Improving the Accuracy and Reliability of Models Used to Predict Multilayer Packaging Film Properties

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SPE International Polyolefins Conference

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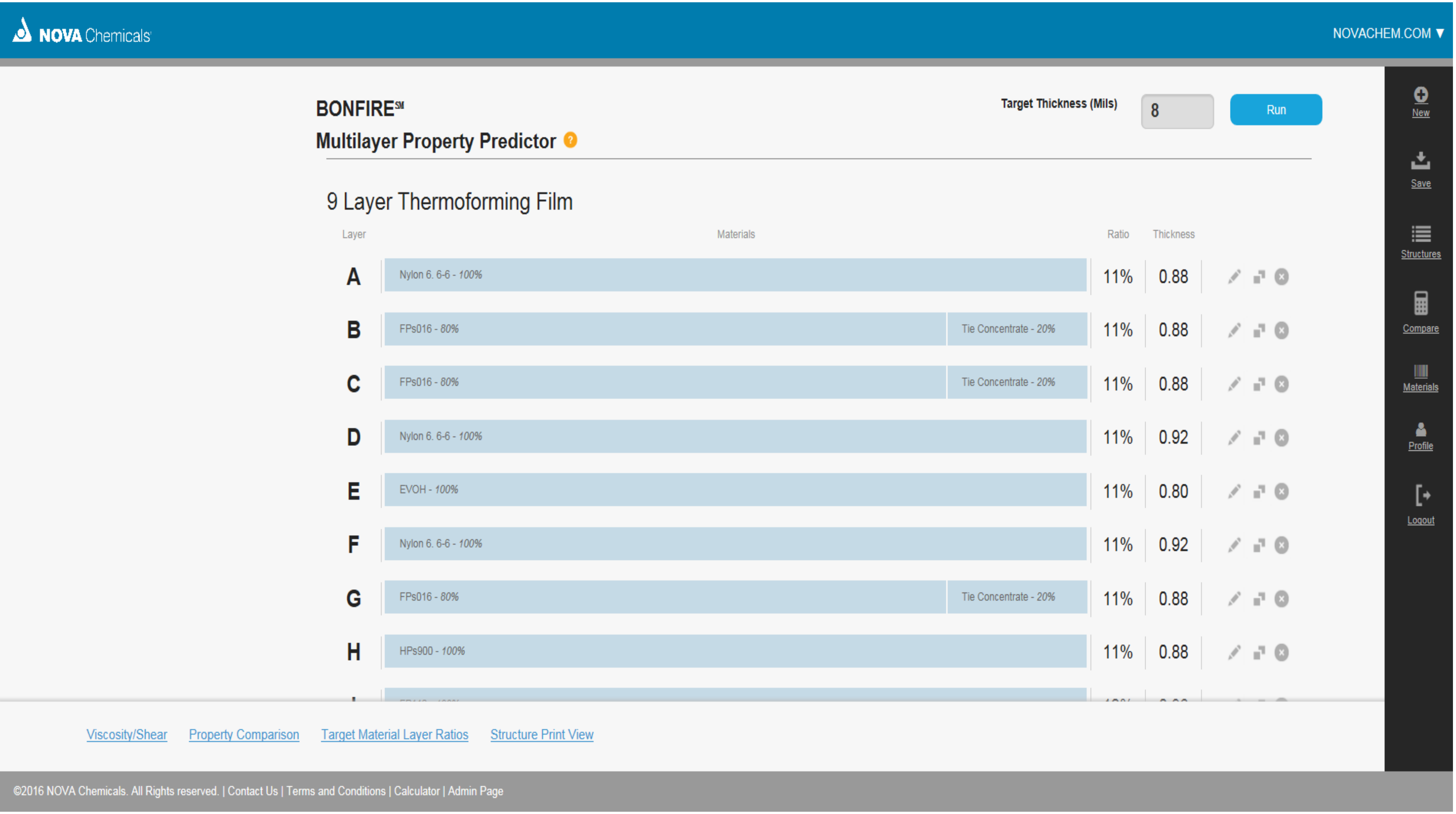
Bonfire℠
Multilayer Property Predictor Structure Input Screen



