

Original Article

Investigation of Compatibility of Multi-Component Systems Based on Polyolefins and Heterocyclic Polymers

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Abstract - In this work, industrial rollers' adaptation, structure, and properties and their dependence on the factors were determined. the purpose of the research is to develop the theoretical basis of compatibility, determine the laws of thermodynamics, create polymer systems on the necessary technical aspects by combining various multifunctional components with the optical properties of the final material.

To develop a technology for obtaining new composite materials based on high-pressure polyethylene (HPP), polyvinyl chloride (PVC), polyurethane thermoelastoplast (PUTEP), butyl rubber (BR), industrial polymetallic polymers, the degree of their compatibility with each other was calculated and calculated. How the spinodal parameter changes depending on the age of the mixture has been studied, and the study showed that the spinodal parameter of hello ma increases with decreasing concentration of any component in the mixture.

Keywords - Adaptation, Polyolefin, Free mixing energy, Spinodal parameter, Solubility, Thermodynamics of polymer mixturesç.

I. INTRODUCTION

The problem of obtaining polymeric materials with the necessary properties to work in extreme conditions is currently solved in two ways; the Synthesis of new polymers and the creation of polymer compositions that complement each other in the properties of individual components [1]. Preparation of polymer compositions is an urgent task. Shikhaliyev (the urgency and importance of this problem is determined by the fact that the creation of the theory of multi-component systems is very poorly reflected in the literature, although it is difficult to assess the importance of such materials in modern technology. Study of the properties of polymer compositions developed in existing technological equipment and their processing conditions, creation of multi-component polymer systems with the required technical complex, creation of important

properties with appropriate detection of thermodynamic regularities by the development of theoretical bases of compatibility, a combination of various selected multifunctional components[8-16] the direction is relevant in practical terms[2-3],[5],[6],[7]. Development of scientific bases of industrial technology for the production of composite materials with wide gamma-operational properties based on polyolefins and hetero sex polymers using existing production facilities and technological equipment [4-],[18],[19]. To achieve this goal: it is necessary to determine the most important Thermodynamic regularities of mixtures of industrially produced polyolefins and hetero sex polymers, and on this basis, the scientific basis of their compatibility, the creation of multi-component composite materials with the required complex performance properties has been the main focus of recent research,[20][21].

II. METHODOLOGY

By studying the thermodynamics of polymer mixtures, their large molecular weight distinguishes them from other systems. According to the laws of thermodynamics, the entropy of mixing polymers is characterized by the free mixing energy of sugar.

$$\Delta G_{\text{scratching}} = \Delta q_{\text{scratching}} - T\Delta S_{\text{scratching}} \quad (1)$$

- (1) Adaptation of polymer mixtures is possible when the free mixing energy is negative. Still, the polymers' high molecular weight does not help create favorable conditions for combinatorial entropy.
- (2) the analysis of equation (1) is given by Flori-Haggins theory:

$$\Delta G_{sm} = RTV \left\{ \frac{\Phi_A \ln \Phi_A}{V_a} + \frac{(1 - \Phi_A) \ln(1 - \Phi_A)}{V_b} + \chi_{AB} \Phi_A (1 - \Phi_A) \right\}$$

where Φ_A - volume fraction of polymer; A, V - i-th component mol. volume; χ_{AB} - interaction parameter.



The first two terms of this equation are the combinatorial entropy of the mixture.

If we consider that both polymers have the same molecular weight, then we can write equation (2) as follows:

$$\Delta G_{CV} = \frac{\rho_B PT}{M_{kn}} \left\{ \frac{M}{M} k p [\Phi_A \ln \Phi_A + (1 - \Phi_A) \ln(1 - \Phi_A)] + 2\Phi_A (1 - \Phi_A) \right\} \quad (2)$$

The upper and lower curves correspond to the mixing temperature and mixing entropy. the remaining curves show the change in the mixing energy of components with different molecular weights.

As can be seen from the figure, the free energy tends to have a positive value, which corresponds to the result of equation (1).

Thus, a negative value of Bargar is a key condition for the adaptation of the polymer-polymer system.

A single-phase mixture is thermodynamically stable if it meets the following conditions:

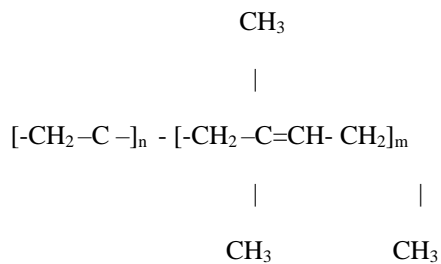
$$(\partial^2 \Delta G_{sm} / \partial \phi^2) T, p > 0 \quad (3)$$

As shown above, the determination of the interaction parameter XAB depends mainly on the solution parameters δA and δB

