Algerian Journal of Chemical Engineering

ISSN: 2773-3068

Journal homepage: http://www.ajce.periodikos.com.br/

Original Article

Platform for studying properties of blend systems

Latifa Bouzid[a]*, Fatma Zohra Fouddad[a], Said Hiadsi[a]

[a]*Laboratory of Electronic Microscopy and Materials Science, Physics Department-Faculty of Science USTO.*

BP. 1505 El M'Naouar, 31100 Oran, Algeria.

ARTICLE INFO

Article history:
Received 22 March 2021
Revised 03 May 2021
Accepted 20 May 2021

Keywords:
Java;
Polymer blend;
Miscibility;
Tg;
Specific volume;
DAEM.

ABSTRACT

In this work, JAVA and MATLAB languages were used to coding a platform that is capable to study different physical properties of polymer blends such as thermal properties (glass transition temperature Tg and simulation for pyrolysis process...), miscibility (by using interaction parameter) …etc. The Flory-Huggins interaction parameter χ is an important value to reflect the miscibility of polymer. If it is negative or very small, the two compounds prefer to mix. Else, the constituents prefer to phase separate (immiscibility). In this paper, the interaction parameter was calculated by using the solubility parameter. Furthermore, the glass transition temperature Tg can be also an important element to predict miscibility of polymer blends, whereas for a miscible system one single Tg take place. Our software permits also to pick up glass transition temperature Tg from the curve of specific volume versus temperature. In addition, our software is capable to study the pyrolysis process after the experimental work by using the distributed activation energy Model (DAEM) with just three heating rates. The software contained a help and special puzzle and other elements.

1. Introduction

The study of the pyrolysis method of materials by non-isothermal thermogravimetric analysis (TGA) was usually known. [1-5] Comparing with other methods, pyrolysis represents more beneficial points. [6] There is lot of model to find the kinetics of pyrolysis, whereas and in this study, the Distributed Activation Energy Model (DAEM) has been used. [7] Due to the important roles of temperature, the properties differ. In fact, glass transition temperature (Tg) of polymers is usually considered by isobaric condition. Since the 1950's, different theories about the Tg were first developed by Fox & Flory. [8]

A polymer blend is a mixture of minimum two polymers to get a new system with different physical properties that can be not found in one single polymer of them. [9] Molecular mechanics (MM) can study lot of polymer blend properties. Also, the MM can help researchers to study the molecular structure and their properties. The simulations have all pursued two different points: the study of miscibility and/or the miscible system properties. [10]

In the nature, it is difficult to find a miscible polymer blend. Instead of lose time and money in experimental work to research a new miscible polymer system; it is preferred to use the simulation to make things easier. For this purpose, we thought to code our own plate-form that is capable to simulate the miscibility of polymer blends by applying different ways.

In this paper, JAVA was used to create software that is capable to obtain glass transition temperature (Tg) of polymer system by using the curve of specific volume *versus* temperature. The glass transition temperature can be a good factor to study the miscibility of a blend system. Whereas, in the case of miscible polymer blend, one single glass transition temperature can take place. If the polymer system contains two different glass transition temperature flanked between those of constituents, the studied bled is immiscible. [11]

In addition, and with another way, our code can simulate

* *Corresponding author.* L. Bouzid
E-mail address: malek_latifa@yahoo.fr

Peer review under responsibility of University of Echahid Hamma Lakhdar.
http://dx.doi.org/10.5281/zenodo.4776593

the miscibility of polymer blends by using the solubility parameter δ. Mason proves that if two different polymers have the same value of solubility parameter, they will be miscible. [12] Furthermore, the interaction parameter χ_{FH} is used to confirm the miscibility of the blends.
The theory of Fox is used also in our Software to calculate the glass transition temperature Tg with another method.
In order to improve our work, a code programmed in MATLAB is added in our platform to study the pyrolysis process after an experimental work by using the modified Distributed activation energy Model (DAEM) with just three heating rates. To verify the credibility of our Software, the miscibility of different polymer systems (P3HT:PCBM, P3HT:CNPh-PPV and PMMA:PS) was simulated and compared with other results found in previous works.
A lot of works improved that the use of simulation is practical in the study of the different properties of materials. [13-18], including headings where appropriate.

