Structure Design, Performance Simulation and Plasticizing Properties of Bio-Based Copolyesters Plasticizer on PVC

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Abstract
Plasticizer is an important assistant in the production process of polyvinyl chloride (PVC), which can effectively improve the plasticity of PVC. However, the durability and plasticizing effect of traditional phthalate plasticizers need to be further improved. In this paper, a variety of copolyesters are designed and synthesized from succinic acid, hexanediol and other four different diols. The plasticizing performance of the copolyester is characterized by FT-IR, H-NMR, XPS and DMA. It is found that the side chain groups in the structural units of the copolyester have a great influence on its plasticizing properties. The glass transition temperature of PVC plasticized by polybutylene succinate 3-chloro-1,2-propanediol ester (PSCH) is 8.1 °C lower than the temperature of PVC which is plasticized by DOP, and the elongation at break is increased by 104.7%. The obtained copolyester plasticizer with flexible long alkane chains and polar C–Cl groups shows improved solvent extraction resistance and better compatibility between plasticizer and PVC compared DOP. It is verified that the hydrogen bonding interaction between the C=O group of plasticizers and α-hydrogen of PVC exhibited in FT-IR, XPS and solubility parameters DS is the main reason for the effective plasticizing efficiency of PSCH on PVC.

Keywords Copolyester · Plasticizer · PVC · Durability · MS simulation

Introduction
Poly (vinyl chloride) (PVC) is one of the most useful manufactured plastics [1], and its products are widely used in a large range of applications, including food packing [2, 3], medical devices [4], toys [5] and architecture [6, 7]. PVC plays an important role in plastic industry, however, it must be combined with additives, such as plasticizer (DOP) and thermal stabilizer, before processing with the virtues of toughness, abrasive resistance, acid and alkali resistance [8]. Because of the strong polar effect among PVC chains, pure PVC exhibits rigidity, brittleness and a high melt viscosity, resulting in a relatively high processing temperature and a high screw torque. PVC compounded with plasticizers is often used for applications that require flexibility. The addition of a plasticizer to PVC can improve its workability, decrease its processing temperature, and achieve the desired toughness [9–12].

Plasticizer is one of the largest additives in terms of production and consumption [13]. It plays an indispensable role in providing high-quality plastic products for human beings [14]. For a long time, plasticizers have been mainly based on phthalate products. With the increasing application of phthalates in food, medicine and other industries, people pay more and more attention to its toxicity [15, 16]. Based on the results of the National Cancer Institute, the U.S. Environmental Protection Agency has restricted the use of 6 o-phenyl plasticizers in areas with higher environmental and sanitary conditions. As phthalates are the main plasticizers of polyvinyl chloride when they are used in medical devices, children's toys and food packaging materials, they can easily leak out of products and pose a serious threat to human health [17–20]. Therefore, plasticizers are developing towards high molecular weight, functional, non-toxic and environmentally friendly polyester plasticizers with good heat resistance and durability [21].

At present, the environmental friendly plasticizers mainly can be divided into haplotype plasticizer and polymerization plasticizer [22–25], which mainly include polyol ester...
plasticizer, epoxy plasticizer, citrate plasticizer and polyester plasticizer and so on. Research on environmental friendly plasticizers mainly focuses on haplotype plasticizers such as epoxy soybean oil and citrate [26–29]. Although this kind of plasticizer avoids the carcinogenic risk of phthalate plasticizers (DOP, DOTP, etc.). Unfortunately, epoxy soybean oil and citrate are still low molecular weight compounds, which can also easily migrate from PVC with the loss of plasticizing properties, and its migration and volatilization resistance performance has not been fundamentally improved. As we know, increasing the molecular weight of plasticizer is an attractive approach to improve the migration resistance of plasticizers. For example, Zhang et al. [30] synthesized a kind of succinic acid glycol ester with good migration resistance effect and Jia et al. [31] synthesized a new rosin based plasticizer, which has excellent solvent resistance and plasticizing effect. However, although this kind of polyester has better migration resistance than traditional DOP, its plasticizing efficiency is still lower than that of benzene plasticizers. The reason is attributed to the lack of intermolecular hydrogen bonding between molecular skeletons of polyester plasticizer and PVC. Therefore, seeking for bio-based polyester plasticizers with excellent plasticizing property to replace traditional petroleum-based plasticizers. In this work, with the objective of seeking for an efficient and environmentally friendly plasticizer, four copolyester plasticizers (PSCH, PSPH, PSNH, PSBH) with different side chains are designed. The plasticizing effect of different plasticizers on the mechanical properties, durability, thermodynamic properties and plasticizing efficiency of PVC was discussed, and the plasticizing parameters of the plasticizer are simulated by Materials Studio (MS) and compared with commercial plasticizer DOP.

