Assignment of mechanical properties of basalt-LDPE composite materials using experimental and computer aided simulation methods

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In this study, an experimental study and a computer aided simulation (CAE) have been performed to predict some mechanical properties of basalt filled low density polyethylene (LDPE) composite materials. This study uncovered that the basalt addition in the LDPE matrix affected the mechanical properties of the composite. In addition, the computer aided study results showed a consistency with the experimental study. These and similar studies are beneficial to the material determination of machine components, building structures, molds, dies, etc. Consequently, some satisfactory results have been obtained about the mechanical properties of LDPE composite up to 30% of basalt addition. Furthermore, a comparison has been realized between experimental and computational results. This study is promising about using computational design processes instead of the experimental procedures. Thus, both time spent will be able to significantly shorten and costs can be reduced.

Key words: Plastics, fillers, molding, mechanical properties, microstructure, CAE.

INTRODUCTION

Filled polymer forms are a specific class of composites, which are tending to replace many traditional material properties. Fillers have always played an important role in the plastics' industry. The original purpose of using fillers was to lower the cost of molding compounds. Nowadays, it is established that fillers are important for selective modification of properties. Various kinds of fillers are used and all of them fit well with the required application. Fillers are solid additives, differing from matrices of plastics in composition and structure, which are added to polymers to increase and improve bulk properties. Generally, inorganic materials and the few organic materials that occur frequently can be used for filler materials. Inorganic fillers are an important class of fillers in the plastics industry and various types of inorganic fillers are already being used commercially to modify the properties of compounds of the plastics. The inorganic fillers being used are calcium carbonate, various clays, barium sulphate, fine powders of some metals, aluminum trihydrate, aluminum hydrate, etc. Thermoplastics and thermoset industries have been using these fillers traditionally. These inorganic fillers have some limitations of use due to greater specific gravity and lower compatibility with the polymers. The use of the fillers should help lower the cost of many plastic products (Zurale, 1998). The polymer matrix composite based on the modified polyethylene have high physico-mechanical characteristics and low combustibility, which places them in the class of construction materials for engineering and technical applications (Naumova et al., 1999).

Polymers have been used as the large-scaled and widely spread due to at least two main basic characteristics of these materials like low density and
ease of processing. In fact, polymers can be shaped to different forms more cheaply and easily than metals or ceramic materials. It is a constant quest to develop lightweight building and machine materials with good mechanical properties. Lightweight materials can reduce the deadweight of structures, provide better thermal insulation for buildings, and cost less to transport and erect when prefabricated structural components are made in a factory. Using lightweight aggregates is one of the most common ways for making lightweight building materials (Wu and Sun, 2007). Mechanical properties are very important to investigate more controllable and effective methods of low-density polyethylene (LDPE). Previous reports show that the material used in construction of the die has great influence on sharkskin formation of polyethylene (Wu et al., 2004). The building industry is also a particular segment that is taking advantage of the use of polymers. Interior panels, nonstructural frames, and roofs are typical examples. These applications usually require, nevertheless, the use of additives to protect against UV degradation and fire (Sainn et al., 2004). Polyethylene (PE) was tested in three-point bending, and the incorporation of the additives always produced a decrease of the flexural strength. In particular, polypropylene (PP) or PE blend showed a promising mechanical performance. The study was undertaken on the application of thermoplastic polymers for interior panels. For low-strength interior panels used in the construction of low-cost housing applications as building and furniture (Petrucci et al., 2006).

In the earlier study, LDPE was considered as a potential replacement of wooden blocks used in a novel steel study design for building applications. The blocks would serve as thermal and, possibly, sound barriers in the all-steel assembly in contact with exterior or interior walls. Furthermore, short-term mechanical properties, performance requirements such as long-term flexural creep, thermal conductivity and flammability were determined and compared with wood (Xanthos et al., 2002).

Basalt is a fine grained compact rocks and tuffs, which are the major constituent of ocean islands and common component of the continental masses as well (Sainn et al., 2004; Beall and Rittler, 1976; Karamanov et al., 2009). Superior abrasion, wear and chemical resistant basalt-based materials are used in many applications. They can be used wherever the transport of material causes mechanical or chemical abrasion as well as mineral wool for heat, noise and fire insulation. Basalt finds wide application in industry as abrasion, wear and chemical resistant materials. It can also be used as filler material for production of the polymer matrix composites (Beall and Rittler, 1976; Yilmaz et al., 1996; Znidarsic and Kolar, 1991; Findik et al., 2002).