III. RESULTS AND DISCUSSION

A. Butyl rubber at a temperature of 298K - calculation of compatibility for high-pressure polyethylene (BR- HPP) system

Given the density of GC under 250C p = 0, 92x103 kg / m3, isoprene content - 5%, constant HPP p = 0, 96x103 kg / m3, calculate the dissolution parameters of each component of the mixture using the table values of molar constants involved in different chemical groups of resin. in the calculation, we do not consider the distribution of the final groups and the molecular mass distribution. BK formula (n = 0.95; m = 0.05)



Isoprene attracts molar constants

$$\begin{aligned} \Sigma F &= 133,2 + 93 + 214 + 28 = 415 \\ M &= 5 \times 12 + 8 \times 1 = 68 \end{aligned}$$

Molar gravity constants are isobutylene

$$\Sigma F \text{ - CH}_2\text{-CH}_3 \quad \backslash /$$

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$$\begin{aligned} \Sigma F &= 133 + 2 \times 214 = 468 \\ M &= 12 \times 4 + 5 \times 1 = 53 \end{aligned}$$

Then the BK solution parameter

$$\delta_{bk} = 0,92/0,95 \cdot 468/53 + 0,05 \cdot 415/68 - 8,0$$

the following equation is used to calculate the critical value of BR- HPP

$$\text{XKR} = 1/2 [1 / \text{XA}1 / 2 + 1 / \text{XB}1 / 2]$$

Contains the degree of polymerization of each polymer expressed in terms of relative volume. the degree of polymerization can be calculated based on the degree of polymerization x when the molar volume of the polymer repeated by the equation is known.

$$\text{HA} = (V / Vp) x$$

A fairly good approach obtained from a ratio

$$\text{HA} = \text{MA} / 100$$

Ma is where the molecular weight of the polymer is.

So we have:

$$\text{BR} = \frac{350000}{100} = 3500$$

$$\text{HPP} = \frac{300000}{100} = 3000$$

Here is the equation to calculate the critical value:
 $(\text{BR- HPP})_{kr} = 1/2 \times 1 / 3500^{1/2} + 1/3000^{1/2} = 6.18 \times 10^{-4}$

Determine the probability of the origin of the phase division, for which we will calculate BR- HPP for differentphase combinations. Results Table .1.

Table 1. Melting parameters of the BR- HPP system

Φ_{BR}	mixing	Φ_{BR}	$(X_{BR-HPP})_{mix.}$
0,00	-	0,5	7.56 x10
0,05	3.636 x10	0,60	7.86 x 10
0,10	1.932 x10	0,65	8.352 x10
0,15	1.38x10	0,70	9.12x10
0,20	11.076 x10	0,75	10.284x10
0,25	9.528x10	0,80	1.212x10
0,30	8.568x10	0,85	1.536x10
0,35	7.98 x10	0,90	2.196x10
0,40	7.62x10	0,95	4.176x10
0,45	7.44x10	1,00	-
0,50	7.428 x10		

As can be seen, as the concentration of any component in the mixture decreases, the spinodal parameter of hello ma increases and dissolves better than HPP at home BC. Concentrations have been determined by variation, in which case an absolute combination is possible. It will be deducted 0.08%. 0.06% for PS and BR.

Thus, the calculation method shows that the BR- HPP system is practically incompatible. To find the critical point of the system in the phase diagram, it is necessary to calculate the GCM for the different components of the system. the calculation was performed for t = 298K, and the results are given in Table 2.

Table 2 BR- HPP mixing temperature

Φ_{BR}	Gear	Φ_{BR}	Gear
0,00	-	0,55	4.104 x10
0,05	7.896 x10	0,60	3.996 x 10
0,10	1.5 x10	0,65	3.792 x10
0,15	2.124x10	0,70	3.492x10
0,20	2.664 x10	0,75	3.12x10
0,25	3.12x10	0,80	2.664x10
0,30	3.492x10	0,85	2.124x10
0,35	3.792 x10	0,90	1.5x10
0,40	3.996x10	0,95	7.896x10
0,45	4.104x10	1,00	-
0,50	4.152 x10		

The calculation data show a so-called symmetrical situation for the BR- HPP system with low critical solution temperature (CSKT). Based on the principle of additivity, we have TKR 503K.

Thus, it can be concluded from the above calculation: 1. the BR- HPP system is practically incompatible; Up to 2.0.06% and 0.08%, HPP is possible in the concentration of BR.

To adjust the compatibility of polymer mixtures, the calculation of compatibility parameters for the PVC and HPP polar components system depending on the polarity of the components was carried out (comparison with the cash-BR incomplete system).

B. Polyvinyl chloride-polyurethane thermoelastic plasticizer (PVC-PUTEP) Calculation of suitability for the system at a temperature of 298K

Calculate the solubility parameters of each component of the mixture using the table values of molar constants to attract different chemical groups of resin, taking into account the density of PVC at 298K.

