



WWJMRD 2017; 3(11): 40-45  
www.wwjmr.com  
International Journal  
Peer Reviewed Journal  
Refereed Journal  
Indexed Journal  
UGC Approved Journal  
Impact Factor MJIF: 4.25  
e-ISSN: 2454-6615

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## Comparing thermal resistivity between semi-crystalline and amorphous polymers

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### Abstract

The aim of this work is to determine the heat transfer in semicrystalline and amorphous polymers. The method is based on ASTM 5334 using a dual needle sensor. The thermal resistivity will be determined due to its reliability in the used technique. The polymers studied were polycarbonate, polypropylene and polyoxymethylene. The obtained results indicated that the semicrystalline polymers have a lower thermal resistivity than the amorphous polymers. Essentially, it was because of the vibrations of the phonons and distance between energy atomic levels. The efficiency was larger in semi-crystalline lattice, especially for polymers which had few attached side functional groups. Other important factors contributing to improved heat transfer were the amount of material around the sensor and the orientation of the flow when the polymer is flowing during extrusion process. Eventually, the method was found efficient and robust, and contributed to increase in depth the knowledge of polymers in this field of research.

**Keywords:** thermal properties, crystallinity, amorphous, thermal diffusivity, thermal conductivity

### Introduction

Commonly used plastics, such as polypropylene (PP) or polyamide (PA) are electrical insulators with a low thermal conductivity. Whilst thermal conductivity measurements on metals date back at least to the late eighteenth century, it was not until 1898 that a quantitative method for studying poor conductors or thermally insulating materials was developed by Lees<sup>[1]</sup>.

Current research work is focused on thermal resistivity ( $R$ ,  $\rho$ ) more than commonly used thermal conductivity ( $\lambda$ ) measurement due to the heat-insulating capacity of the polymer material. In addition, thermal resistivity measurements according to the application of the material, these are in common use in the construction and textile industries. The construction industry makes use of units such as the R-value (resistance) and the U-value (transmittance). Although related to the thermal conductivity of a material used in an insulation product, R- and U-values are dependent on the thickness of the product.

Likewise the textile industry has several units including the *tog* and the *clo* which express thermal resistance of a material in a way analogous to the R-values used in the construction industry.

Hence, since decades the polymer materials have been characterized by a low thermal conductivity, or in others words a high thermal resistivity. Currently, it is known that low heat transfer of the polymers is because of the large distance between the valence layer and the energy conduction layer. Summarizing this evidence, it is the distance which the atoms should cross so that the energy be transferred between them; i.e. along to the molecular structure. To understand how the atoms are working on the heat transfer, it is explained that each isolated atom has electron orbitals named as energetic levels (e.g. s, p, d, f...). These energy levels are well defined and they are occupied by electrons according to their quantum numbers. In general, these atoms are forming the material they are organized in a mixture of orbitals or layers. The atoms in these layers are organized from lesser to higher energy. Furthermore, note that highest energy level containing electrons is known as the valence layer. On the other hand, lowest energy level which does not contain electrons is called the

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conduction layer. Consequently, heat transfer occurs when the electrons of the valence layer cross up to the conduction layer, then the material is able to transfer a heat flow. Whereas, if the space between the two layers is wide enough and the electrons are not able to cross between levels, the material will have insulate properties. Polymers are a very good example of these properties.

Although their insulated heat transfer they offer substantial number of advantages. Primarily, using polymers may decrease cost, volume and weight of the device. Other useful properties include flexibility, resistance to fouling and corrosion and the ease with which they can be tailored to application needs [2]. Enhancing thermal conductivity of polymers has been a huge challenge for a certain time which is why robust understanding of mechanism of heat transfer in polymers is desired.

