



## Empirical equations for viscosity and specific heat capacity determination of fatty acids



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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. Saturated fatty acids are one of the most used PCM in TES systems, as they have high phase change enthalpy but in addition they do not present subcooling nor hysteresis and have proper cycling stability. The simulations and design of a TES system require the knowledge of the thermophysical properties of materials. Thermal conductivity, viscosity, specific heat capacity ( $C_p$ ) 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 determined by empirical equations. In this paper, three empirical equations are given to calculate the viscosity, solid  $C_p$ , and liquid  $C_p$  of the whole fatty acid family of PCM.

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### 1. Introduction

The increasing energy demand and the global warming are the two most important issues that researchers in the energy field have to face nowadays. The reduction of the fossil-fuel energy consumption, and therefore CO<sub>2</sub> emissions too, is the main trend in which researches are focusing their work [1,2]. As a result of the wide research lately done in the field, energy storage is presented as a potential solution to fulfil the exposed goals, as it allows overcoming the gap existing between energy demand and the supply sources [3,4]. From the different thermal energy storage (TES) systems, latent heat systems use the latent heat of phase change materials (PCM), between solid and liquid states, to store or release heat depending on the application needs, being one of the most effective and promising solutions so far. Domestic hot water (DHW) installations, building comfort and solar power plants are examples of applications in which TES systems are used. Paraffin, salts and fatty acids are the most implemented PCM [5–9] in these systems.

Fatty acids are carboxylic acids with a long aliphatic chain that have an unbranched chain of an even number of carbon atoms,

from 4 to 28. They can be saturated (no double bonds between carbon atoms) or unsaturated (one or more double bonds between carbon atoms, cis and trans configurations). Saturated fatty acids have high energy density storage capacity due to the high values of latent heat of phase change, along with a mostly stable and well defined phase temperature range, which makes them one of the most suitable and used materials in TES systems [10–12]. However, their design requires knowing other material properties such as the viscosity and the specific heat capacity ( $C_p$ ) to simulate and optimize their performance.

The estimation of properties with empirical equations is used in chemical engineering. These are material and time saving tool to know in advance the material behaviour with no need of experimental tests [13–15]. However, the TES community does not use this tool widely. As Table 1 shows, some researchers have worked in the development of empirical equations of some fatty acid properties, but results are for specific fatty acid mixtures and fatty acid by-products. Moreover, no general equation for fatty acid PCM can be found.

On the other hand, empirical equations for the determinations of viscosity, and solid and liquid  $C_p$  can be found in more general literature not related to PCM. For viscosity, Lide and Kehiaian [24] gave two different equations, one for gases (Eq. (1)) and another for liquids (Eq. (2)); Furbo [25] presented an equation for water to be

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**Table 1**  
State-of-the-art on empirical equations for fatty acid materials.

Material	Property assessed	Highlights	Reference
Fatty acid alkyl esters	$C_p$ and Viscosity	No specific conclusions on specific heat measurements and calculations	[16]
Ternary and quaternary polyunsaturated fatty acid compounds	Viscosity	The use of UNIMOD model often gives satisfactory viscosity predictions for fatty mixtures	[17]
Pure liquid organic and some inorganic compounds.	$C_p$	Review on heat capacity calorimetry methods. Classification of materials by recommended heat capacity values	[18]
Vegetable oils from fatty acid composition	Viscosity	Equation as a function of the amount of PUFA or monounsaturated FA	[19]
Hexadecanoic acid, octadecanoic acid, and cis9-octadecenoic acid.	$C_p$	A comparison between two methods applied was presented.	[20]
Fatty Acids, Triacylglycerols, and Vegetable oils.	$C_p$	Estimation for all types of vegetable oils provided the fatty acid composition.	[21]
High-chain fatty acid esters of 1-octadecanol.	$C_p$	Coefficients for polynomial equations for liquid and solid states are given.	[22]
Saturated and unsaturated fatty acid methyl ester.	$C_p$	The use of an ideal mixing rule may be of use to formulate a predictive equation	[23]

