Properties of Plastic Cellulosic Composites through Simulation Techniques Using Accelrys Materials Studio 6.1

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Abstract

Molecular dynamics simulations permit the study of complex, dynamic processes that occur in biological systems. It is the most detailed molecular simulation method which computes the motions of individual molecules. This technique solves equations of motion for a large number of particles in an isolated cluster or bulk and has become a powerful tool for answering scientific problems as numerical experiments for new materials without synthesizing them. Recently attention has been drawn to the utilization of bio-reinforced composites in several applications due to an increased concern for sustainability. Recent studies in Wood Plastic Composites (WPCs) that use materials other than wood with are taking a special emphasis on the utilization of more basic foundations such as Cellulose which is important component produced by every plant and it is the most abundant biological molecule in the world. This study investigates the miscibility and mechanical properties of pairings of cellulose and lignin with several different polymer matrices such as HDPE using molecular dynamics simulation techniques with the Accelrys Materials Studio 6.1 software.

Introduction

Applications of WPC

- Decking and railing
- Industry
- Automotive
- Construction

Benefits

- Environmentally friendly
- Low maintenance
- More dimensional stable and lower absorption than wood

WPC Market

- In 2004, the EPA restricted the residential use of CCA treated wood decking
- 2005 market size $956 million
- Forecasted market for 2013 was $5 billion
- Competition
    - Trex: $2.12/ linear ft.
    - ChoiceDek: $1.83 - $2.00/ linear ft.
- Wood fibers represent 40% to 60% of an average size chile plant which represent approximately 51% of chile wood fibers after drying

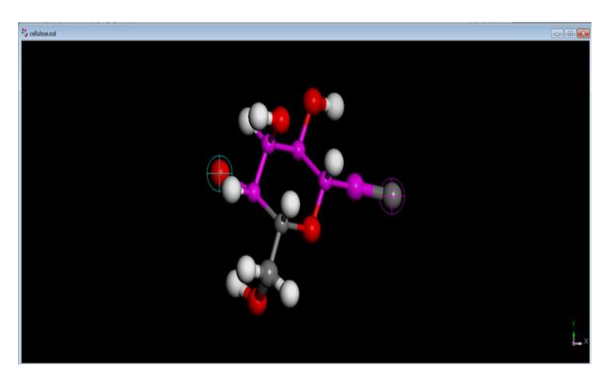
Hypothesis/Objectives

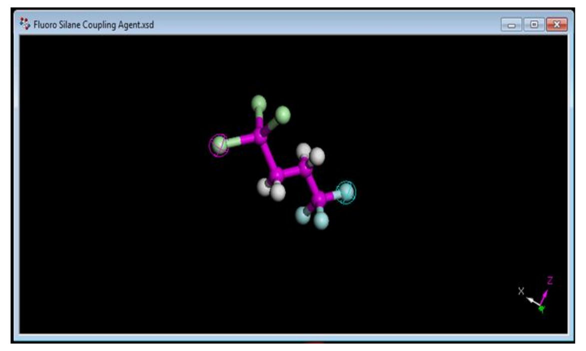
- Using experimental data to build a simulation model to imitate experimental methods with the expectations to get same results.
- Use the Simulation model to predict experimental results

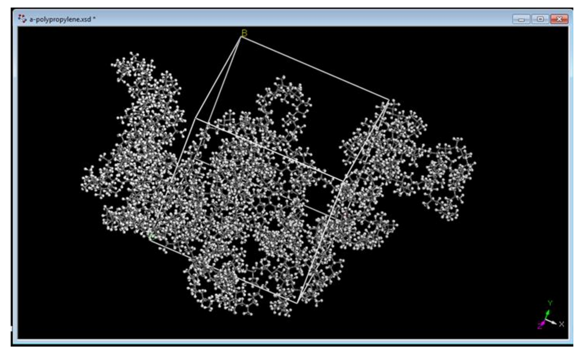
Methods

	100%PP	63.75%, 21.25%, 11.25%, 3.75% *Combination #1*	70%PP 20%W 5%FR 5% Coupling *Combination #2*	60% PP, 30% W, 10% coupling *Combination #3*
		30mesh	*30mesh*	*30mesh* (590μm)
Average UTS (MPa)	32.78539	19.3143	24.9531	16.960
Ave Yield Stress (MPa)	22.64914	8.9452	9.2084	19.05665

Category	Factor	Value
Material	Composition: % of Wood	21.25%, 20%, 30%
	% Polypropylene	100%, 63.75%, 70%, 60%
	Grain size of Wood	30 mesh
	Fire retardant	11.25%, 7.5%
	Coupling Agent	7.5%. 3.75%
	UV stabilizer	0%, 3.75%
Processing	Barrel and nozzle temperature	400 ˚F
	Injection Time	15 sec
	Melting residence time	20 min
	Mold Temperature	140 ˚F