Heat transfer takes place when thermal energy is exchanged between two physical objects. Thermal energy can be defined as a sum of kinetic energy of atomic motions and potential energy of distortion of interatomic bonds [3]. Heat is transferred from high to low temperature areas of the material and can occur in three different modes: conduction, convection and radiation. Conduction is a result of interactions between electrons, vibrating atoms and molecules. Transferring heat by conduction requires direct contact and occurs in all phases of matter. Convection takes place when a mass of liquid or gas is transported due to density differences or under the influence of external force. Heat transfer by radiation takes place when the body (solid or fluid) is emitting electromagnetic waves as a consequence of its temperature [4] [5]. The main focus on this research is put on heat transfer in solid state polymers by means of conduction mode.

Ability of the material to conduct heat can be described by thermal conductivity  $\lambda$ , which is a coefficient in the Fourier's law. The unit of thermal conductivity is  $\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ .

$$q = -\lambda \frac{\partial T}{\partial x} \quad (1)$$

Where  $q$  is the heat flux i.e. the amount of thermal energy transferred through a unit of area per unit of time,  $\lambda$  is the thermal conductivity in  $\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ , and  $\partial T/\partial x$  the thermal gradient.

In physics, thermal conductivity is the property of a material's ability to conduct heat. It appears primarily in Fourier's Law for heat conduction. Thermal conductivity or its inverse thermal resistivity predicts the rate of energy loss or not release (in watts, W) through a piece of material. In the window building industry "thermal conductivity" is expressed as the U-Factor, which measures the rate of heat transfer and tells you how well the window insulates. Therefore, the lower the U-factor, the better the window insulates.

Thermal conductivity is temperature dependent. Other factors that may influence thermal conductivity include pressure, chemical phase, thermal anisotropy, density, magnetic field, morphology, orientation, additives, impurities, and moisture [6] [7].

A physical property that characterizes unsteady state heat conduction is called thermal diffusivity  $\alpha$ . It describes the ability of a material to transmit a thermal disturbance [8]. In other words, it describes how quickly the heat is propagated

in the material during temperature change. Thermal diffusivity is simply related to thermal conductivity by Equation 2. The unit of thermal diffusivity is  $\text{mm}^2\cdot\text{s}^{-1}$ .

$$\alpha = \frac{R}{\rho \cdot C_p}; R = \frac{1}{\lambda} \quad (2)$$

Where  $\alpha$  is the thermal diffusivity,  $\rho$  is the density of the specimen, and  $C_p$  is the specific heat capacity i.e. the amount of energy needed to increase the temperature of one kg of mass by 1 °K. Eventually,  $R$  (rho) is the thermal resistivity.

Heat is transferred by electrons and phonons (waves of lattice displacement). Since polymers are non-metallic substances with no free electrons the heat transfer occurs mainly due to lattice vibrations [3]. Debye described the relationship between thermal conductivity and lattice oscillations by Equation 3 [9].

$$\lambda = K \cdot \rho \cdot C_p \cdot v \cdot l \quad (3)$$

Where  $K$  is a dimensionless constant around 0.33,  $v$  is the transfer speed for elastic oscillations i.e. the sound speed within the mass material, and  $l$  is the free length of elastic oscillations i.e. the atomic distance for amorphous thermoplastic region.

According to Equation 3, factors that influence thermal conductivity of a polymer are type and strength of the bonds located in the direction of heat transfer.

Besides of these equations, also to calculate the thermal resistivity (R) value the Equation 4 by IEEE 442 is suggested such as follows;

$$R = 4\pi \frac{(T_2 - T_1)}{\left[2.303q \cdot \log\left(\frac{t_2}{t_1}\right)\right]} \quad (4)$$

Where  $T_1$  is the temperature measured at some arbitrary elapsed time,  $T_2$  is the temperature measured at another arbitrary elapsed time,  $q$  is the heat flux dissipated per unit of length,  $t_1$  is the elapsed time at which a temperature measurement was recorded and  $t_2$  is the elapsed time at which another temperature measurement was recorded. The analytical model (Eq. 4) used to calculate thermal resistivity was derived assuming that a line heat source of infinite length dissipates heat in an infinite medium.