2. Simulation Methods

Glass transition temperature Tg of a polymer system is an important value which verifies the miscibility of elements. Miscible blends gives one single Tg between the Tgs of the constituents, where immiscible polymer blends represent two different glass transition temperatures (Tgs) between those of the compounds. [19]

The glass transition temperature can be obtained from the curve of the specific volume versus temperature. The specific volume for each temperature is simulated by using Materials Studio 6.0 software package of Accelrys, Inc. [20]
Because of the great volume of polymer chain, the molecular mechanic (MM) and molecular dynamic (MD) are used in the computer simulation. The two methods (MM and MD) are based on the applied of a force field. The used force field has a great effect on the obtained results. In the tests of the present paper, COMPASS has chosen as a force field.

In this work, the polymers studied as a test were embedded in a cell with periodic boundary conditions. Then a minimization is applied with 20000 iterations to eliminate all indesirable energies and to ensure the stability of our structure. A series of dynamics with the ensemble NVT and NPT were applied on our polymer chains for 100 ps for each blend, with a step of 1 fs by using the Verlet–leapfrog algorithm. [11, 14]

The obtained specific volume for each temperature in the studied structure is used by our Software to plot the curve of specific volume versus temperature to pick-up the glass transition temperature Tg.
In addition, the glass transition temperature Tg of polymer system can be also calculated in our plate-form by using the theory of Fox by the relation:

$$\frac{1}{T_g} = \frac{X_A}{T_{g_A}} + \frac{X_B}{T_{g_B}} \qquad (1$$

Where:
X_A, X_B : volume fraction
Tg_A, Tg_B : Tg of polymers A and B.

The solubility parameter δ is an essential element in the study of miscibility of polymer blends. First, it was employed for polymer/solvent systems. Thereafter, the approached for polymer/polymer systems was developed by Bohn [21]. The solubility parameter δ can be obtained by using the following relations:

$$\delta = \sqrt{\frac{E_{coh}}{v}} = \sqrt{\frac{(E_s - E_b)*C}{V_c}} = \sqrt{CED} \qquad (2$$

Where:
CED : the Cohesive Energy Density
E_s : is the single chain energy
E_b : is the energy of the same chain in periodic system
V_c : the volume of the cell in cubic angstrom.
C : is the unit conversion factor. [22]

If two different polymers have not similar values of solubility parameter δ, we say that they are immiscible. In the case where the polymers have the same value of solubility parameter δ, they are miscible. [23] The solubility parameter δ can be employed to find the interaction parameter χ by applying the mathematical formula [19]:

$$\chi_{\mathrm{FH}} = \mathrm{V_{seg}} \cdot \frac{(\delta_1 - \delta_2)^2}{RT} \qquad (3$$

Where:
V_{seg} : the volume taken to be close to the molar volume of the smallest unite between the two constituents.
δ_1 , δ_2 : the solubility parameters for the two polymers.

To study the thermal properties of an element, the nonisothermal thermogravimetric procedure can be used. In our plate-form the number of heating rate is limited by three for each sample. The user is free to choose the heating rate because it is not fixe in the code. This last helps to find the very proper kinetic parameters of material pyrolysis by using the modified distributed activation energy model (DAEM) [17]. The method used in our plate-form is based on the modification of the classic DAEM procedure to obtain both of activation energy (E_a) and frequency factor (k_0).

3. Software

Fig.1 shows the interface of our software with different buttons and menu bar.

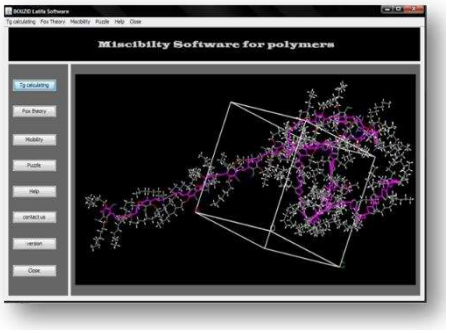

Fig 1. The interface of our software.

The platform permits to simulate the miscibility of a polymer blends by using the interaction parameter and the solubility parameters (Fig.2). Our software permits also to plot curves of specific volume versus temperature in the goal to obtain the glass transition temperature (Tg) that is an important element in the study of miscibility of polymer systems (Fig.3).

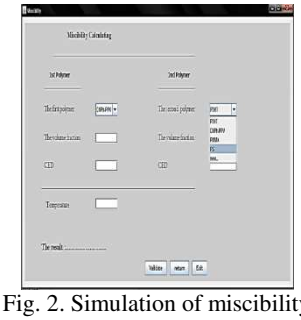

Fig. 2. Simulation of miscibility

Fig. 3. Simulation of glass transition temperature.

