Effect of olefin block copolymer on the toughness of microcellular polypropylene composite

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Abstract
Microcellular polypropylene (PP) materials have wide applications in the automotive industry and other fields due to their low density, high heat resistance, and environmental friendliness. To improve the toughness of foamed PP materials, the olefin block copolymer (OBC) toughened foamed PP materials, PP-G-MAH as compatibilizer, were prepared by foaming injection molding (FIM) to study the influence of OBC elastomer on the toughness of foamed PP composites. The crystallization behavior showed that the addition of OBC could increase the crystallinity and reduce the spherulite size of PP0, which benefited the improvement of toughness. The rheological measurement demonstrated that the melt viscosity of various PP0/OBC samples was significantly improved in contrast to those of PP0, which was good for the formation of the cell. The microstructure images showed that the cell sizes of the core layer and transition layer in the vertical section reached respectively 40.4 μm and 27.3 μm, as the content of OBC was 20 wt%. When 20 wt% OBC was added, the impact toughness of PP composites increased by 2.3 times, and the plastic deformation of the cell wall in the impact profile increased maximum, which could absorb a lot of energy and benefit for toughening. The representative volume element (RVE) model of PP/OBC foamed materials was established to simulate its impact and tensile process, taking into account the effect of elastomers and cells. The simulation results showed that the stress concentration factor of foamed PP under impact load increased from 1.80 to 1.93 by adding 20 wt% OBC content and 15 vol% void fraction, while the stress concentration factor of foamed PP under tensile load increased from 1.6 to 2.07 by adding 15 wt% OBC content and 15 vol% void fraction. The impact toughness of foamed PP composites with 20 wt% OBC and the tensile toughness of that with 15 wt% OBC reached the maximum with a 14.2% void fraction.

1. Introduction

With the development of the automotive industry, the numbers of cars increase continuously year by year, which brings many environmental problems. To decrease vehicle weight and energy consumption, many lightweight plastics are widely used to manufacture automobile parts. For purpose of further development in lightweight automobiles, lots of researchers have explored the use of lighter foamed plastics.

Polypropylene (PP) has become a commonly used plastic in automobiles due to its advantages of low cost, high strength, chemical resistance, and easy molding [1, 2]. In the past years, the poor toughness and low-temperature brittleness limited further development and application of pure PP. To overcome the
shortcomings, many researchers have devoted themselves to studying the toughening and strengthening mechanism of PP composites [3–7]. At present, the most effective way to toughen the PP is by adding elastic particles. Previous studies have shown that elastomers can also improve cellular structure parameters. In recent years, researchers have studied many kinds of elastomers for toughening plastic materials, such as EPR, EPDM, SBS, SEBS, POE, OBC, and propylene-based elastomers [8–12]. The crazing & shear band theory, which becomes the mainstream elastic particle toughening theory, says that crazing and shear band are two different forms of energy consumption. When the crazing stress $\sigma_c$ is smaller than the shear yielding stress $\sigma_h$, the fracture mode is mainly crazing and brittle. When $\sigma_c > \sigma_h$, the fracture mode is mainly shear yield and toughness, when $\sigma_c = \sigma_h$, the matrix is at the ductile brittle transition point.

Recently, the effect of toughening on microcellular has been confirmed [13–15], which has aroused our interest. Past research showed that rubber particles can greatly improve the impact strength of foamed PP composite while reducing the weight. At the same time, it is also found that the addition of rubber particles can affect the cellular structure. The cellular structure and elastomers have an obvious function on the toughness of microcellular materials, but few reports focused on the synergistic toughening effect of cells and elastomers currently. Bao et al. studies the influence of cellular structure parameters on the impact and fracture toughness of isotactic polypropylene (i-PP) and found that cells with a size of 10$\mu$m have a good toughening effect [16]. Moreover, elastomer could influence the cellular structure, and in turn, the cell could affect the distribution of elastomer, in which this synergistic function could exert a good toughening effect.