The main objective of the present study was to investigate the mechanical effect of the basalt addition as a filler material to the LDPE and comparison of the results with computer aided engineering (CAE) simulation methods.

### MATERIALS AND METHODS

#### Materials and experimental methods

Four different weight percentages of basalt (10 to 70 wt%) were introduced to LDPE to investigate the mechanical computer aided simulation relationships between LDPE and basalt combinations. The polymer matrix material that was used in this study is a commercial grade LDPE supplied from Turkish Polymer Industry. Natural basalt volcanic rocks obtained from Konya desert in the Middle Anatolia region of Turkey was used in polymer matrix composites.

Basalt composition used in the study was given in Table 1. The basalt was ground using a ring grinder and sieved within the range of 170 to 200 mesh. Test samples were manufactured as rectangle plates of the dimensions of 160 × 20 mm. For production of basalt filled polymers an Injection moulding machine which has three different heating stages of 165, 175, 180°C were used. Injection and molding pressures were applied as 5 and 9 MPa, respectively. The mould temperature was fixed at 30°C and the pressure was applied for 30 s. The tensile and flexural tests were realized using a universal Instron 3367 device with the standards of ASTM D 638 and ASTM D 790. The SEM studies of the basalt filled polymers were obtained by using Jeol JSM-6008LV Scanning Electron Microscopy. Before the SEM studies, the gold coating was applied on the samples surface for conductivity.

#### Computer aided simulation

##### Finite element method (FEM)

FEM is an approximate calculation method of the computer age, solves sophisticated engineering structure problems as making discretion to simple finite parts. Thus, the solution is carried out in each simple element of the structure separately. Afterwards, these solutions are assembled in a matrix algebra form and obtained partial results become a total result of the structure system.

Figure 1 represents a finite element region simulates a two-dimensional structure. Thus, a typical element labeled (e) and associated with nodes 1, 2, 3 and 4 is examined. The forces acting at the nodes are defined by the displacements of these nodes, the distributed loading on the element (p). The forces and corresponding displacements are defined by suitable elements (U, V and u, v) in a common coordinate system (x, y). The forces acting on all the nodes of the element (e) as a matrix:

<table>
<thead>
<tr>
<th>Compound</th>
<th>Wt.%</th>
</tr>
</thead>
<tbody>
<tr>
<td>SiO₂</td>
<td>45.88</td>
</tr>
<tr>
<td>Al₂O₃</td>
<td>18.20</td>
</tr>
<tr>
<td>Fe₂O₃</td>
<td>9.95</td>
</tr>
<tr>
<td>CaO</td>
<td>9.28</td>
</tr>
<tr>
<td>MgO</td>
<td>6.62</td>
</tr>
<tr>
<td>K₂O</td>
<td>1.64</td>
</tr>
<tr>
<td>Na₂O</td>
<td>4.76</td>
</tr>
<tr>
<td>P₂O₅</td>
<td>1.04</td>
</tr>
<tr>
<td>LOI</td>
<td>2.63</td>
</tr>
</tbody>
</table>
Figure 1. A two-dimensional structure assembled from individual finite elements and interconnected at the nodes.

\[
q^e = \begin{pmatrix} q_1^e \\ q_2^e \\ q_3^e \\ q_4^e \end{pmatrix}, \quad q^i = \begin{pmatrix} u_1 \\ v_1 \\ u_2 \\ v_2 \end{pmatrix}
\]

and nodal displacements:

\[
u^e = \begin{pmatrix} u_1^e \\ u_2^e \\ u_3^e \\ u_4^e \end{pmatrix}, \quad u^i = \begin{pmatrix} u_1 \\ v_1 \\ u_2 \\ v_2 \end{pmatrix}
\]

Characteristic equation of linear elastic behavior of the element:

\[
q^e = K^e u^e + f^e
\]

Here \( f^e \) represents the nodal forces required to stabilize the distributed loads on the element. Of course, same arguments and definitions can be applied generally. Therefore:

\[
q^n = \begin{pmatrix} q_1^n \\ q_2^n \\ \vdots \\ q_{4n}^n \end{pmatrix} \quad \text{and} \quad u^n = \begin{pmatrix} u_1^n \\ u_2^n \\ \vdots \\ u_{4n}^n \end{pmatrix}
\]