The glass transition temperature Tg can be simulated in our software with another way by using theory of Fox; where we must give the percentage of the first polymer and the code will calculate automatically the percentage of the second polymer. The window is shown in Fig.4.

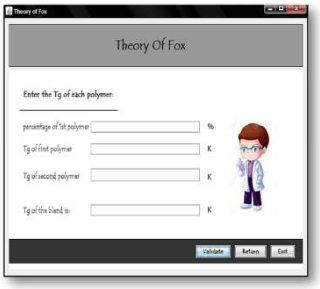

Fig 4. Simulation of Tg by using theory of Fox.

In addition, a programmed code in MATLAB is integrated in our software in order to study the pyrolysis process by using the Distributed activation energy Model (DAEM) with three heating rates. The window is shown in Fig.5.

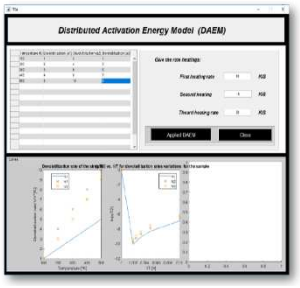

Fig 5. Simulation by using DAEM model.

As all platforms, our code contains a Help to facilitate the work on the platform to users (Fig.6). A simple game (PUZZLE) is added in our software (Fig.7).

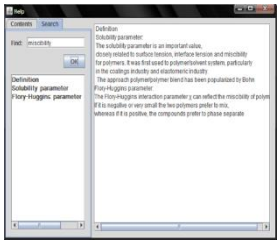

Fig 6. The Help.

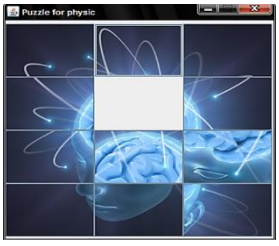

Fig 7. PUZZLE.

4. Results and Discussion

In the order to verify the credibility of our plate-form, the miscibility of PMMA:PS, P3HT:PCBM and P3HT:CNPh-PPV systems was tested and compared with available results in the literature. All blends in this study were considered with the percentage of 50% for each constituent. Our values of glass transition temperature Tg (by using Fox Theory and simulation) and the interaction parameter for the studied polymer blends were shown in Table.1 and compared with found results in other works.

Table.1 our simulated glass transition temperatures and χ parameters at 300 K, compared with the found results in other papers.

	P3HT:CNPh-PPV	P3HT:PCBM	PMMA:PS
Our plate-form			
Tg Fox Theory	312	334.37	368
χ	0.1	0.03	0.04
Blend	miscible	miscible	miscible
Other works			
Synthia (k)	-	-	369 [14]
Tg_{sim} (k)	339 [11]	317 [11]	375 [24]
Tg_{exp}(k)	-	313 [25]	-
χ	0.2[11]	0.00644[11]	0.12 [14]
Blend	miscible	miscible	miscible

By the analyze of Table 1 we can remark that P3HT:CNPh-PPV, P3HT:PCBM and PMMA:PS polymer blends are miscible that is in accordance with available values in the other papers. The simulated glass transition temperature Tg of P3HT:CNPh-PPV system by our platform is not far to the calculated glass transition temperature for the same blend in other work. Also the value of the interaction parameter for P3HT:CNPh-PPV in this paper is very near to the computed value in other study.

For P3HT:PCBM and PMMA:PS blends, our simulated values of glass transition temperatures and the interaction parameters are also near to the found results in other papers.

The validation of part that works with the modified Distributed activation energy Model (DAEM) needs an experimental study. The same procedure and the same mathematical relations were used and proved their credibility with polymer structure in other works [17].

From all above results and analyzes, we can insure the credibility of our platform.

5. Conclusion

JAVA was used to code our software. This last is capable to simulate the miscibility of blends by using different methods. The software permits to plot the curve of the specific volume versus temperature in the goal to obtain the glass transition temperature Tg; whereas the Tg is an important element in the study of miscibility of polymer systems. A code written in MATLAB was added to our software in order to study the pyrolysis process after the experimental work by using the Distributed activation energy Model (DAEM) with three heating rates. The Software contained a help and special Puzzle.