The block copolymer with both rigidity and toughness is a good toughening agent. The hard segment has a higher melting temperature than the soft segment, which can be used as a heterogeneous nucleation point to improve cellular structure. The soft segment has better flexibility than the hard segment and can play a toughening role. Therefore, this type of elastic particle will be the mainstream of toughening agents in the future. The olefin block copolymer (OBC) is a new elastomer prepared based on POE [17–19]. OBC is composed of crystallizable hard segment (ethylene octene) with low $\alpha$-olefin content and amorphous soft segment (ethylene octene) with high $\alpha$-olefin content [20]. The hard segment has a higher melting and crystallization temperature, while the soft segment has a lower glass transition temperature [21]. Due to its special structure, OBC is a good toughening agent for plastic materials [22]. In the past, researchers have studied the toughening effect of various common elastomers. However, few works had focused on the toughening effect of block copolymers in foamed materials, not to consider the synergistic effect of elastic particles and cells.

In order to reveal the mechanism of synergistic effect between cell and elastomer, the solid and foamed PP/PP-G-MAH/OBC (PP0/OBC) samples were prepared by injection molding. The influences of elastic particles on the cellular structure and synergetic toughness of PP blends were studied in the aspects of crystallization behavior, rheological properties, toughening properties, impact profile, and the microstructure of particles and cellular structure. Finally, the representative volume element (RVE) model of foamed material was established based on the range statistics of cells in SEM to explain the strengthening and toughening mechanism of PP blends.
2. Experiment and method

2.1. Materials
Polypropylene (K8303) with a melt flow index of 3 g/10 min was provided by SI-NOPEC Yanshan Petrochemical Co., Ltd (Beijing); OBC (9100) elastomer with a melt flow index of 1 g/10 min was supplied by Dow Chemical; PP-G-MAH with grafting rate of 1.2% was provided by Dongyuan Ziheng Plastics Co., Ltd. High-pressure nitrogen with 99% concentration was provided by Wuhan Xiangyun Industry and Trade Co., Ltd. Corrosives xylene, commercially available.

2.2. Samples preparation and foaming process
In this experiment, five groups of samples including solid and foamed samples were set. The first sample was pure PP with 5 wt% PP-G-MAH, for the convenience, the first sample was called PP0. The second to fifth samples were based on the first sample with 5 wt%, 10 wt%, 15 wt%, and 20 wt% OBC respectively. The PP-G-MAH was added to improve the compatibility of the elastomers with the matrix [23]. The raw materials were dried in a drying oven (Shanghai Guangdi Instrument & Equipment Co., Ltd 101A-1, China) for 8 h, then mixed evenly with an agitator, finally granulated by a twin-screw extruder (Nanjing Giant Machinery Co., Ltd SHJ-20, China). Before the injection using an injection molding machine (Ningbo Hai-da Plastic Machinery Co., Ltd HDX50, China), the composite masterbatch should be dried at 80 °C for 8 h. The injection temperature section is 190 °C−200 °C−200 °C−190 °C. The injection pressure is 80 MPa, the gas saturation pressure is 16 MPa, and the cooling time is 16 s.

Figure 1 show the process of microcellular foaming. The supercritical N2 was injected into the barrel and mixed with the molten polymer to form a single-phase solution under the shear action of the screw. Then the solution was injected into the mold cavity and the thermodynamic instability caused by the pressure drop induced the nucleation of the cell. Finally, gas diffusion and coalescence of the cell nuclei made the cellular nuclei grow into stable cells.

2.3. Characterization
2.3.1. Mechanical performance test
Tensile tests were carried out in accordance with GB/T 1040–2006 at a speed of 50 mm min⁻¹; The notched Izod impact strength of the samples was tested in accordance with GB/T 1843–2008 with an impact energy of 2.75 J; All tests were performed at room temperature, and took the average of 10 tests as the experimental results.
2.3.2. Characterization of cellular structure

The microstructure and distribution of the elastomer particles and cells were characterized by scanning electron microscopy (SEM) of JSM-IT300 (JSM-IT300, JEOL Ltd, Tokyo, Japan). The solid and foamed samples were immersed in liquid nitrogen for 3 h in order to fracture at low temperatures. Before using SEM for observation, the samples were sprayed with platinum using a high vacuum ion sputtering instrument. Image-Pro was used to calculate the size and density of the cells on the fractured section.