With each \( q^n \) and \( u^n \) have the same number of components or degrees of freedom. The stiffness matrices of the element \( e \) will clearly always be square:

\[
K^n = \begin{bmatrix} K_{11}^n & K_{12}^n & \cdots & K_{1n}^n \\ K_{21}^n & K_{22}^n & \cdots & K_{2n}^n \\ \vdots & \vdots & \ddots & \vdots \\ K_{n1}^n & K_{n2}^n & \cdots & K_{nn}^n \end{bmatrix}
\]

\( K_{11}^n, K_{22}^n, \) etc., are submatrices which have size \( l \times l \). \( l \) is the number of force and displacement components to be considered at each nodes, if \( u \) is assumed as the nodal displacements of the structure (Figure 1):

\[
U = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}
\]

Now for the whole structure in which all the elements participate, satisfies the first condition. This is necessary to establish equilibrium conditions at the nodes of the structure. The organized equations will contain the displacements as unknowns. The internal forces in elements, or the stresses, can easily be found by using the characteristics established for each element by the equations. The forces of all the components for a typical node \( a \):

\[
\sum_{n=1}^{N} q_{na}^n = q_1^a + q_2^a + \cdots = 0
\]

Here, \( q_{na}^n \) is the partial force to node \( a \) by element \( n \) and superscripts of the \( q \) are the number of elements.

If the forces contributing to node \( a \) from the Equation (3) and nodal variables \( u_a \) are common:

\[
\left( \sum_{n=1}^{N} K_{11}^{an} \right) u_1^{an} + \left( \sum_{n=1}^{N} K_{12}^{an} \right) u_2^{an} + \cdots + \left( \sum_{n=1}^{N} K_{1n}^{an} \right) u_n^{an} = 0
\]

If all such equations are assembled we simply have:

\[
K u + f = 0
\]

Submatrices of \( K \) and \( f \) are:

\[
K_{ab} = \sum_{n=1}^{N} K_{ab}^{an}
\]

and

\[
f_{a} = \sum_{n=1}^{N} f_{a}^{an}
\]

This is basic assembly process of all finite element calculations (Zienkiewicz et al., 2005).

**Boundary conditions**

In the structure of Figure 1, both components of displacement of Nodes 5 and 6 are zero and therefore:

\[
u_5 = u_6 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}
\]

can be expressed. This causes the reduction of the number of equilibrium equations by deleting the fifth and sixth pairs.
presented as contour form in tensile and bending areas show LDPE matrix. Computational tensile and scanning electron microscope (SEM) (Figure 3). The experimental results about the mechanical properties of the structural system can be solved to obtain nodal displacements and the internal forces for each element.

For the tensile analysis, geometry of the finite element model which was used in this study is a quarter shape of the experimental specimens. Thus, total element numbers and CPU times will decrease.

Material model

In this study, bilinear isotropic hardening (BISO) technique uses the von Mises yield criteria coupled with an isotropic work hardening assumption for large strain analyses has been adopted to simulate the behavior of the basalt filled LDPE. This material model assumes a bi-linear region in the Stress-Strain (σ-ε) diagram as elastic and plastic behavior (Figure 2). Here, $E_t$ is a plastic (tangent) modulus to characterize the plastic behavior of the material. This model gives the strain rate-independent reasonable results, especially in the determination of yield strength for basalt filled LDPE such as tensile and bending. Some studies were realized for different materials with similar techniques (Caliskan, 2006; Buyukkaragoz et al., 2008; Ivanyi and Ivanyi, 2009). ANSYS FEA software has been used for the simulations in this study.

RESULTS

Experimental results about the mechanical properties of basalt filled LDPE are in Table 2. Fractured surfaces of composite materials, including 10, 30, 50 and 70% basalt compositions. Flexural strength test was analyzed using scanning electron microscope (SEM) (Figure 3). The lighter areas reflect the basalt particle, and the darker areas show LDPE matrix. Computational tensile and bending results were shown in Table 3.

In Figures 4 and 5, stress and strain results were presented as contour form in tensile and bending analyses.

DISCUSSION

Addition in the LDPE as a filler material resulted to higher flexural strength, higher elastic modulus, and lower tensile strain to fracture, lower toughness and lower fracture energy. The reduction in the elongation with increasing basalt content in the basalt filled LDPE may have resulted from poor bonding strength of the basalt particles to the LDPE matrix. If the polymer chains have enough time and amorphous regions, the crystalline phase formation and orientation of chains during tests start immediately, and this causes an increase in elastic modulus of composite (Micusik et al., 2006; Luyt et al., 2006). Also, the filler added to the polymer matrix restricts the motion of polymer chains and thus lowers the tensile strain to fracture, sharply.