The goal of this study was to determine the influence of chemical structure and morphology of different polymers on heat transfer, as well as to assess how the dimensions of the sample have influence on the thermal resistivity value of the polymer. This will increase the knowledge of heat transfer mechanisms in polymers.

## Materials and methods

Samples required to carry out the research work were two semi-crystalline polymers and one amorphous polymer as follow;

### Polycarbonate

Polycarbonate Tecanat (PC) is a transparent, thermoplastic polymer. It can be characterized with high stiffness and high impact-resistance. Polycarbonate is amorphous under normal processing conditions. The literature value of thermal resistivity at 23 °C falls into range from 5.26 to 4.54

$m \cdot K \cdot W^{-1}$  and thermal diffusivity at  $25^\circ C$  equals  $0.14 \text{ mm}^2 \cdot s^{-1}$  [10].

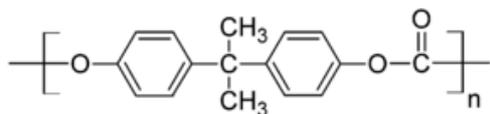


Fig. 1: Chemical structure of polycarbonate

### Polypropylene

Polypropylene Moplen HP556E (PP) is a thermoplastic polymer with a regular and flexible structure which favors crystallization. Most of commercial polypropylene have intermediate degree of crystallinity. The literature value of thermal conductivity at  $23^\circ C$  falls into range from 10 to  $4.54 \text{ m} \cdot K \cdot W^{-1}$  [11] and thermal diffusivity at  $25^\circ C$  equals  $0.096 \text{ mm}^2 \cdot s^{-1}$  [12].

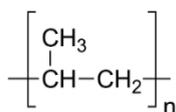


Fig. 2: Chemical structure of polypropylene

### Polyoxymethylene

Polyoxymethylene or polyacetal Resal Yuncon M25 (POM) is a rigid, hard, thermoplastic polymer. The white color of the material comes from high level of crystallinity. The literature value of thermal conductivity at  $23^\circ C$  falls into range from 4.54 to  $4.16 \text{ m} \cdot K \cdot W^{-1}$  for homopolymer, and from 4.35 to  $3.33 \text{ m} \cdot K \cdot W^{-1}$  for copolymer [13]. Thermal diffusivity equals  $0.18 \text{ mm}^2 \cdot s^{-1}$  [14].

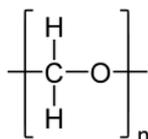


Fig. 3: Chemical structure of polyoxymethylene

The methodology used in this research was based on the transient method of the hot wire. The framework of the method is based on the fact that the temperature of a thin hot wire rises exponentially when a constant power (heat flow) is applied while it is drawn in the center of a sample of infinite length. This allows calculating the thermal conductivity of the material based on the heat flow (power and intensity), the characteristics of the heating wire (length, radius and resistance) and the increase of temperature in the wire in a certain time [15].

ASTM D5334 and IEEE 442 gather and improve this technique. Both American's standard D5334 and IEEE 442 are applicable for all type of specimens, yet this test method is suitable only for isotropic materials, usually [16] [17]. This test method is applicable to dry materials over a wide temperature range from below 0 to more than  $100^\circ C$ , depending on the suitability of the thermal needle probe construction to temperature extremes. This method may also be used for specimens containing moisture. However, care must be taken to prevent significant error from the redistribution of water due to thermal gradients resulting from heating of the needle probe, and the phase change (melting) in specimens with temperatures higher their

melting point. Both of these errors can be minimized by adding less total heat to the specimen either through minimizing power applied to the needle probe and/or minimizing the heating duration of the measurement [16] [17]. In order to obtain a reliable thermal dataset, a simple laboratory methodology needs to be adapted and depicted, according to existing standards and owing to neither the manufacturer nor the standard present whatever methodology to investigate on polymers. The present work describes the first step towards the development of a laboratory procedure to obtain reliable, accurate and rapid thermal properties dataset in polymers, taking into account the current accepted standard [18] is based on.