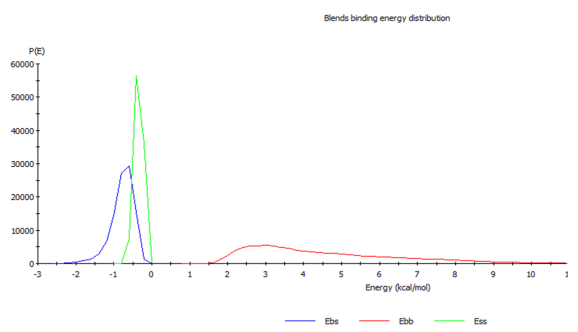






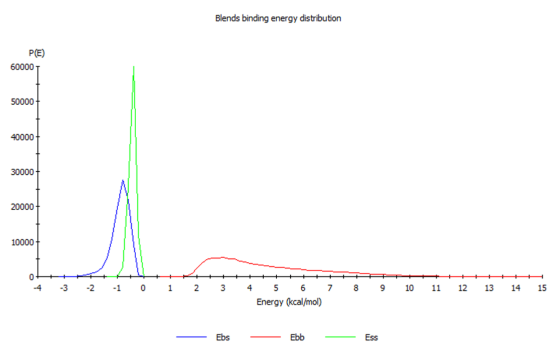
Data and Results

Analysis of Cellulose and Polyethylene Miscibility – Blends binding energy distribution



Values of important Parameters
Chi (298K) Emix(298K)
-14.39051422 -8.52188317

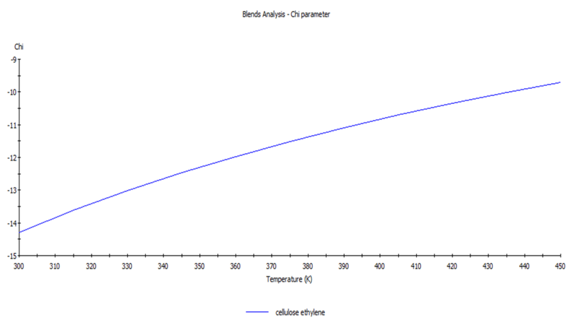
Analysis of Cellulose and Polypropylene Miscibility – Blends binding energy distribution



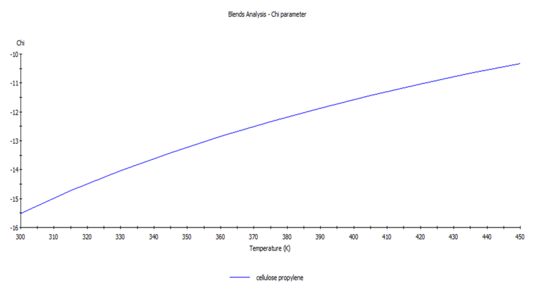
Values of important parameters:
Chi (298K) Emix(298K)
-15.61885338 -9.24929031

- These quantities suggest that polypropylene and cellulose do not mix properly

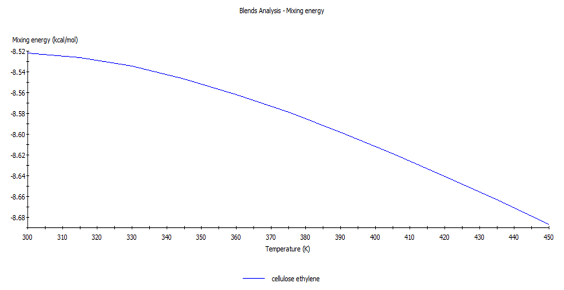
Analysis of Cellulose and Polyethylene Miscibility – Blends Analysis – Chi Parameter



Analysis of Cellulose and Polypropylene Miscibility – Blends Analysis – Chi Parameter



Analysis of Cellulose and Polyethylene Miscibility – Blends Analysis – Mixing Energy



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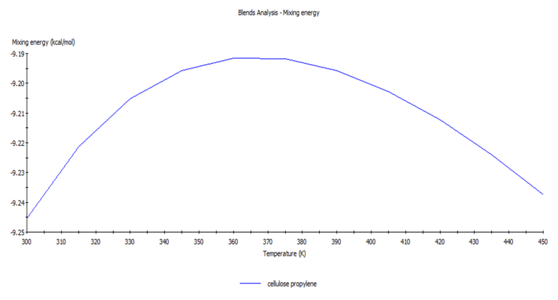

Conclusions

- Through molecular dynamic simulation we can obtain a valid model, thus reducing time and cost, testing different ratios in a faster and more efficient manner, and predict the miscibility and mechanical properties of the different components in wood-plastic composites.
- A Chi parameter analysis from 300K to 450K suggests that, although the miscibility of cellulose_ethylene increases as temperature increases, not enough miscibility takes place.
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- From literature we know that this is true.

Future Research

- To investigate degradation pathways and profiles as a function of composition and manufacture.
- Identify degradation models to provide an explanation of the behavior the samples exposed to UV light.
- To investigate UTS and yield stress.
- To develop simulation models that make predictions of physical properties.

Acknowledgments

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