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Bonfire℠
Property Estimates and Structure Comparisons

New
Save
Structures
Compare
Materials
Profile
Logout

Property Comparisons

9 Layer Thermoforming Film - Reduced Nylon	9 Layer Thermofor	Delta	Units
0.01 OTR	0.01 OTR	1%	cc/100in2-day-atm
0.24 WVTR	0.25 WVTR	-6%	g/100in2-day
1049.6 1% MD Sec Modulus	1393.3 1% MD Sec Modulus	-25%	MPa
3.3 Penetration Energy	2.6 Penetration Energy	24%	Joules
918.4 MD Tear	739.2 MD Tear	24%	Grams
389.2 Bending Stiffness	560.3 Bending Stiffness	-31%	N-µm
1.56	1.72	-9%	$ / LB

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Model *Starting* Assumptions and Calculations

1. Most material physical properties are linear and proportional to gauge

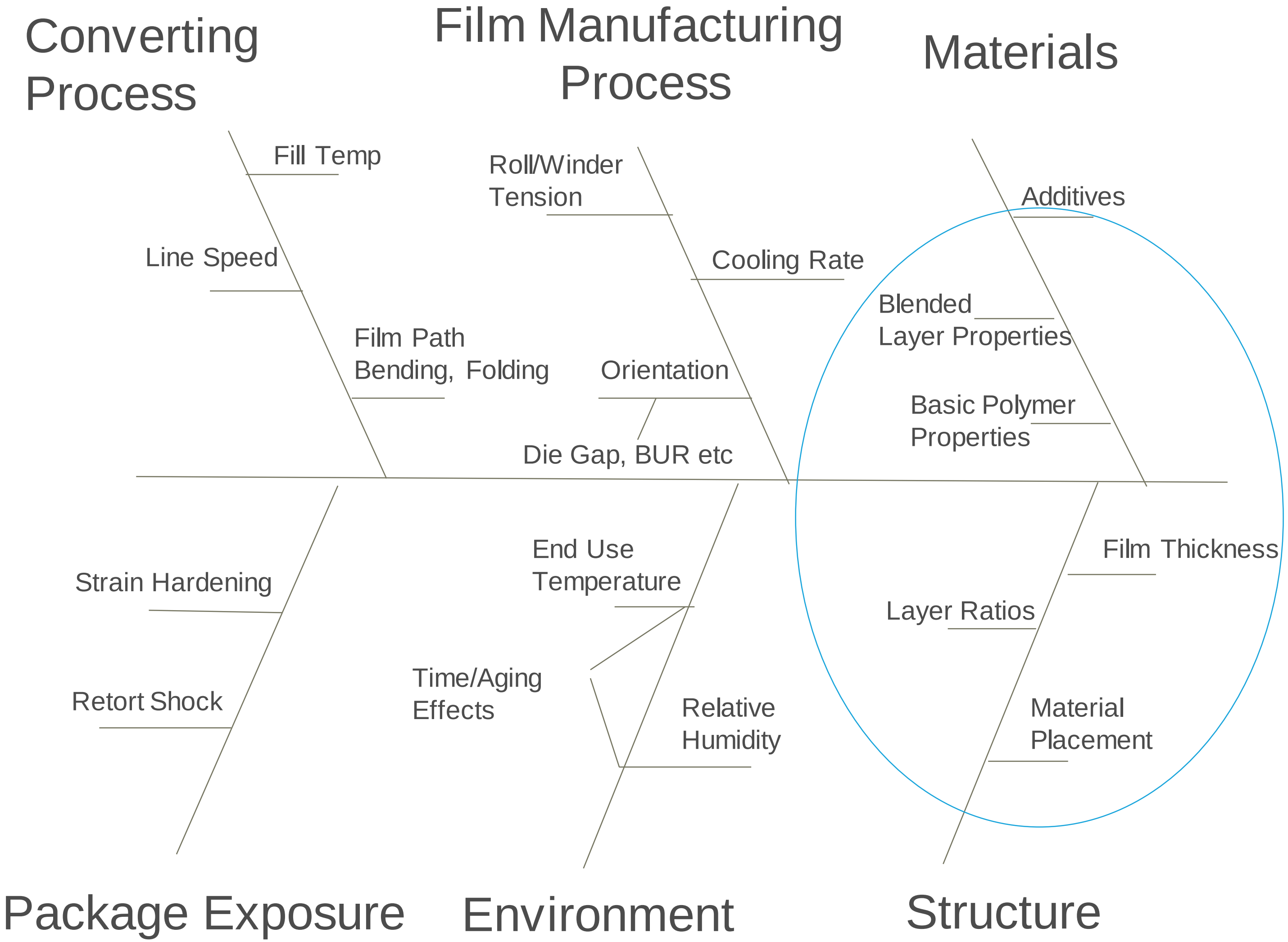
2. Properties of individual layers are additive. (No layer interactions)