The average size of the cells was determined by the following formula:

\[ D = \frac{\sum_{i=1}^{n} d_i}{n} \]  

Where \( D \) is the average cell size, \( d_i \) is the size of a single cell in a given region, and \( n \) is the number of cells in a given region.

The cell density can be determined by the following formula [24]:

\[ N = \frac{\rho_s}{\rho_f} \left( \frac{n}{A} \right)^{\frac{2}{3}} \]  

Where \( N \) is the density of cells (unit /cm\(^3\)), \( n \) is the number of cells in a given region, and \( A \) is the area of shooting area in SEM (cm\(^2\)). \( \rho_s \) and \( \rho_f \) are respectively the density of solid and foamed samples, which satisfy the following relationships,

\[ \frac{\rho_s}{\rho_f} = \frac{1}{1 - \phi} \]  

Where \( \phi \) is the void fraction of foamed samples.

The cells parallel to the melt flow direction were subjected to greater shear force during the growth process, large deformation would occur. In this paper, the ratio of length-diameter (d) and the offset angle (\( \theta \)) of the cells are used to characterize the amount of deformation of the cells, as shown in figure 2. The larger the ratio of length-diameter, the greater the deformation degree of the cell. The calculation formula of the ratio of length-diameter (d) is as follows:

\[ d = \frac{b}{a} \]  

The offset angle is defined as the angle between the long axis of the cell and the melt flow direction.

2.3.3. Crystallization behavior and morphology

The differential scanning calorimetry (DSC 214, Netzsch, Germany) was used to study the non-isothermal crystallization behavior of the material. The sample mass was about 10 mg, the purge atmosphere was N\(_2\), and the temperature was raised to 230 °C at a heating rate of 20 °C min\(^{-1}\) and then kept constant for 5 min. After the thermal history was eliminated, the temperature was reduced to 40 °C at a cooling rate of 10 °C min\(^{-1}\). The formula for calculating crystallinity is as follows:

\[ \chi_c = \frac{\Delta H}{\Delta H_0 \times \phi} \times 100\% \]  

Where \( \Delta H \) and \( \Delta H_0 \) are the melting enthalpies of the blend and the enthalpy of 100% crystallization. In this paper, the enthalpy for complete crystallization of PP is 209 J g\(^{-1}\), and \( \phi \) is the content of PP (After considering the content of PP-G-MAH, the obtained crystallinity is approximate crystallinity).

POM (carlzeiss/Germany Axio Scope Al A, Germany) was used to observe the spherulitic morphology of PP composites. First, the pre-dried pellets were heated to 230 °C at 20 °C min\(^{-1}\), kept at a constant temperature for 5 min, and then lowered to room temperature at 10 °C min\(^{-1}\), last observed the spherulitic structure under orthogonally polarized light.

2.3.4. Rheological behavior test

A capillary rheometer (CR6000, China) was used to measure the rheological properties of the material. The pre-dried masterbatches of about 12 g made by the extruder were put into the cylinder and heated to 230 °C. Then the shear rate and viscosity values corresponding to the seven descending rates were collected.

2.4. Multiscale simulation process

Both elastomer and cell have an important influence on the toughness of materials in the foamed composites. Previous studies have shown that elastomers can act as stress concentration points to induce crazing-shear yielding of the matrix and dissipate the energy of the matrix during impact. The cells can also act as stress
concentration points to induce the shear yield of the matrix and play a role in toughening the foamed material. In recent years, research on materials has continued to develop in the microscopic field, and multi-scale simulation has become one of the methods to link the macro and micro properties of materials [25]. As shown in figure 3, the effects of elastic particles and cell structure parameters on the properties of foamed composites were studied based on multi-scale simulation technology and the construct of Representative volume element (RVE).

The multiscale simulation required the acquisition of basic physical property parameters of materials, as shown in table 1. During the simulation, the following basic assumptions should be followed:

1. The elastoplastic model is used for PP, while the linear elastic model is used for elastomers;
2. The distribution of elastomers in the matrix is uniform and periodic;
3. The cell is spherical or ellipsoid in the matrix material to analysis expediently;
4. The uniaxial and shear peak strain $\varepsilon_{11} = 0.03$ was used for model loading.