**Experiment Section**

**Materials**

Cyclohexane and petroleum ether were purchased from Yantai Far East Fine Chemical Co. Ltd. activated carbon, DOP and heat stabilizer were purchased from Sinopharm Chemical Reagent Co., Ltd. poly(propylene glycol adipate) and PVC (industrial grade) were obtained from Henan lianchuang chemical Co., Ltd. 3-Chloro-1,2-propanediol was obtained from Zhengzhou Alpha Chemical Co., Ltd. 1,2-Propanediol, 1,2-Butanediol, Neopentyl glycol, Succinic acid and hexanediol were obtained from Shanghai Macklin Biochemical Co., Ltd. All the reagents were used as received unless otherwise noted. 3-chloro-1,2-propylene glycol, 1,2-propylene glycol, 1,2-butanediol, neopentyl glycol, succinic acid, hexanediol, succinic acid, 1,6-hexanediol were added in a certain proportion to the three-necked flask equipped with nitrogen circulation system and water separator, and tetrabutyl titanate was added to the flask as catalyst. The reaction temperature was raised to 175 °C, and nitrogen was injected into the flask for protection. After the reactants in the flask entered the molten state, after about 8 h of reaction, no more water was evaporated, and the esterification reaction was over. The product was decompressed at 175 °C to remove the remaining water in the reaction product.

Four environmental friendly polyester plasticizers, polyhexamethylene glycol succinate 3 chloro-1,2 propylene glycol ester (PSCH), polypropylene glycol succinic acid 1,2 propylene glycol ester (PSPH), polyhexamethylene glycol succinate 1,2 butanediol ester (PSBH) and polyhexylene glycol succinic acid neopentyl glycol ester (PSNH) were synthesized. The synthesis route is shown in Fig. 1.

**Preparation of PVC Blends**

PVC/plasticizer films were prepared by solution casting. The compositions of different formulas were shown in Table 1. PVC, plasticizer and thermal stabilizers were dissolved in 80 ml THF at 40 °C for 2 h, and the prepared solutions were casted on clean petri dishes and dried at ambient pressure, room temperature for 2 days to remove most of THF. The solid films were taken out and put into vacuum oven for another 2 days to eliminate residual THF. Finally, films were packed in aluminum foils and kept in desiccators for further testing.

**Characterization and Testing**

Fourier Transform Infrared Spectroscopy (FT-IR). FT-IR spectra of PSXH/PVC were recorded on a Thermo-Nicolet Avatar-360 apparatus in the wavelength range of 4000–400 cm⁻¹ with resolution of 2 cm⁻¹.

Tensile Testing. The tensile properties of PVC blends were evaluated by determining tensile strength and elongation at break. Tensile tests for the composites were carried out by the Universal Testing Machine (AI-7000S, China) equipped with a 10 KN electric load cell. The crosshead speed was 50 mm/min.

Extraction Test. To appraise extraction stability of the plasticizer, the samples of PVC blends with dimension 10 × 10 × 1 mm³ were immersed in 100 mL liquids at 25 °C. The liquids were selected as water, ethanol, cyclohexane, petroleum ether. After extraction, the samples were fully dried under vacuum until the weights of the samples were constant.

Migration Test. The migration stability was characterized by detecting the amount of plasticizer migrated out from samples. The samples were placed between the rubber for two weeks at a constant temperature (40 °C). The extraction,
Volatilization and migration were characterized by mass loss, calculated by the following equation:

\[
\text{Mass loss(\%)} = \frac{W_1 - W_2}{W_1} \times 100
\]

where \(W_1\) and \(W_2\) were the weights of the samples before and after the tests, respectively.

Dynamic Mechanical Analysis (DMA). DMA of plasticized PVC was studied on a DMA 242E apparatus (NETZSCH, Germany). Samples were subjected to tension with amplitude of 20 µm and at a frequency of 1 Hz. The temperature was set from -80 °C to 120 °C with a rate of 5 °C/min.