3. The properties of blended layers average out proportionally to blend ratios by weight.

4. Film processing effects and package end-use conditions are “standard” or constant and not considered initially.

STRATEGY: Start with a flexible modeling platform that can easily incorporate new findings, properties and relationships.

Factors Affecting Final Film Properties



END GOAL:

Develop an integrated model that accurately predicts a broad range of film properties from basic relationships and accounts for important interactions, manufacturing and end use conditions

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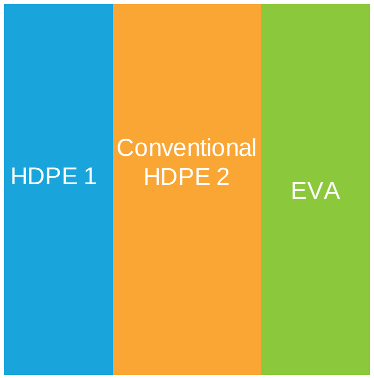
Case Study #1: Blend Effects

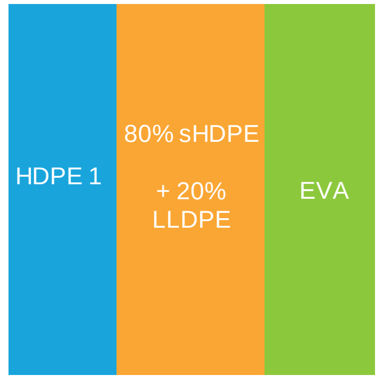
Estimating Permeability in Coex Films with Blended HDPE Layers

3-Layer Coex film for Cereal Liners and Dry Food Packaging

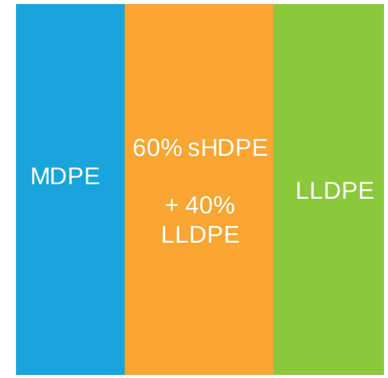
Traditional Structure



Test Structure # 1



Test Structure #2



	Traditional Structure		Test Structure 1		Test Structure 2 (modified structure)	
Property	**Actual Value**	**Predicted Value**	**Actual Value**	**Predicted Value**	**Actual Value**	**Predicted Value**
Gauge (mils)	2.2	-	2.0	-	1.9	-
Cost (cents/MSI)		5.58		5.86		5.01
WVTR (g/100in2-day)	0.18	0.19	0.12	0.26	0.15	0.45