### 3. Result and discussion

#### 3.1. Crystallization behavior

Crystallization behaviors have a significant influence on cell nucleation and cell growth in foamed polymers, among which crystallization temperature ($T_c$) and melting temperature ($T_m$) could give an important indicator for selecting foaming temperature. In general, the polymer interface between the crystallization regions and amorphous regions could be regarded as heterogeneous nucleation points, affecting the cell nucleation. The crystallization region could be acted as a physical cross-linking point to affect the cell growth. Therefore, it is necessary to study the crystallization behavior of PP composites.
Figure 4 plotted the DSC thermograms of the PP composite material, and the relevant parameters were summarized in Table 2. Results show that the crystallinity reaches 44.92% with the content of 20 wt% OBC. It could be seen from Figure 4 and Table 2 that the addition of OBC particles shifted \( T_c \) to the right, which indicated that the addition of OBC improved the crystallization ability of PP and makes PP crystallize prematurely. In addition, the addition of OBC also made \( T_m \) move to the right, indicating that the addition of OBC reduced the supercooling required for crystallization and promotes crystallization. The main reason of the temperature shift was that OBC had a large crystallization temperature and a lower melting temperature, while PP-G-MAH had a large crystallization temperature and melting temperature [19, 26]. Therefore, the thermal behavior of the blends was affected by the three phases of PP, OBC and PP-G-MAH.

Figure 5 showed the spherulitic morphology of PP composite taken under orthogonally polarized light. It can be seen that the PP0 has a clearer grain boundary, larger grain size, and fewer crystallization regions. With the addition of OBC particles, the size of spherulites gradually decreases, and the interface between spherulites became more blurred. The main reason lies in the heterogeneous nucleation of OBC, which makes PP form a small spherulite structure during the crystallization process. Another reason is that the soft segment of OBC hinders the diffusion and accumulation of PP molecular segments, impedes the growth of crystal grains, and destroys the spherulitic structure of PP.

The interface between crystallization regions could be regarded as the physical cross-linking point to affect cell growth. Therefore, reduced spherulites mean more cross-linking sites to support the cell nucleation and growth.

### 3.2. Rheological behavior

Figure 6 plotted the shear viscosity curves of PP composites. During the injection molding process, the viscosity of the polymer changed as a result of the temperature field and shear forces. Figure 6(a) showed that the increase of shear rate decreased the viscosity of the system, which could reflect the rheological properties of the polymer at the barrel of the injection molding machine, the needle valve and the inside of the mold. The viscosity of OBC is higher than that of PP, so the addition of OBC could improve the viscosity of PP blends [27]. Figures 6(b) and (c) showed the partially enlarged view at low and high shear rates. Figure 6(b) showed that the blends had higher viscosity at low shear rates, and the viscosity gradually increased with the content of OBC. Meanwhile, the addition of OBC led to the increase of the slope of the viscosity curve at a low shear rate, which indicated that the addition of OBC increased the sensitivity of the blends to shear rate. However, it could be noticed from figure 6(c) that the viscosity of PP blends decreased firstly then increased at the same shear rates. The viscosity of blends decreased by less than 1% compared to PP0 with the
addition of 5 wt% OBC, while the viscosity of the system increased by 12% in comparison to PP0 with the adding of 20 wt% OBC. It indicated that a small amount of OBC could improve the flowability of PP, while an excessive amount of OBC increased the viscous resistance to the movement of PP molecular chains. At the same time, the variation of OBC content at high shear rates, compared to low shear rates, made the blends less sensitive to shear rates. The viscosity also played an important role in the growth process of the cell. Low-viscosity polymers had little resistance to cell growth and thus resulted in larger cells, while high-viscosity polymers had a large resistance to cell growth and led to smaller cells. Therefore, it was necessary to study the rheological behavior on the effect of the cellular structure of PP composites. In addition, the dispersibility of OBC and air in PP would also cause a variation in the cellular structure.