X-ray photoelectron spectroscopy (XPS). The chemical composition was characterized by using XPS analysis on an ESCALAB 250Xi apparatus (Thermo, America). X-ray source used monochromatic Al Ka alpha rays (\(h_\nu = 1486.6\) eV) with the power of 150 W, and the beam spot was 500 µm.

Solubility parameters of plasticizer and PVC were studied by the small Eq. (2). Furthermore, the solubility parameter of mixed plasticizer was calculated in terms of the additivity rule in Eq. (2).

\[
\Delta\delta = \delta_{\text{pvc}} - \frac{\rho \sum F}{M}
\]

Results and Discussions

Characterization of Oligomeric Copolyester

The chemical structure and \(M_n\) of four copolyester plasticizers, PSCH, PSPH, PSBH and PSNH, are shown in Fig. 2. As shown in the Fig. 2a, the strong absorption peak at about 1170 cm\(^{-1}\) is assigned to the characteristic peak of the stretching vibration of \(C-O-C\) bond in the polyester, while the peak at about 1725 cm\(^{-1}\) is ascribed to the stretching vibration of carbonyl, indicating the successful synthesis of polyester. Meanwhile, the evident peak of \(C-\text{Cl}\) appears near 729 cm\(^{-1}\) in the infrared spectrum of PSCH, indicating that the \(\text{Cl}\) is successfully introduced into copolyester.

Figure 2b shows the number-average molecular weight and molecular weight distribution index of the synthesized copolyester
plasticizers. It can be seen from Fig. 2b that the molecular weight of the four synthesized copolyester plasticizers is 3447, 3996, 3636 and 3049, respectively. Besides, their PDI are 1.252, 1.234, 1.166 and 1.322, respectively, indicating that the molecular weight distribution of the synthesized low-poly copolyester plasticizer is narrow and the molecular weight distribution of the plasticizer is uniform.

### Plasticizing Property

The mechanical properties of PVC blends plasticized by the four copolyesters including tensile and impact strength are measured and compared with the commercial plasticizer DOP. The stress–strain curve from the tensile test can be used to characterize the mechanical properties of PVC films. A typical stress–strain curve of the PVC film is shown in Fig. 3a. And compared with DOP and the other copolyesters, PSCH has the highest plasticizing effect which can be deduced from the data of elongation at break (292.46%). The result might be attributed to the molecular features of PSCH plasticizer. More polar groups (C–Cl) of PVC blends plasticized by PSCH were incorporated into the PVC matrix than PVC blends plasticized by other copolyesters. The polar groups of plasticizers could interact with the polar parts of PVC molecule and induce dipole–dipole interaction between the plasticizer and PVC, reducing the PVC-PVC interactions at sites where polymer chains could associate and increase the space between polymer molecules.

Glass transition temperature ($T_g$) is an effective index for the evaluation of plasticizing efficiency, and lower $T_g$ usually means better compatibility between plasticizer and PVC. The $T_g$ of PVC blends is determined by DMA measurement and the obtained DMA curves of PVC blends plasticized by the copolyesters and DOP are shown in Fig. 3b. Based on the definition of plasticization, the $T_g$ of PVC blends is expected to be decreased with the addition of a plasticizer, and as observed from Fig. 3b, $T_g$ of PVC blends plasticized by copolyester is close to or lower than that of DOP, which indicates the novel copolyester plasticizer could have the same performance as DOP in many applications. It is worth mentioning that $T_g$ of all the PVC blends plasticized by copolyester plasticizer is below 5 °C verifying that the system is completely flexible at room temperature and can be used for soft PVC products. PVC blends plasticized by PSCH has the lowest $T_g$ (−7.34 °C) which is decreased by 8.01 °C compared with DOP, and this trend is also consistent with the stress–strain results shown in Fig. 3a.

XPS is used to obtain the binding energy of C–Cl in PVC blends and the possible interaction forces between PVC and plasticizers is determined. According to XPS analysis result in Fig. 3c, the binding energy of C–Cl of PVC/PSCH blend is 199.53 eV, which is 0.87 eV–2.07 eV lower than that of pure PVC. The XPS analysis of pure PVC was 200.4 eV–201.61 eV. The carbonyl group in the copolyester can form hydrogen bond with the hydrogen on the carbon connected with chlorine atom in PVC, which can reduce the polarity of C–Cl bond. It’s worth noting that PSCH has the best plasticizing efficiency attributed to the C–Cl bond on the side. According to the similar compatibility principle, except for hydrogen bonding, the existence of C–Cl bond in PSCH increases the compatibility of plasticizer and PVC. To sum up, it can be stated that the decreased binding energy of C–Cl and weakened polarity of PVC molecules make the plasticity of PVC samples increased.