6 % Difference   > 100% Difference   300% Difference

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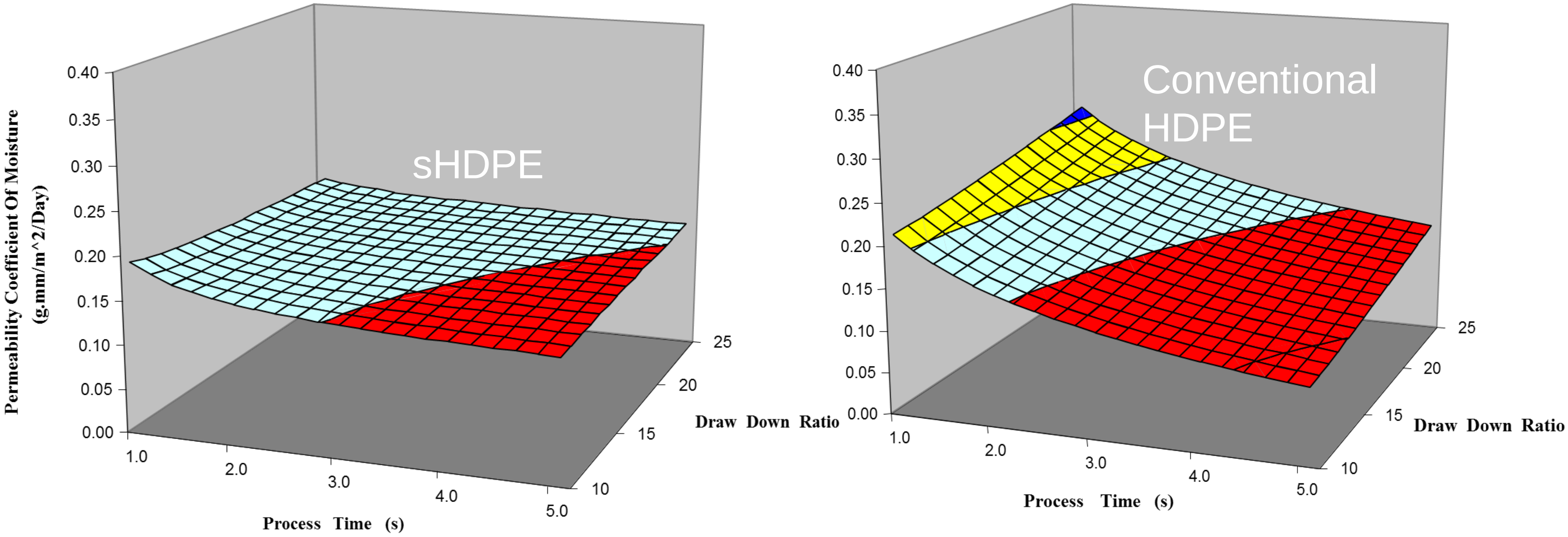
Processing or Orientation Effects?