Inside the barrel of the injection molding machine, the PP blends were in a low viscosity state due to the high shear of the screw, which facilitated a more homogeneous mixing of the gas and melts. In the injection foaming process, the degree of homogeneity of the gas and melt greatly affects the final cellular structure. After the melt was injected into the mold, the blends were in a high viscosity state. At this time, the growth of cells was resisted and smaller cells were obtained. Therefore, the high shear state in the early stage affected the cell nucleation, while the low shear state in the later stage affected the cell growth, and both stages had a direct effect on the final cellular structure.
The viscosity curve could also reflect the melt strength of the blends in some extent. The poor melt strength of PP0 could not support the growth of the cell and resulted in the rupture of the cell. The addition of adequate OBC could improve the melt strength and thus boost the nucleation and growth of the cell. Meanwhile, the increase of melt strength avoided the rupture of the cell.

3.3. Elastomer distribution
Figure 7 showed the elastomer distribution of PP/OBC. OBC presented a relatively regular spherical, and a uniform 'sea-island' distribution in the PP matrix. With the addition of OBC, the mean particle size of OBC in solid samples gradually decreased. The mean particle size of OBC reached 368.81 nm with a content of 20 wt% OBC, which can effectively prevent the expansion of the crazing. OBC, acting as a stress concentration point of the matrix, could induce a large number of crazes and form shear bands. The crazes and shear bands formed between adjacent OBC particles interfered and overlapped with each other, which hindered the development of the crazes into destructive cracks. Meanwhile, small particle size provided more nucleation sites for the blends, which could boost the nucleation of cells and increase cell density.

Interestingly, the mean particle size of foamed samples changed in contrast to the solid samples. The mean diameter of OBC in foamed PP increased from 368.81 nm to 491.50 nm in contrast to solid samples with 20 wt% OBC. The reason for the change in particle size lies in the result of the mutual influence of cell growth and melt solidification. In the process of solidification and crystallization of the melt, due to the different times required for the complete solidification of the elastomers and matrix, the growth of cells caused dispersion or aggregation of the particles, which in turn led to the change of the particle size.

Previous research had shown that the toughness of composites is closely related to the size of elastomer particles [7, 28]. Therefore, the cell could influence the toughness of the matrix by affecting the size of the elastomer particles.

3.4. Cellular structure
Figure 8 showed the cellular morphology of the vertical section and parallel section, and corresponding cellular structure parameters were plotted in figure 9. Due to the different cooling rates of the skin layer and core layer,
Figure 8. Cellular structure: (a) ~ (c) vertical section, (a’) ~ (e’) parallel section, (a), (a’) PP, (b), (b’) PP/5 wt% OBC, (c), (c’) PP/10 wt% OBC, (d), (d’) PP/15 wt% OBC, (e), (e’) PP/20 wt% OBC.

Figure 9. Cellular structure parameters: (a) The cell diameter of vertical section, (b) The cell density of vertical section, (c) The cell diameter of the parallel section, (d) The cell density of parallel section, (e) The ratio of length-diameter and offset angle of transition layer in the parallel section, (f) Void fraction.
the cell morphology presented an obvious multi-layer distribution including skin layer, transition layer, and core layer. The skin layer had a little cell, so the cellular structure parameters of the transition layer and core layer were summarized. From the figures 9(a) and (b), it could be noticed that, when 20 wt% OBC was added, the cell diameter of the core layer and transition layer in the vertical section decreased respectively to 40.4 μm and 27.3 μm, and the cell density improved respectively to $3.77 \times 10^5$ units cm$^{-3}$ and $7.42 \times 10^5$ units cm$^{-3}$.

Figures 9(c) and (d) plotted the cellular structure parameters of the parallel section. In parallel section, when 20 wt% OBC was added, the cell diameters of the core layer and transition layer decreased respectively to 58 μm and 43 μm, and the cell density improved respectively to $2.28 \times 10^5$ units cm$^{-3}$ and $6.45 \times 10^5$ units cm$^{-3}$. In addition, the cell of the transition layer in the parallel section presented a thin strip shape with an offset angle concerning the flow direction. When the 20 wt% OBC was added, the ratio of length-diameter and offset angle of cell reached respectively the minimum 3.5 and 4.9°.

