The reason for this research

PET is a form a plastic in a class of polymers called polyesters. They are called polyesters because they are long molecules with lots of structures that organic chemists call esters. The prefix poly means many. So, poly ester = many esters, or polyester. The letters PET come from its formal name which is diethylene terephthalate. PET is used for lots of things from clothing to soft drink bottles.

Just how long the PET molecules are is important to people in companies who make PET and the people and other companies that use it. The length of the molecules changes the properties of the plastic, so it’s important to be able to test the product to make sure that it has the molecule length that is wanted.

Determining the average length of these PET molecules is usually done by mixing samples is a suitable liquid and testing the viscosity of that mixture.

The viscosity is then compared to a correlation curve which is a kind of graph or math equation that tells the average length of the chains in the sample.

Hypothesis

Our hypothesis is: If the concentration of PET dissolved in PCA is increased, then—because of increased attractions between molecules—efflux time of the solution will increase and will do so in a way that can be used to determine the average molecular mass of PET samples.

The reason for this research

PET is typically manufactured with one of 2 catalysts: a titanium salt or an antimony salt. A catalyst can be defined as a substance that changes how fast a reaction proceeds but is not consumed by the reaction itself. The problem is that minute particles of the catalyst remain in the structure of the PET. Since PET is used as food and drink packaging, there is concern about the presence of these materials.

Titanium poses little risk, but antimony is a heavy metal with a serious health effect. Antimony is used as a catalyst because PET produced with it is almost clear while titanium catalysts produce PET with an undesirable yellow or gold color. The antimony exists in the PET packaging but in extremely small amounts and usually remains trapped in the polymer structure so its poses little risk.

Never-the-less, eliminating the need for any metallic catalysts—such as titanium and antimony—would be valuable development to the PET industry and consumers.

Conclusions

Even though we were faced with a number of technological challenges (some of which were unavoidable) the data and analysis of our experimental, scientific research were sufficient to conclude that propylene carbonate (PCA) is a suitable solvent for use in determining the average molecular mass of polyethylene terephthalate (PET).

A reasonable Mark-Houwink equation, which we determined to be [η] = 0.000624 x M<sup>0.608</sup>, can now be used to predict the molecular mass of PET samples. A reasonable correlation equation manufacturer’s [η] = [η] x [0.5657] also exists to further verify or refine our analysis and conclusions.

Future work:

Now that the feasibility of using PCA as a solvent for the average molecular mass determination of PET has been shown, more accurate measurements, of viscosity of PET in PCA should be done to determine more accurate viscosity values and correlation between viscosity and the average molecular mass of the PET samples produced.

Determing whether polyethylene carbonate can be used as a safer solvent for finding the size of molecules in polyesters

PET is a group of really long molecules built from a lot of smaller molecules. PET has to be built in a tank under very high temperatures and very low pressures. The structure above shows a very small section of those molecules. The water functional groups have been highlighted for you.

Hypothesis

Our hypothesis is: If the concentration of PET dissolved in PCA is increased, then—because of increased attractions between molecules—efflux time of the solution will increase and will do so in a way that can be used to determine the average molecular mass of PET samples.

Determing whether sodium dimethylsulphonate can be used as a substitute for heavy metal catalysts in synthesizing polyesters

Figure 2. This is a diagram of long molecules. Solutions, solvents, or esters are placed in the bottom. A vacuum is used to draw the liquid into the tube with the 2 tubes near the top. The liquid is heated using the top of the liquid to pump from one of 2 lines to the other. The viscometer looks like the temperature bath is filled with water. The temperature inside must be kept at 25.0°C.

Figure 3. This is what the mixing looks like when it’s in the constant temperature bath.

Figure 4. PET is a group of really long molecules built from a lot of smaller molecules. PET has to be built in a tank under very high temperatures and very low pressures. The structure above shows a very small section of those molecules. The water functional groups have been highlighted for you.

Figure 5. Repeat: test of PET.

Figure 6. The solution (PET) and the solvent (PCA) must be heated to about 210°C to get them to mix together into a solution. Once they cost, the mixture forms a suspension if the PET molecules are very large. They can be used as a solution when the PET molecules are small enough.

Figure 7. This is what the mixing looks like when it’s in the constant temperature bath.

Figure 8. This is a diagram of long molecules. Solutions, solvents, or esters are placed in the bottom. A vacuum is used to draw the liquid into the tube with the 2 tubes near the top. The liquid is heated using the top of the liquid to pump from one of 2 lines to the other. The viscometer looks like the temperature bath is filled with water. The temperature inside must be kept at 25.0°C.

Figure 9. This is a diagram of long molecules. Solutions, solvents, or esters are placed in the bottom. A vacuum is used to draw the liquid into the tube with the 2 tubes near the top. The liquid is heated using the top of the liquid to pump from one of 2 lines to the other. The viscometer looks like the temperature bath is filled with water. The temperature inside must be kept at 25.0°C.

Figure 10. This is a diagram of long molecules. Solutions, solvents, or esters are placed in the bottom. A vacuum is used to draw the liquid into the tube with the 2 tubes near the top. The liquid is heated using the top of the liquid to pump from one of 2 lines to the other. The viscometer looks like the temperature bath is filled with water. The temperature inside must be kept at 25.0°C.

Figure 11. This is a diagram of long molecules. Solutions, solvents, or esters are placed in the bottom. A vacuum is used to draw the liquid into the tube with the 2 tubes near the top. The liquid is heated using the top of the liquid to pump from one of 2 lines to the other. The viscometer looks like the temperature bath is filled with water. The temperature inside must be kept at 25.0°C.

Figure 12. This is a diagram of long molecules. Solutions, solvents, or esters are placed in the bottom. A vacuum is used to draw the liquid into the tube with the 2 tubes near the top. The liquid is heated using the top of the liquid to pump from one of 2 lines to the other. The viscometer looks like the temperature bath is filled with water. The temperature inside must be kept at 25.0°C.

Figure 13. Reaction vessel (left) and autoclave (right) to prepare for testing in the viscometer.

Figure 14. Reaction vessel without the heating mantle and insulation.

Figure 15. First PET product removed from the reaction vessel using DMA.

Figure 16. Ray Tedder adds liquid nitrogen (which has a temperature of -196°C) to a special container called a Dewar. The liquid nitrogen to keep a flask in the vacuum system extremely cold to collect side products of the PET synthesis.

Figure 17. Liquid nitrogen boils at ~196°C around the flasks that is capturing side products of the PET synthesis reaction.

Figure 18. Ray Tedder tightens one of the fittings around the piston where it is a heat sealed reaction vessel to eliminate a leak. Leaks must be minimized because the pressure inside the vessel must be kept below 6190 psi at normal atmospheric pressure.

Figure 19. Dr. Posey is using a head gun to melt some side product solids that have collected at the end of the reaction while Tedder watches. These low molecular mass materials are boiled in the reaction vessel but they tend to test the vacuum system and must be removed.

Figure 20. Dr. Posey (left) and John Svec (right) remove PET product from the reaction vessel after the synthesis process has ran it's course.