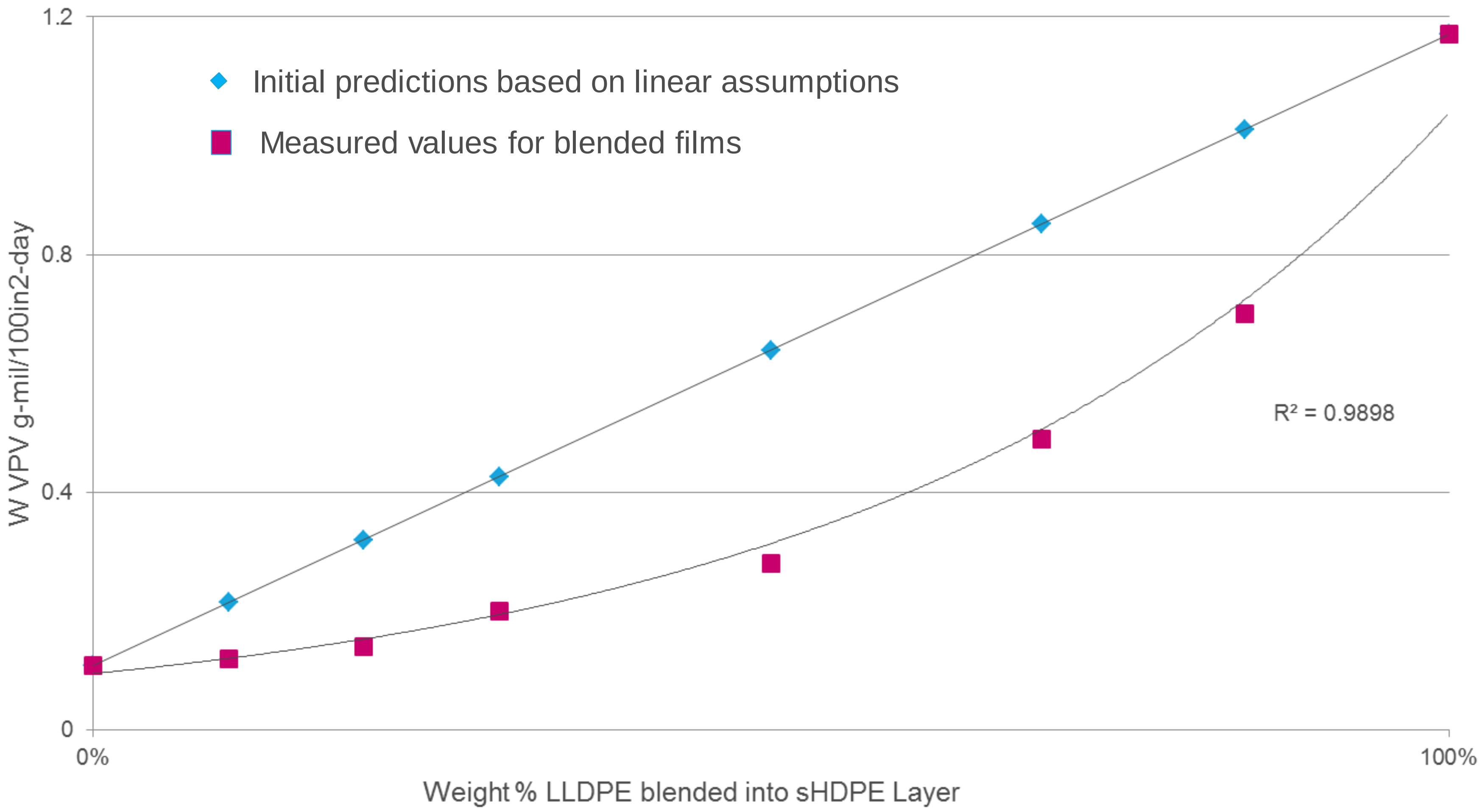


Aubee, N. and Lam, P., *Influence of Blown Film Process Conditions on Moisture Barrier Properties of HDPE*
TAPPI PLACE CONFERENCE (2006)

Effects of other layers? *Layer Interactions or surface effects etc.*

Blend effects? ***Weighted ratio assumption is inaccurate for sHDPE + LL blends.***

Predicted and Actual Water Vapor Permeation Values of sHDPE Blends with LLDPE



Blend data provided by Norman Aubee, NOVA CHEMCIALS CORPORATION

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Improved Permeability Estimations in sHDPE Structures

Incorporate Conditional Formatting (logic gate) into calculation

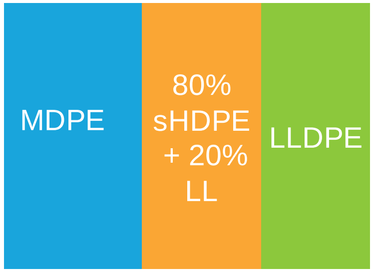
=IF (Component 1=“sHDPE“& Component 2= LLDPE),use equation 2
=IF NOT, use equation 1

	Test Structure 1			Test Structure 2		
Property	**Actual Value**	**Initial Predicted Value**	**Revised Predicted Value**	**Actual Value**	**Initial Predicted Value**	**Revised Predicted Value**
WVTR	0.12	0.26	0.13	0.15	0.45	0.16

5% Difference

7% Difference

Optimized Structure
- ✓ Lowest MSI cost
- ✓ Meets barrier specs
- ✓ Good balance of physical properties