The main reason for the above phenomenon was that, in addition to the shear force of the screw, the melt of the transition layer in the parallel section was also subjected to the force of the inner wall of the mold, which resulted in a larger ratio of length-diameter and offset angle during the injection process. Due to the shear action of the screw, the gas was dispersed into more droplets, and thus more cell nucleiated. Figure 2 showed the schematic diagram of the shear gradient, which indicated the transition layer had higher shear force resulting in larger cell deformation. The resulting curve showed that the maximum and minimum ratio of length-diameter and offset angle of cell would be got with the content of 15 wt% and 20 wt% OBC. The main factors affecting the ratio of length-diameter and offset angle are temperature and melt viscosity. The lower the temperature and the melt viscosity, the larger the offset angle and the ratio of length-diameter.

3.5. Toughening properties

Figure 10 showed the morphology of the impact profile and impact strength. It can be noticed that the addition of OBC particles could effectively improve the impact strength of PP0, but when the content of OBC reached 10 wt%, the increasing trend of impact strength slowed down. The impact strength of the foamed samples was higher than that of the solid samples at 0 wt% and 5 wt% of OBC content, indicating that the presence of cells had a toughening effect on the matrix. However, as the content continued to increase, the impact strength of foamed samples became lower than that of solid samples. The main reason was that the existence of cells changed the dispersibility of the particles. Previous studies had shown that the toughening of elastic particles was closely related to the diameter and the volume fraction, so this result was produced under the combined action of the cell and the elastomer.

It can be seen from figure 10 that foamed PP0 presents a smooth surface without obvious plastic deformation, which is closed to brittle fracture. However, with the addition of OBC particles, the cell wall
appeared to have significant plastic deformation, presenting typical ductile fracture characteristics. After the addition of 20 wt% OBC, the plastic deformation of the cell wall led to the largest extent with a much-tearing phenomenon.

Figure 7 showed that a large number of elastic particles dispersed in the cell wall, and these dispersed elastic particles had a good toughening effect on the matrix. Firstly, when subjected to external force, the stress concentration at the crack tip accelerated the crack expansion, and the cells could blunt the crack tip as well as form secondary cracks, consuming a quantity of energy through cell deformation; Secondly, when the crack expanded to the cell wall, a large number of elastic particles dispersed in it could act as stress concentration points to induce crazes and shear bands, hindering the expansion of cracks, or formed secondary cracks to consume energy. In fact, the presence of cells can also induce crazes and shear bands, which have a similar effect to elastic particles, but the toughening effect of cells is not as obvious as that of elastic particles. The main reason was that the existence of cells reduced the content of PP molecular chains per unit volume, which made it easier for molecular chains to move under external force, resulting in a decrease of toughness.

Figure 11 showed the tensile stress-strain curve of the solid and foamed PP composite. It can be found that the curve was a straight line at the beginning and the composite lied in the elastic stage. As the strain increased, the composite material yielded, but it could be found that the yield point of the foamed material was earlier than that of the solid material. It was mainly because of the plasticizing effect of cells on the matrix. The reason for plasticization was that the presence of cells reduced the content of PP in the same volume. At the same deformation, the PP molecular chains in foamed materials moved more than the solid materials, which led to an advancement of the yield point.

Moreover, the tensile strength of PP composites continued to decrease with the increase of OBC content. When 20 wt% OBC was added, the tensile strength of foamed PP0/OBC samples had decreased from 28 MPa to 15.5 MPa compared to solid PP0 samples. The reason is that the low tensile strength of OBC particles, and the decrease of the bearing area caused by the existence of cells. The strain of the foamed material is lower than that of the solid material. The reason lies in the difference between OBC and cells. OBC itself has a high fracture strain and can rely on its own volumetric strain to absorb energy, while cells mainly rely on the passivation and diversion of microcracks to improve the toughness of the matrix. In addition, according to past research, the fracture toughness of foamed materials is related to their solid strength, cellular structure parameters and relative density [29]. The relative density of foamed materials is always less than 1, and the weight of this item is higher than the vesicular structure item, which causes the majority of foamed materials have lower tensile strain at fracture than solid materials.

3.6. Multiscale simulation analysis
There is a relationship between cell diameter, cell density, and cell void fraction by mathematical deduction, as shown in the following formula:

\[
\phi \approx \frac{\pi}{6} D^3 N
\]

Where \(\phi\), \(D\) and \(N\) are respectively cell void fraction, cell diameter (cm), and cell density (units cm\(^{-3}\)).