The measurements were taken using dual-needle sensor, and measurements were collected through reader-logger. The dimensions of the sensor are; 1.3 mm diameter, 3 cm long and 6 mm spacing between the two needles. SH-1 thermal sensor measures the three thermal properties by employing the dual needle heat pulse method (DNHP).

For each type of polymer 8 samples with different dimensions were measured (Table 1). Data was collected with two different heat flow directions; these depended on sensor orientation, which was in regard to the direction of polymer flow during extrusion, i.e. perpendicular to the direction of polymer flow during extrusion and parallel to the direction of polymer flow during extrusion (Figure 4).

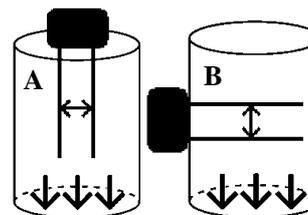


Fig. 4: Samples set up, heat flow measurement and sensor location. Arrows indicate the polymer flow direction. A = perpendicular; B = parallel.

All measurements were carried out at room temperature, around  $25^\circ C$ . Five measurements were taken for each sample. The read time was set for 2 minutes and the interval between successive measurements was 45 minutes. The reader logger was used in high power mode to gather all the data. Two different dual-needle sensors were used to take measurements, thus the sensors reliability and accuracy were verified as well.

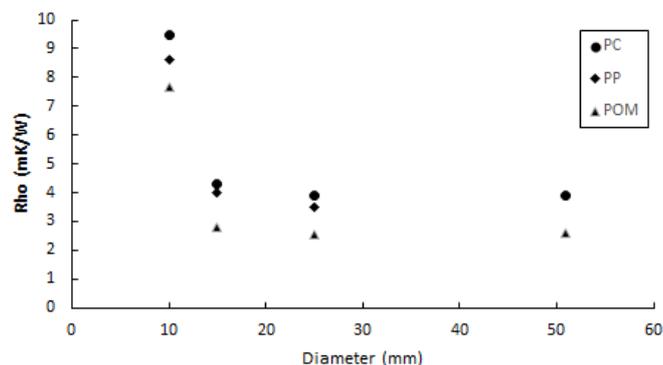
Table 1: Sampling design for the three polymers used. PC=polycarbonate; PP= polypropylene, and POM=polyoxymethylene

Sample	Perpendicular		Parallel	
	Height	Diameter	Height	Diameter
	(mm)			
PC		25	25	
	35	15	15	50
		10	10	
	40	51	40	51
PP		25	25	
	35	15	15	50
		10	10	
	40	51	40	51
POM		25	25	
	35	15	15	50
		10	10	
	40	51	40	51

## Results & Discussion

Thermal resistivity showed tendency to increase with decreasing height (heat flow parallel to the direction of polymer flow during extrusion) or diameter (heat flow perpendicular to the direction of polymer flow during extrusion) of the sample. Samples with the smallest diameter or the smallest height exhibit major rise in their thermal resistivity value. The reason of this behavior is probably due to the heat escaping from polymer samples. The amount of ambient material around the sensors was too small which allowed the heat to escape easily outside polymeric sample. It provided an anomalous behavior of the heat transfer inside the sample. Neither both standards nor manufacturer guide are not clear about the quantity of material in terms of polymer materials which must be allowed parallel to the sensor in all directions because the sensor emits heat pulses, otherwise the error will occur.

When the direction of heat flow was perpendicular (Figure 5) the values of thermal resistivity for the samples with dimensions; 35 mm high, 25 mm diameter and 40 mm high, 51 mm diameter were similar but the smaller (35 mm high, 25 mm diameter) showed slightly lower values. The difference might be owing to different initial temperatures prior to thermal measurements. Polycarbonate samples with above-mentioned dimensions exhibited the biggest difference in thermal resistivity. The initial temperatures of both samples were practically the same; therefore a possible explanation might be the use of different sensors, with a non-accurate calibration.