Plasticizing efficiency of the copolyesters is calculated by elongation at break using Eq. (3) [34], and the results of plasticization efficiency are shown in Table 2.

![FT-IR spectrum (a), $M_n$ and PDI (b) of the four copolyesters](image)
where $E_{\Delta \varepsilon, \text{copolyester}}$ is plasticizing efficiency of the plasticizer and $\Delta \varepsilon_{\mu}$ represents the difference of elongation at break between plasticized PVC and pure PVC. What’s more, the plasticizing efficiency of DOP for PVC is defined as 100%.

As it is shown above Table 2, the greatest improvement in plasticizing efficiency for PVC is observed with the addition of PSCH (142.6%), and compared with DOP, the plasticizing efficiency is increased by about 40%. Besides, the plasticizing effect of PSBH, PSPH and PSNH plasticizers is also slightly better than DOP. The main reason is the hydrogen atoms and carbonyl groups in the polyester molecule interact with the hydrogen on the carbon connected with chlorine atom in PVC, which reduces the interaction between the PVC molecules, thereby reducing the hardness of the PVC material. All in all, the copolyesters synthesized in this study have a good effect on improving the plasticity of PVC.

### Compatibility

FT-IR is a reliable and facile method for analyzing the miscibility between PVC and plasticizer. After adding into PVC, the carbon group absorption band of plasticizer will shift to lower position due to the dipole–dipole interaction between the C=O of plasticizer and $\alpha$-hydrogen of PVC, which is important to assess the miscibility of PVC and polyester blends.

The offset of carbonyl peak of low polyester plasticizer after plasticizing PVC calculated by FT-IR can be used to calculate the enthalpy change of the system before and after plasticizing PVC of low polyester, as shown in Formula 4 [35].

![Stress–strain (a) and loss modulus (b) of PVC blends plasticized by copolyesters and c Cl 2p scan of PVC plasticized by PSCH](image)
The FT-IR of PVC blends exhibits a definite peak shift and broadening of the carbonyl band of plasticizer as well as the C–H rocking band of PVC as the blend composition is varied. Figure 4 shows the positions shift of the carbonyl peak of different plasticizers blends with PVC, and the positions of carbonyl group absorption band before and after blending are listed in Table 3. The carbonyl group absorption band is at 1732.21 cm$^{-1}$ for pure polyester plasticizers. As can be observed from Fig. 4b, after blended with PVC, the carbonyl group absorption of copolyester plasticizers shifts to the lower band. Especially, when PSCH is used as the plasticizer (Plasticizing mechanism is shown in Fig. 4a), the absorption peak of C=O is shifted from 1739.47 to 1716.49 cm$^{-1}$. Figure 4 shows the shift of the plasticizer’s C=O absorption peak due to the interaction between plasticizer C=O and PVC α-hydrogen molecules, and Table 3 shows the C=O absorption positions of the four plasticizers before and after plasticizing PVC. As can be clearly seen from Fig. 4, compared with pure PSCH, the C=O absorption peak of PVC/PSCH moved to the low-frequency region, confirming the strong interaction between PVC and plasticizers. In FT-IR spectra, the greater the deviation of the carbonyl absorption band and C–H rocking band, the better the solubility of the mixture. It can be seen that the carbonyl peak of PVC plasticized by oligomeric copolyester shifts to low wave number, and the enthalpy of interaction (calculated by formula 4 and listed in Table 3) of plasticized system is negative, which proves that oligomeric copolyester and PVC can be highly compatible from the perspective of thermodynamics.