used between 10 °C–100 °C (Eq. (3)):

$$\mu [Pa \cdot s] = A(1) + A(2) \cdot T[K] + A(3) \cdot (T[K])^2 + A(4) \cdot (T[K])^3 + A(5) \cdot (T[K])^4 \quad (1)$$

$$\ln(\mu [Pa \cdot s]) = A(1) + \frac{A(2)}{A(3) - T[K]} + A(4) \cdot \ln(T[K]) \quad (2)$$

$$\mu [m^2/s] = 1.477 \cdot 10^{-6} \cdot \exp(-1.747 \cdot 10^{-2} \cdot T) \quad (3)$$

where  $\mu$  is the viscosity,  $A(n)$  are the equation constants, and  $T$  the temperature at which the viscosity wants to be known.

Regarding the specific heat capacity for solids, Lide and Kehiaian [24] proposed Eq. (4), while Smith and Van Ness [26] gave Eqs. (5) and (6):

$$C_p = A(1) + A(2) \cdot T[K] + A(3) \cdot (T[K])^2 + A(4) \cdot (T[K])^3 + A(4) \cdot (T[K])^4 \quad (4)$$

$$C_p = A(1) + A(2) \cdot T[K] + A(3) \cdot (T[K])^2 \quad (5)$$

$$C_p = A(1) + A(2) \cdot T[K] + \frac{A(3)}{(T[K])^2} \quad (6)$$

For liquids, Eq. (7) proposed by Kubaschewski [27] can be found:

$$C_p = A(1) + A(2) \cdot T[K] + \frac{A(3)}{(T[K])^2} + A(4) \cdot (T[K])^2 \quad (7)$$

The equations presented above are not specific for PCM, and in most of the cases the equation constants for fatty acids and other PCM are not provided. Consequently, disperse results are obtained with them when used with TES materials, leading in many cases to important errors in systems simulations and design.

Empirical equations play an important role in the improvement of the system design stage by providing reliable low error data, saving time and resources and conducting to better simulations and thereby, better designs. As fatty acids are one of the most used PCM families and to fill the existing lack of empirical equation for TES materials, this study presents three low error empirical equations that respectively describe the viscosity, solid  $C_p$  and liquid  $C_p$  of the whole fatty acid PCM family as a function of temperature, for use in TES systems modelling and simulation.

## 2. Materials and methods

### 2.1. Materials

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 °C, 54 °C, and 66 °C, to formulate the empirical equations presented. In addition, palmitic acid (hexadecanoic acid, 98%,  $C_{16}H_{32}O_2$ ), with melting point of 62 °C, was used to validate the equations. All of them are widely used PCM in thermal energy storage.

### 2.2. Viscosity analyses

A Brookfield RST Controlled Stress rheometer was used to measure the viscosity of the materials. The measurements consisted on consecutive 1 min isothermal stages, increasing the temperature 1 °C 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.

The viscosities of the three fatty acids were measured in liquid state, starting the measurements after the phase change was complete and the material was totally melted. Capric acid viscosity was measured between 40 °C and 60 °C, while myristic acid measurements were conducted between 60 °C and 80 °C and stearic acid viscosity was acquired in the 75 °C–95 °C temperature range. Validation measurements with palmitic acid were done from 65 °C to 85 °C.

### 2.3. 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  $\mu$ l aluminium crucibles and sample mass around 10 mg weighed in a Mettler Toledo AG135 analytical balance with a precision of 0.01 mg. The DSC areas method described by the authors in [28,29] for  $C_p$  determination was used to calculate the  $C_p$  of each material with 3% of error. This method consists on consecutive isothermal stages, as Fig. 1 shows.

Each of the peaks of the DSC signal corresponds to every temperature step of the method. The temperature difference between isotherms is of 1 °C. Integrating the peak on the DSC curve for both sapphire and material and using Eq. (8), the  $C_p$  can be determined:

$$C_{pm} = \frac{C_{ps} \cdot A_m}{A_s} \quad (8)$$

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