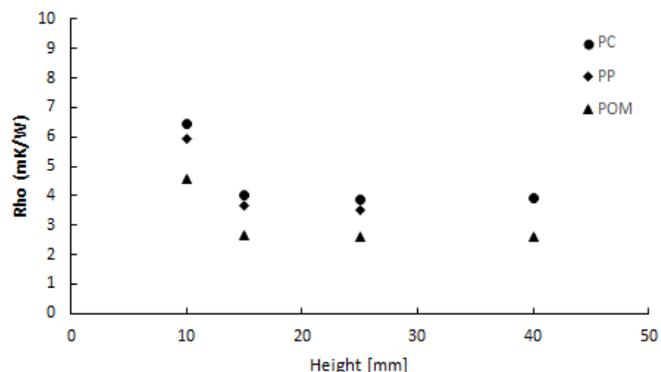
**Fig. 5:** Relationship between thermal resistivity and diameter samples on polymer flow perpendicular direction. Height = 35 mm.

When the direction of heat flow was parallel (Figure 6) the values of thermal resistivity for the samples with dimensions; 25 mm high, 50 mm diameter and 40 mm high, 51 mm diameter were similar, as well. Heat transfer behavior on the whole of the samples was exactly equal, i.e. decreasing the R value when the height increased.

Comparing values of thermal resistivity for the samples with biggest dimensions in different directions of heat flow, observed that generally values were very similar but in the direction perpendicular to the direction of polymer flow during extrusion, values of thermal resistivity were few higher. Minor resistivity values might be attributed to the fact that during extrusion polymer chains were partially aligned in the direction of polymer flow because of the tensile stress which was created during forcing polymer through a nozzle [19]. The orientation of polymer chains provided an increase of thermal diffusivity, i.e. an increase of heat transfer through the sample in the direction of polymer flow during extrusion because longer phonon

meant free paths were provided parallel to the direction of chain alignment. Strong covalent bonds along polymer chains transport heat more efficiency than physical interactions (as van der Waals force for instance) perpendicular to the backbone.

Comparing different polymer samples, the highest values of resistivity were obtained for polycarbonate samples and the lowest for polyoxymethylene samples. Probably the most important factor which influences heat transport is degree of crystallinity. The value of thermal diffusivity increased with increasing degree of crystallinity, thus thermal resistivity value decreased. Disorder and lack of regularity increases the effectiveness of phonon scattering in heat transfer mechanism and thus increases heat resistance; i.e. the material becomes more insulating.



**Fig. 6:** Relationship between thermal resistivity and diameter samples on polymer flow parallel direction. Diameter = 50 mm.

Polycarbonate is amorphous and has a high-disorder structure which leads to higher thermal resistivity and lower thermal diffusivity than obtained for highly-crystalline polyoxymethylene. Polypropylene usually has intermediate degree of crystallinity which is why its values of thermal resistivity were in between of those measured for polycarbonate and polyoxymethylene (Figure 5 and 6). Another factor that might influence heat transport mechanism in studied samples was the size of side groups grafted to polymer backbone. The bigger the size of functional groups, the bigger the disorder therefore thermal resistivity increases. For instance, methyl ( $\text{CH}_3$ ) groups attached to polypropylene main chain increase the disorder and increase thermal resistivity compared to polyoxymethylene backbone with no side groups.

However, obtained values of thermal resistivity for all polymers by both standards slightly differ from the values found in literature and these are higher. Nonetheless, authors such as Radhakrishnan et al. and Karger-Kocsis found the same thermal resistivity values in polypropylene filled with silica [20]. The reason might be the use of different method to calculate thermal properties on polymers. Furthermore, the morphology of the samples used in literature was not defined, and this could be a crucial point on these values.