In this work, the RVE model of the microcellular PP composites was established to study the cell diameter and cell void fraction on the mechanical properties, as shown in figure 3. Table 3 showed the stress cloud...
It can be noticed from figure 13 and table 3 that the cell size has little effect on the mechanical properties of the PP composites at the same volume fraction. From a horizontal perspective, in the elastic stage, the cell size did not affect the stress-strain of the PP composites, while at the yield stage, the cell size had a slight effect on the PP composite. Vertically, with the increasing content of OBC, the strength of PP composites gradually decreased, which was mainly due to the low strength and low modulus of OBC itself.

The toughening mechanism of elastomer and cell can be explained by craze & shear band theory. The stress concentration is the incentive to produce craze and shear band. The greater the stress concentration, the greater the tendency to produce crazes and shear bands. In order to analyze quantitatively the influence of elastomer and cell on the mechanical properties of PP, the stress concentration factor was introduced to characterize the stress distribution of the foamed composites.

\[
\alpha = \frac{s_{\text{max}}}{s_n}
\]

Where \(\alpha\) is the stress concentration factor, \(s_{\text{max}}\) is the maximum equivalent stress, and \(s_n\) is the average equivalent stress.

As can be seen in figure 12(f), the effect of cell diameter on the stress concentration factor varied considerably for different material systems. PP with a cell size of 20\(\mu\)m has a high \(\alpha\), however, due to the low viscosity and foaming ability of pure PP, it is difficult for pure PP to get excellent cell size. In fact, the real curve beneficial to the experiment process existed a shift in contrast to the theoretical curve, as shown in figure 12(f). The main reason lied in the multi-layer distribution of cellular structure in foamed samples.
Table 4 showed the stress cloud diagram of the RVE body model with different cell void fractions when the cell size was 20 μm, and the stress-strain relationship in the x-direction as shown in figures 13(a)–(e).

It can be seen from table 4 and figure 13 that, as the cell void fraction increased, the yield point of the material advanced, and the strength decreased at the same material system. The simulation showed that the tensile strength of PP composites with 20 wt% OBC and 15 vol% void fraction decreased to 15.51 MPa compared to pure PP. This is mainly because the increase of cell void fraction reduces the load area per unit, and at the same time, the decrease of matrix per unit volume results in the increase of displacement relative to the solid material under the same load, leading to an earlier yield point and a decrease in strength. At the same void fraction, with the increase of elastic particles, the strength of the material decreased, and the yield point advanced, which was consistent with the experiment.

In addition, table 4 and figure 13(f) could reflect the toughening effect of the cells on the matrix. It can be noticed from table 4 that, at the same material system, as the cell volume fraction increased, the stress percolation between cells increased. According to previous studies [30], the toughening of elastic particles depended on the thickness of the ligaments between the particles. The increase of cell void fraction reduced the thickness of the ligaments between the cells, making the stress state transition from the plane strain state to the plane stress state, resulting in increased toughness. From figure 13(f), as the cell volume fraction increased, the stress concentration factor increased, which was conducive to the formation of the craze & shear band. The stress

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Figure 12. The effect of cell diameter on uniaxial tensile stress-strain of PP composites with the same void fraction (0.1): (a) PP, (b) PP-5 wt% OBC, (c) PP-10 wt% OBC, (d) PP-15 wt% OBC, (e) PP-20 wt% OBC, (f) Stress concentration factor.
concentration factor of PP composites with 15 wt% OBC and 15 vol% void fraction reached the maximum 2.07 compared to the pure PP, which was consistent with the experiment.

Unlike the tensile process, the impact process can be simplified to a planar model, limiting the crack extends to the same plane for easy analysis. Table 5 showed the stress clouds of the RVE face model for different cell diameters when the void fraction was 0.1. It can be seen that the stress percolation in the loading direction gradually strengthened with the decrease of the cell diameter.

Table 6 showed the stress clouds of the RVE face model for different void fractions when the cell diameter was 20 μm. It can be seen that the stress percolation in the loading direction gradually strengthened with the decrease of the void fraction.

