the properties under study in order to calculate this properties for other materials of these PCM groups and these empirical equation can be extrapolated for PCM with higher or lower phase change temperatures within a lower relative error 4%.

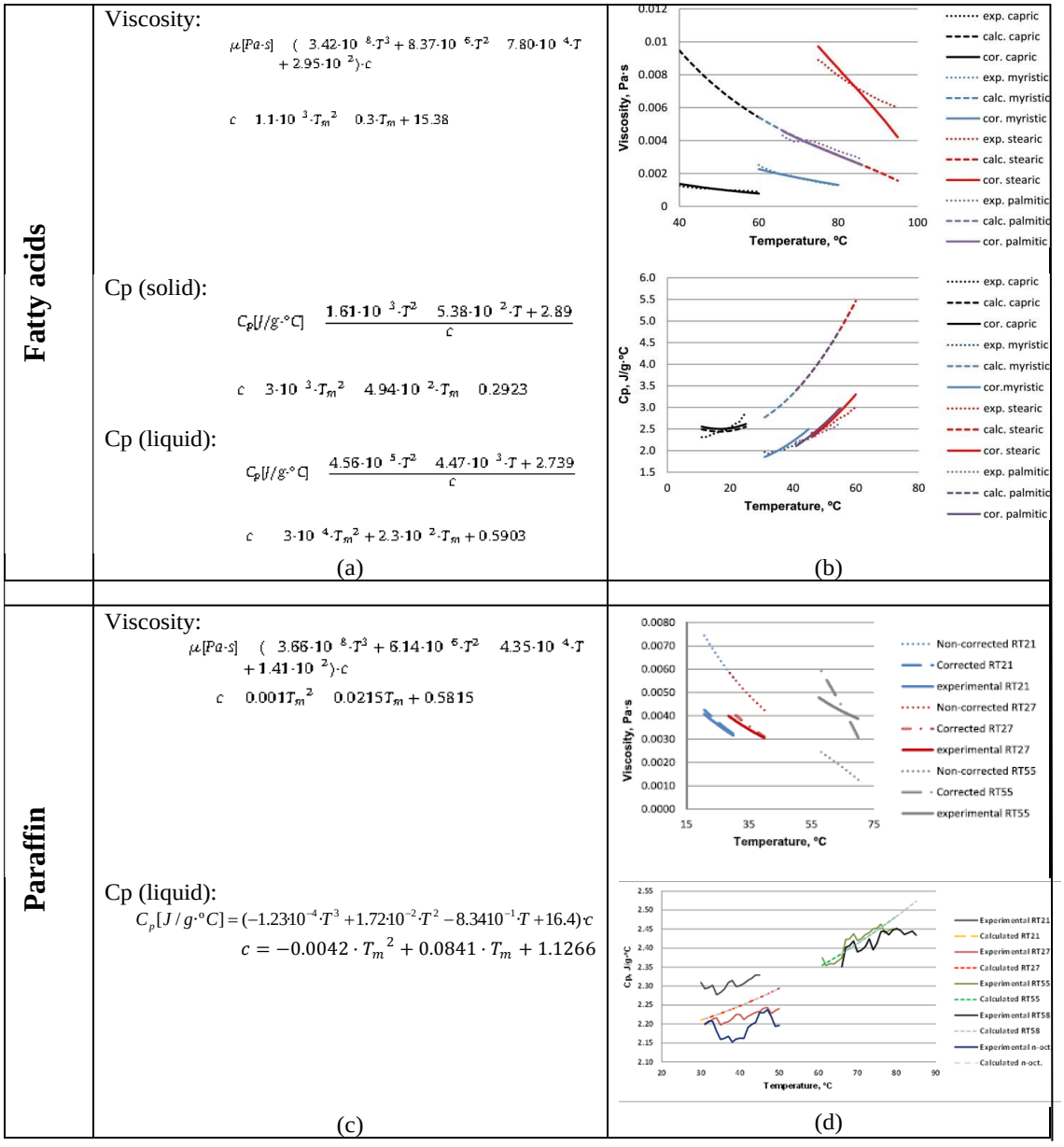


**Figure 1.** (a) Empirical equation with corrector factor for viscosity and $C_p$ of fatty acid-PCM calculations. (b) Viscosity and $C_p$ measurements of fatty acid-PCM vs. values calculated with empirical equations. (c) Empirical equation with corrector factor for viscosity and $C_p$ of paraffin-PCM calculations. (d) Viscosity and $C_p$ measurements of paraffin-PCM vs. values calculated with empirical equations. From the literature [8-10].

## 4. Conclusions.

Empirical equations to calculate the viscosity, solid $C_p$, and liquid $C_p$ of the whole fatty acid family and general polynomial 3 equation is the one that fits better for viscosity and polynomial 2 equation is the best one for $C_p$ measurements. A common polynomial 3 equation for the whole paraffin family has been calculated for viscosity values. Results in its primary form are not proper enough, thus a correction parameter as a function of the melting temperature. A general polynomial 2 equation was formulated for $C_p$ (liquid) for the whole paraffin family. Good results were obtained, with great adjustment of the

calculated values. These equations represent an important advance for simulation and system design purposes in the thermal energy storage field. These are reliable tools that provide the viscosity, solid $C_p$ and liquid $C_p$ of the materials in advance without the need of experimental runs.

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