(P25 = 1, 41x103 kg / m3). the calculation will consider that the number of limited groups is insignificant, and the molecular weight distribution is not taken into account. PVC single link - [- CH2-CCL -] n

Molar attraction constants

$$-CH_2 - CH = Cl -$$

$$\sum F = 133 + 28 + 270 = 431$$

$$M = 12,2 + 1,3 + 35,5 = 62,5$$

Then the PVC hellolma parameter will be: $\delta_{PVX} = 1.41 \times 431 / 62.5 = 9.72$

The solubility parameter of PUTEP, taking into account the density of overpasses with 250C (P25 = 1, 1x103 kg / m3). the only Ring of PUTEP

$$[-(CH_2)_6 - OCOHN - (CH_2)_4 -]_n$$

$$- (CH_2)_6 - - COO - - NH - - (CH_2)_4$$

$$\sum F = 133,6 + 310 + 180 + 133,4 = 757$$

$$M = 12,11 + 1,21 + 16,2 + 14 = 199$$

$$\delta_{PUTEP} = 1,10 + 1820 + 199 = 10,06$$

the parameter of the interaction between the polymers in the system is calculated according to the equation:

$$X_{AB} = V_n / RT (\delta A - \delta B)^2$$

Where r-gas is constant, equal to 1,987 kcal * mole-1 * degree-1; t-temperature K; Vn-comparative volume (cm3 / mol) is usually assumed to be equal to 100 cm3 / mol. Thus, the equation for t = 298K assumes the form:

$$X_{AB} = (\delta A - \delta B)^2 / G$$

in this case, for the PVC-PUTEP system there are:

$$X_{PVC-put} = (10.06 - 9.72)^2 / 6 = 0.019$$

the krKR equation is used to calculate the critical value (Xpvx-pulp)

$$X_{KR} = 1/2 [1 / X_1 / 2A + 1 / X_{B1} / 2] 2$$

Contains the degree of polymerization of each polymer, expressed by the comparable VN volume. the degree of polymerization can be calculated based on the actual degree of polymerization x when the molar volume of the polymer is known according to the equation:

$$HA = (V / V_p) x$$

A fairly good approach obtained from a ratio

$$HA = MA / 100$$

Ma is where the molecular weight of the polymer is.

So we have:

$$X_{PVC} = \frac{90000}{100} = 900$$

$$X_{PUTEP} = \frac{18000}{100} = 180$$

Here is the equation to calculate the critical value:

$$(X_{pvx-putep})_{kr} = 1/2 \times 1 / X_A (fA / GP) + 1 / HV (FV)_{sp} \text{ (table3)}$$

Table 3. Price of PVCsignal parameter for mixed connections of different phases

NoNo	PVC	mixing
1.	0,00	-
2.	0,05	3.336x10 ⁻³
3.	0,10	1.68x10 ⁻²
4.	0,15	10.368x10 ⁻³
5.	0,20	8.364x10 ⁻³
6.	0,25	7.5x10 ⁻³
7.	0,30	7.116x10 ⁻³
8.	0,35	6.984x10 ⁻³
9.	0,40	7.032x10 ⁻³
10.	0,45	7.224x10 ⁻³
11.	0,50	7.548x10 ⁻³
12.	0,55	8.004x10 ⁻²
13.	0,60	8.616x10 ⁻³
14.	0,65	9.444x10 ⁻³
15.	0,70	10.548x10 ⁻³
16.	0,75	1.212x10 ⁻²
17.	0,80	1.428x10 ⁻²
18.	0,85	1.752x10 ⁻²
19.	0,90	2.304x10 ⁻²
20.	0,95	3.408x10 ⁻²
21.	1,00	-

Since 0.019 is significantly larger than 0.006, i.e., $X_{pvc-putep} > (X_{pvc-pulp})_{KR}$, this system must be incompatible with many compositions.

Using the equation:

$$(X_{AB})_{sp} = 1/2[1/X_A(FA)_{BM} + 1/X_V(FV)_{BM}]$$

IV. CONCLUSION

A detailed study of new approaches to creating polymer composition systems based on polyolefins and wind-dandruff polymers was conducted and followed, and the most important results were obtained.

Polyethylene (PE), polyvinyl chloride (PVC), polyurethane thermoelastoplast (PETEP), butyl rubber (BK), chlorocarboxylate polyethylene (ChCPE), ethylene-propylene rubber (EPR) developed new composite materials based on industrial multi-polymers.

The solubility parameters of four polymers at different poles were determined by turbidimetric titration (TSH) and coated gas chromatography methods. According to the temperature dependence of the solubility parameter obtained on the storage times of sorbates, the amount of

solubility parameter was calculated as equal to 298 K and compared with the amount obtained by the TDG method at the same temperature. An increase in the difference between the polarity of the polymer and the magnitude of the solvent parameters obtained by the two methods has been shown. the observed Effect is explained by the diametrically opposite state of the "polymer-solvent" systems understudy

It was determined that the properties of polymer composition systems with properties based on multifunctional polyolefins and hetero sex polymers, the relative content of phases in the mixture, the nature of the polymer matrix, particle shape and size, the structure of the interfacial layer, the phase-to-phase elasticity component.

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