Solubility parameters and solubility parameter of different plasticizers listed in Table 4 are obtained from formula 5 and 6 [36]. High plasticizing efficiency of plasticizer for PVC is attributed to plasticizer’s good compatibility with PVC and its high diffusion in PVC, which result from the interaction between plasticizer and PVC molecules. For plasticization, intermolecular forces between plasticizer molecules must be as strong as those between the plasticizer and the polymer to

\[ \Delta H = 0.236 \times \Delta v \]  \hspace{1cm} (4)

| Material | $F$ | $\delta$ (J cm$^{-3})^{1/2}$ | DS (J cm$^{-3})^{1/2}$ |
|----------|-----|----------------------------|---------------------|
| DOP      | 2459| 9.87                       | 0.21                |
| PSCH     | 3201| 9.72                       | 0.06                |
| PSPH     | 3019| 9.82                       | 0.16                |
| PSBH     | 2998| 9.79                       | 0.13                |
| PSNH     | 3108| 9.92                       | 0.26                |
| PVC      | 431 | 9.66                       | –                   |

Table 3 C=O rocking band analysis of PVC films plasticized by copolyesters

| Material | Wave number of C=O rocking band (cm$^{-1}$) | $\Delta$V of C=O rocking band (cm$^{-1}$) | $\Delta$H (kcal mol$^{-1}$) |
|----------|---------------------------------------------|------------------------------------------|-----------------------------|
| PSCH     | 1739.47                                     | -22.98                                   | -5.42328                    |
| PSPH     | 1733.1                                      | -4.71                                    | -1.11156                    |
| PSBH     | 1732.72                                     | -4.58                                    | -1.08088                    |
| PSNH     | 1732.69                                     | -4.02                                    | -0.94872                    |
be plasticized. The stronger interaction between plasticizer molecule and PVC molecule, the greater the compatibility.

\[
\delta = (CED)^{1/3} = \left[ \frac{\Delta E}{V_i} \right] = \frac{\sum F_i}{M} = \frac{\rho \sum x_i F_i}{M} = \frac{x_1 \sum F_1 + x_2 \sum F_2 + \cdots + x_n \sum F_n}{x_1 V_1 + x_2 V_2 + \cdots + x_n V_n}
\]

(5)

In formula 5, \(\delta\) is the solubility parameter, \(\Delta E\) is energy of vaporization, \(V_i\) is molar volume, and \(F_i\) is the molar attraction constant. \(\rho\) and \(M\) are the density and molecular weight of the plasticizer or chain unit of the polymer, respectively.

Furthermore, according to van Krevelen, good solubility between polymer and plasticizers occurs when difference in value of solubility parameter (Eq. 6) is as small as possible.

\[
DS = \delta_{plasticizer} - \delta_{PVC}
\]

(6)

where \(\delta_{PVC}\) and \(\delta_{plasticizer}\) denote the solubility parameter of the polymer and plasticizer, respectively.

In this study, PSH and 3-Chloro-1,2-propanediol were chemically combined into a new compound, PSCH. The chlorinated paraffin parts of the new compound will also interact with PVC to mask more sites of attachment between PVC molecules and hinder forces holding PVC chains together, partially compensating the decreased plasticizing efficiency. This may why PSCH has such amazing plasticizing efficiency.

**Durability**

PVC samples after plasticization often come into contact with organic or inorganic solvents. In order to test the migration resistance of the synthesized copolyester plasticizer in organic or inorganic solvents, the mass loss rate of plasticizer and the mechanical properties of PVC samples after aging in tap water (inorganic) and cyclohexane (organic) are studied. Figure 5 shows the durability test of plasticized PVC.

Figure 5a and b respectively show the test results of the mass loss rate and elongation at break of the copolyester plasticized PVC samples during the aging process of cyclohexane. As can be seen from the figure, after soaking in cyclohexane for seven days, the mass loss rate reached 20.67%, and the elongation at break of PVC/DOP decreased from 226.37 to 167.41%. As the molecular weight of DOP is small, it is easy to migrate from PVC. After 7 days of aging, the elongation at break of PVC/DOP is 28% lower than the initial value. By contrast, for PVC samples plasticized with copolyester, the elongation at break of PVC/PSCH decreases from 292.46 to 277.37% after soaking in cyclohexane for 7 days, only 5% lower than the initial value, and the mass loss rate of PSCH is only 1.54%, proving that PVC plasticized by PSCH has better migration stability. As shown Fig. 5c, PVC/DOP samples basically lose their flexibility after 60 days of aging in cyclohexane, and more seri-
directions. The strain in each direction of the two systems is similar, indicating that plasticizer and PVC are mixed evenly without plasticizer agglomeration. The simulation value is substituted into the equation below to calculate the Lamé constant of PVC/DOP and PVC/PSCH [36].

\[
\lambda = \frac{1}{3}(C_{11} + C_{22} + C_{33}) - \frac{2}{3}(C_{44} + C_{55} + C_{66})
\]  