Figures 14(a) and (b) showed respectively the stress concentration factor curves based on table 5 and table 6. From figure 14(a), overall, it can be seen that the stress concentration factor of the PP blends increased with the addition of OBC content. When the OBC content was 20 wt%, the stress concentration factor increased from 1.63 to 1.89 concerning pure PP, while it can be seen from figure 14(b) that the effect of the void fraction on the stress concentration of PP blends was greater and more distinct. When the OBC content was 20 wt% and the void fraction was 15 vol%, the stress concentration factor increased from 1.80 to 1.93 relative to pure PP. In the

\[ \text{Figure 13. The effect of volume fraction on uniaxial tensile stress-strain of PP composites with the same cell diameter (20 μm): (a') PP, (b') PP-5 wt% OBC, (c') PP-10 wt% OBC, (d') PP-15 wt% OBC, (e') PP-20 wt% OBC, (f') Stress concentration factor.} \]
actual impact experiments, the impact toughness of PP foamed samples reached the best with the 20 wt% OBC content and the void fraction was 14.2% at this time, which was similar to the simulation results.

4. Conclusion

In this work, solid and foamed PP/PP-G-MAH/OBC (PP0/OBC) composites were prepared respectively via CIM and FIM technology. As the content of OBC increased from 0 to 20 wt%, the impact toughness of foamed PP0/OBC samples improved to 1.7 times in contrast to PP0. The addition of OBC brought about an ameliorative cellular morphology of PP0 and cell size as well as cell density. The cell sizes of the core layer and transition layer in the vertical section reach respectively 40.4 μm and 27.3 μm, and the cell density improved respectively to 3.77 × 10^5 units cm^{-3} and 7.42 × 10^5 units cm^{-3}. The tensile results revealed that the percentage elongation of solid samples increased to 7 times with 20 wt% con-tent of OBC in contrast to solid PP0, which showed that a good toughening function of OBC. The multiscale simulation showed that the stress concentration of foamed PP increased from 1.6 to 2.07 by adding 15 wt% OBC content and 15 vol% void fraction, while the tensile toughness of that improved to 2 times when 15 wt% OBC was added. The stress concentration of foamed PP increased from 1.80 to 1.93 by adding 20 wt% OBC content and 15 vol% void fraction, while the impact toughness of that improved to 2.3 times when 15 wt% OBC was added. However, the cell diameter had little effect on the tensile strength of PP composites at the same void fraction. The void fraction had a significant effect on the tensile strength of PP composites. The larger the void fraction, the lower the tensile strength. The simulation revealed that the tensile strength of PP composites with 20 wt% OBC and 15%vol void fraction was 15.51 MPa, while the actual tensile strength was 15.58 MPa in the experiment.
Table 5. Stress cloud of PP/OBC material with different cell sizes under impact load. (The void fraction = 0.1).

| Material   | 40µm | 60µm | 80µm |
|------------|------|------|------|
| PP         | ![Image] | ![Image] | ![Image] |
| PP-5OBC    | ![Image] | ![Image] | ![Image] |
| PP-10OBC   | ![Image] | ![Image] | ![Image] |
| PP-15OBC   | ![Image] | ![Image] | ![Image] |
| PP-20OBC   | ![Image] | ![Image] | ![Image] |

Figure 14. Stress concentration factor of foamed PP/OBC under impact load: (a) The effect of cell diameter with the same void fraction (0.1); (b) The effect of void fraction with the same cell diameter (20µm).
Table 6. Stress cloud diagram of PP/OBC material with different void fractions under impact load (Cell diameter = 20 μm).

|          | \( \phi =0.05 \) | \( \phi =0.1 \) | \( \phi =0.15 \) |
|----------|-----------------|-----------------|-----------------|
| PP       |                 |                 |                 |
| PP-5OBC  |                 |                 |                 |
| PP-10OBC |                 |                 |                 |
| PP-15OBC |                 |                 |                 |
| PP-20OBC |                 |                 |                 |

**Data availability statement**

The data generated and/or analysed during the current study are not publicly available for legal/ethical reasons but are available from the corresponding author on reasonable request.

**Author contributions**

Huajie Mao: Investigation, Formal analysis, Supervision. Hao Li: Software, writing-original draft, Validation, Writing- Reviewing and Editing. Wei Guo: Conceptualization, Project administration. Min Wu: Resources. Fankun Zeng: Validation.

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Conflicts of interest

The authors declare no conflicts of interest.

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