The addition of basalt shows no remarkable effect on the tensile strength of the composite’s fracture. According to the results, the higher the basalt content, the lower the stress and strain in the flexural test. The results calculated from CAD study were too close to the experimental study for 10 and 30% basalt filled LDPE composites. Over 30% basalt content, the results calculated decreased in the experimental study results.

While there is a small oscillation in the experimental tensile stress results in Figure 6. Figure 7 shows a good tendency between experimental and computational study results. There was a similar oscillation in Figure 8 as seen in Figure 6. In Figures 6 and Figure 8 show that remarkable differences over the 30% basalt content in the basalt filled LDPE composites. Consequently, there is a good equilibrium between experimental and computational results up to 30% basalt content in the composite.

Conclusions

The following conclusions can be drawn from the present study:

1. Basalt addition as a filler material to the LDPE matrix up to 30 to 70 wt % cause an increase in the flexural strength and elastic modulus.
2. Increase in the basalt addition to the LDPE resulted to decrease in the elongation at fracture.
3. Increase in basalt addition, isotropic structure degeneration, and therefore some unexpected results can be seen for over 30% basalt content.
4. These simulation method results have shown that for approximate design, this kind of studies is beneficial, especially for designers. Thus, design process time will significantly shorten, and experimental procedure’s cost will be reduced, and time will shorten. However, experimental studies are still essential in finish design.
Table 2. Experimental tensile and flexural properties of basalt filled LDPE.

<table>
<thead>
<tr>
<th>Basalt content (wt. %)</th>
<th>Tensile strength to fracture (MPa)</th>
<th>Tensile strain to fracture (%)</th>
<th>Flexural strength (MPa)</th>
<th>Elastic modulus (MPa)</th>
<th>Toughness (MPa.m$^{1/2}$)</th>
<th>Fracture Stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>7.29</td>
<td>266.53</td>
<td>6.44</td>
<td>138.68</td>
<td>18.96</td>
<td>81.91</td>
</tr>
<tr>
<td>10</td>
<td>6.96</td>
<td>132.33</td>
<td>6.88</td>
<td>206.77</td>
<td>8.85</td>
<td>35.97</td>
</tr>
<tr>
<td>30</td>
<td>7.08</td>
<td>43.49</td>
<td>8.71</td>
<td>290.08</td>
<td>2.86</td>
<td>11.62</td>
</tr>
<tr>
<td>50</td>
<td>5.87</td>
<td>14.80</td>
<td>10.88</td>
<td>458.94</td>
<td>0.78</td>
<td>3.43</td>
</tr>
<tr>
<td>70</td>
<td>6.87</td>
<td>4.17</td>
<td>12.57</td>
<td>1438.66</td>
<td>0.03</td>
<td>1.10</td>
</tr>
</tbody>
</table>

(a) (b) (c) (d)

Figure 3. The microstructure of the fractured surfaces of the composite ×500, (a) 10 wt % basalt, (b) 30 wt % basalt, (c) 50 wt % basalt, (d) 70 wt % basalt.

Table 3. Computational tensile and bending properties of basalt filled LDPE for a point belongs to fracture line.

<table>
<thead>
<tr>
<th>Basalt content (wt. %)</th>
<th>Tensile stress (MPa)</th>
<th>Tensile strain (%)</th>
<th>Flexural stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>8.045</td>
<td>305.9</td>
<td>7.53</td>
</tr>
<tr>
<td>10</td>
<td>7.568</td>
<td>193.2</td>
<td>7.157</td>
</tr>
<tr>
<td>30</td>
<td>7.164</td>
<td>125.4</td>
<td>6.951</td>
</tr>
<tr>
<td>50</td>
<td>2.763</td>
<td>36.4</td>
<td>2.73</td>
</tr>
<tr>
<td>70</td>
<td>2.451</td>
<td>36.9</td>
<td>3.507</td>
</tr>
</tbody>
</table>
Figure 4. Stress (left-a,c,e,g,i) and strain (right column-b,d,f,h,j) results in tensile analyses for pure LDPE and 10, 30, 50, 70wt.% basalt filled LDPE specimens, respectively.
Figure 5. Stress (left column a,c,e,g,i) and strain (right column b,d,f,h,j) results in bending analyses for pure LDPE and 10, 30, 50, 70 wt % basalt filled LDPE specimens, respectively.
Figure 6. Tensile stress comparison between experimental and computational results.

Figure 7. Tensile strain comparison between experimental and computational results.

Figure 8. Flexural (bending) stress comparison between experimental and computational results.
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