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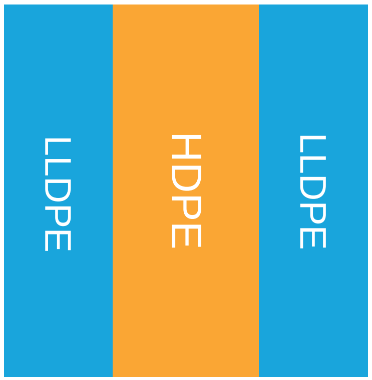
Case Study #2: Layer Interaction Effects

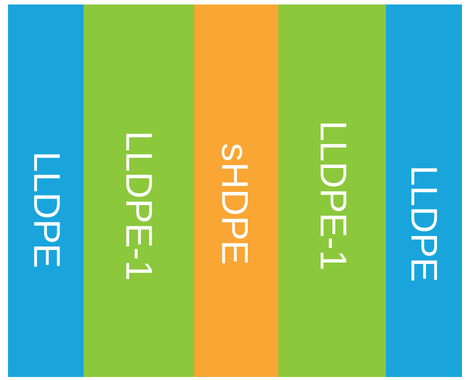
Loss of LLDPE Tear Strength in HDPE Coex Structures

Coex Sealant Web for Frozen Food Packaging

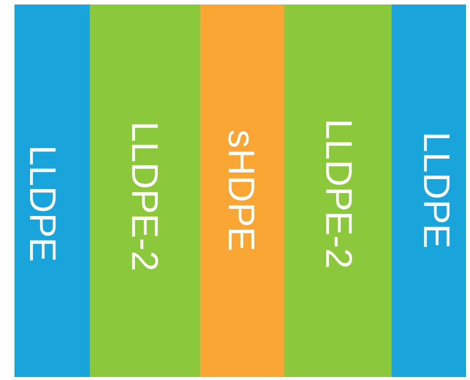
3 Layer Control
3 mil total gauge



5 Layer Test Structure # 1
2.7 mil



5 Layer Test Structure # 2
2.7 mil



	Control Structure		Test Structure 1		Test Structure 2	
Property	**Actual Value**	**Predicted Value**	**Actual Value**	**Predicted Value**	**Actual Value**	**Predicted Value**
Cost (cents/MSI)		7.80		6.83		7.06
O_2 Barrier (cc/100in2-day-atm)	85	81	84	82	85	83
MD Tear Strength (grams)	250	550	136	476	177	625