Moreover, crystallinity has a great impact on heat conduction. Thermal properties, especially thermal diffusivity depends on the degree of crystallinity. Amorphous polymers with high-disorder have higher thermal resistivity than crystalline ones because disorder and lack of regularity increases the effectiveness of phonon scattering [14]. Hence, increasing crystallinity increases the heat transfer as occurs in the study samples, where a

controlled cooling process of the polymer provides better crystal formation and orientation <sup>[20] [21]</sup>.

Mostly important are the morphological and basic molecular properties of the polymers. Strong covalent bonds forces between chain atoms that build polymer chains transport heat more effectively than physical interactions between chains, such as the van der Waals force. Thus, thermal resistivity is lower along the polymer backbone than perpendicular to it <sup>[22] [23]</sup>.

Consequently, orientation of polymer chains caused for example by stretching of the material increases heat conductivity in the direction of chain alignment. Thermal resistivity is lower parallel to stretching direction than perpendicular to it <sup>[22]</sup>. More extended chain morphology results in lower thermal resistivity because it provides longer phonon, therefore it means free paths <sup>[24]</sup>. Defects in polymer structure such as chain ends, entanglements, random orientation, voids and impurities act as stress concentration points and phonon scattering centers <sup>[25]</sup>. Rod-like polymers that are characterized with great stiffness of polymer chains exhibit decrease in thermal resistivity due to tendency for crystallization and therefore chain orientation <sup>[26] [27]</sup>. Hence, exists purely geometrical effect is self-evident. Although, it strictly applies in the case of a perfectly homogeneous distribution of identical tie molecules <sup>[22] [23]</sup>.

As reported before, other factors that can influence the order of polymer structure and thus heat flux transfer are amount and size of the groups grafted the main chain of polymer. The effect caused by the inhomogeneity of the micromorphology of the semicrystalline layers sample must be understood as folded-chain blocks are not perfectly equal in length, width and orientation. The same applies to the amorphous layer sandwiched between the blocks and to the number, length, and lateral displacement of the fixed ends of tie molecules. Moreover, the non-uniform distribution of tie molecules among the amorphous layers and within every single layer causes a wide variation in the cross section area per molecule and hence in heat flux transfer, even if the tie molecules are of identical length <sup>[22] [28]</sup>. Therefore, the rule to drive the heat transfer would be applied to the amount and size of the functional groups. Hence, increasing number of different groups placed along polymer chain as well as branching reduces regularity of the structure and decreases the quantity of heat transferred <sup>[29]</sup>.

## Conclusions

In summary, both chemical structure and morphology of the sample have had a great impact on thermal properties. Probably, the most decisive factor has been a degree of crystallinity of the sample. Hence, higher degrees of crystallinity have determined lower values of thermal resistivity.

In addition, one of the variables that has presented greater relevance on the thermal properties of the material has been the dimension of the sample. The amount of material as ambient boundary conditions around the sensor has shown that it cannot be small; otherwise, an error may occur and the measured values may be distorted. This implies that the value of the thermal resistivity (R) has shown a clear tendency to decrease when the diameter or height of the sample increases. Therefore, the samples with larger diameter or height have had lower thermal resistivity

values, especially since the heat does not escape outside the sample.

Finally, Dual thermal needle probe test used in this study has been found to be a fast and efficient method to obtain thermal resistivity values in particular and thermal properties of polymer materials in general. Although the study of the thermal properties of different polymer samples with different dimensions has allowed to complement the investigations on the mechanism of transfer of heat in polymers, however, additional investigations still have to be done that allow us to understand in a more extensive and detailed way this aspect in the field of polymer science.

## Acknowledgments

The authors thank to the ACCIO Program from Government of Generalitat of Catalonia to grant this research project. Also, authors appreciate the Advanced Technology Centre Eurecat Foundation for its support in this research.

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