A serial of tests was applied on our platform that proved its efficacy with different materials.

Acknowledgements

This work has been partially supported by The BIOLAB in Departement of Thermal Engineering and Fluid Mechanics. University Carlos III of Madrid.

Conflict of Interest

The authors declare that they have no conflict of interest.

References

[1] Singh, S., Wu, C., Williams, P.T. (2012). Journal of Analytical and Applied Pyrolysis, 94, 99–107.
[2] Zhengzhao, M., Jianghao, X., Ningbo, G., Cui, Q. (2018). Journal of the Energy Institute, 1-11.
[3] Mathew, C. (2013). Polymer Degradation and Stability, 98, 2419-2429.
[4] Antonio, S.V., Elke, G., Andrés, M.G., Nestor G.H., Uwe, R. (2017). Energy conversion and Management, 138, 261-272.
[5] Antonio, S.V., Elke, G., Nestor, G. H., Uwe, R. (2018). Algal Research, 3211-29.
[6] Zhihua, C., Mian, H., Xiaolei, Z., Dabin, G., Shiming, L., Zhiquan, H., Bo, X., Jingbo, W., Laghari, M. (2015). Bioresource Technology, 192, 441–450.
[7] Soria-Verdugo, A., Garcia-Hernando, Garcia-Gutierrez, N., Ruiz-Rivas, U. (2013). Energy Conversion and Management, 65, 239–244.
[8] Fox, T.G., Flory P. (1948). J. Am. Chem. Soc. 70 2384.
[9] Thomas, S., Grohens, Y., Jyotishkumar P. (Editors). Characterization of polymer blends: miscibility, morphology and interfaces. (2015). Vol 1. Wiley- VCH, Weinheim, Germany. 994.
[10] U. Burkert, N.L. Allinger, Molecular mechanics American chemical society, Washington DC (1982).
[11] Bouzid, L., Hiadsi, S., Bensaid, M.O., Haddadi, K., Belaid, L., Ghrici, Y.F. (2021). Canadian journal of physics, 99(1),10-15.
[12] Mason, J.A., Sperling, L.H. (1976) Polymer blends and composites, Plenum Press, New York.
[13] Gee, R., Fried, L., Cook, R. (2001). Macromolecules. 34, 3050.

[14] Bouzid, L., Hiadsi, S., Bensaid, M.O., Foudad, F.Z. (2018) Chinese Journal of Physics, 56, 3012-3019.
[15] F., Ahmed, N.S., Akbar. Chinese Journal of Physics. 55 (2017) 1400.
[16] R., Muhammad, M., Tariq, H.M., Rafique, M., Tanveer, F.H., Syed. (2016). Chinese Journal of Physics, 54, 587.
[17] Bouzid, L., Fouddad, F.Z., Hiadsi, S. (2020) Advances in Polymer Technology 2020 Article ID 8865926.
[18] Fouddad, F.Z., Hiadsi, S., Bouzid, L., Ghrici, F.Y., Bekhadda, K. (2020). Materials Science in Semiconductor Processing, 107, 104801.
[19] Paul, D.R., Newman, S. (1978) Polymer blend. New York: Academic Press.
[20] Accelrys Software Inc, Materials Studio Modeling Environment, Release6.0, Accelrys Software Inc., San Diego, 2011.
[21] Bohn, L. (1968) Incompatibility and phase formation in solid polymer mixtures and graft and block copolymers. Rubber Chemistry and Technology, 41, 495-513.
[22] Hua, Y., Li, Z.S., Qian, H.J., Yang, Y.B., Zhang, X.B., Sun, C.C. (2004). Polymer, 45, 453.
[23] Mason, J.A., Sperling, L.H. (1976) Polymer blends and composites, Plenum Press New York.
[24] Chul, H.P., Jae, H.K., Moonhor, R., Byeong-Hyeok, S., Jin, C.J., Wang-Cheol, Z. (2004) Polymer, 45, 4507.
[25] Savagatrup, S., Printz, A.D., Wu, H., Rajan, K.M., Sawyer, E.J., Zaretski, A.V., Bettinger, C.J., Lipomi, D.J. (2015). Synth. Met., 203, 208.

Recommended Citation

Bouzid, L., Foudad, F.Z., Hiadsi, S. (2021). Platform for studying properties of blend systems. *Algerian Journal of Chemical Engineering*, http://dx.doi.org/10.5281/zenodo.4776593