(7)

\[
\mu = \frac{1}{3}(C_{44} + C_{55} + C_{66})
\]  

(8)

The young’s modulus (E) and volume modulus (K) of the plasticized PVC and pure PVC systems are further calculated by using the Ramey constant.

\[
E = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu}
\]  

(9)

\[
K = \frac{2}{3}\lambda + \mu
\]  

(10)

The calculation results are shown in Table 5, from which it can be seen that the PVC system plasticized by PSCH has the lowest Young’s modulus and is the most soft material. The young’s modulus of PVC/DOP and PVC/PSCH decreases by 33.4% and 52.2% respectively compared with that of pure PVC. The volume modulus decreases by 36.4% and 51.4%, respectively. This is attributed to the addition of plasticizer which reduces the rigidity of pure PVC material and increases the plasticity of PVC, and is in accordance with the conclusion of tensile test and surface hardness test. For pure PVC system, due to the presence of a large number of polar functional groups –Cl on the PVC molecular chain, PVC molecules have a strong intermolecular role, and the relative movement of PVC molecules is limited, making PVC materials show hard and brittle properties. When plasticizer is used to plasticize PVC, plasticizer molecules will interact with PVC molecules, making the interaction

Fig. 5 Durability test of plasticized PVC samples in cyclohexane. a Mass loss rate, b elongation at break, c Stress–strain after 60 days of aging
Fig. 6  a Radial distribution function of PVC/DOP. b Radial distribution function of PVC/PSCH. c Mean square displacement of different plasticizing models. d Solubility parameters of PVC/plasticize and e Binding energy of PVC/plasticize.
between PVC molecules weakened. For DOP, the group that can interact with PVC molecule is C=O, in contrast, the groups that can interact with PVC molecules in copolyester plasticizers are C=O and –Cl, and the density of C=O in copolyester plasticizers is higher than DOP, so the Young’s modulus of PVC/PSCH is lower than that of PVC/DOP.

Taking the PVC/PSCH system as an example, the binding energy of the system is the energy required for the separation of PSCH and PVC. The higher the binding energy is, the stronger the interaction between plasticizer and PVC is, and the more difficult it is for plasticizer to migrate out of the PVC system. In plasticized PVC system, its expression is as follows:

$$E_{\text{bind}} = E_{\text{total}} - E_{\text{PVC}} - E_{\text{Plasticizer}} \quad (11)$$

where in, $E_{\text{total}}$ is the total energy of binary mixed system, while $E_{\text{PVC}}$ and $E_{\text{Plasticizer}}$ are the energy of PVC and plasticizer (DOP and PSCH) separately. The energy of each system is calculated by MS simulation, as shown in Fig. 6e. Put the energy of each system obtained by simulation into formula (11) to calculate the binding energy of DOP and PSCH with PVC is 82.2 kcal/mol and 274.4 kcal/mol, respectively. It can be seen that DOP has the minimum binding energy with PVC. Compared with PSCH, DOP, as a traditional small-molecule plasticizer, has lower molecular weight and lower carbonyl density, which makes its interaction with PVC weaker. According to the lubrication mechanism, after adding small molecules of DOP between large molecules of PVC, DOP can act as the lubrication molecules between PVC molecules, reduce the interaction force between PVC molecules, and make PVC molecules slip more easily so as to achieve the plasticizing effect. However, the non-polar PSCH segment blocks the PVC molecules, and the polar groups C=O and C–Cl interact with PVC, thus reducing the interaction force between PVC molecules and achieving plasticizing effect.

### Conclusion

In this paper, the mechanical properties, durability, glass transition temperature and other properties of PVC plasticized by oligomeric polyester are studied. The plasticizing effects of oligomeric polyester and DOP are simulated by molecular dynamics using MS, and the relevant performance parameters of PVC plasticized by oligomeric polyester and DOP are calculated. The results show that the plasticizing efficiency of PSCH plasticizer is superior to that of other polyester plasticizers, up to 153%. The difference of solubility parameters DS between PSCH and PVC is the smallest, and the decrease of C–Cl bond energy in XPS also proves that PSCH can effectively reduce the polarity of PVC molecules. The binding energy simulation results of plasticizing system show that the binding energy between PSCH and PVC molecules is the highest, and PVC/PSCH samples still have good flexibility after 60 days of aging in cyclohexane, reflecting a great improvement in durability of PVC.

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### Declarations

Conflict of interest There are no conflicts to declare.

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