>100% Difference

~300% Difference

350% Difference

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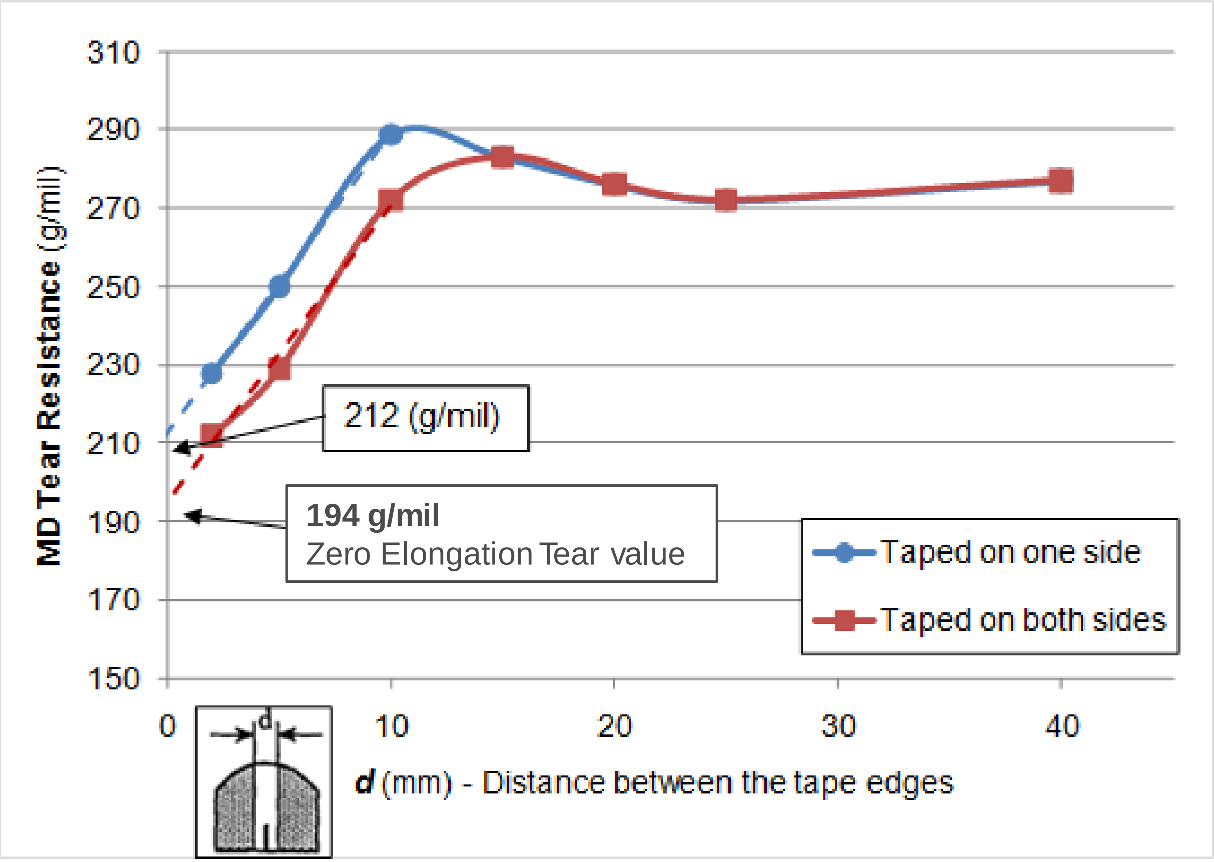
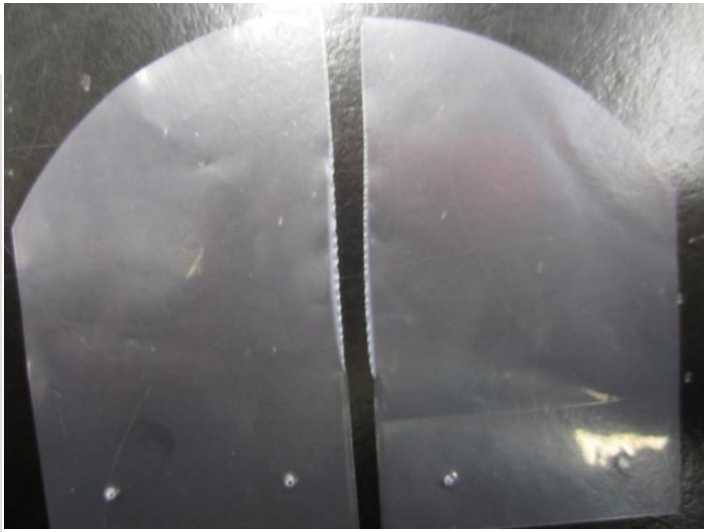
Restricted Elongation Affects the Tear of LLDPE Layers and Structure





REFERENCE: Tearing resistance of multi-layer plastic films
R.-Y. WU 1 , L,D. McCARTHY 1 and Z.H. STACHURSK
International Journal of Fracture 68:141-150, 1994.

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Improving Tear Estimations in LLDPE/HDPE Coextrusions

Determine "zero-elongation" tear values for LLDPE layers
Incorporate Conditional Formatting Into Calculation

= IF (Layer X = HDPE & Layer Y = LLDPE), use zero elongation tear

= IF NOT, use standard tear

	Test Structure 1			Test Structure 2		
Property	Actual Value	Initial Predicted Value	Revised Predicted Value	Actual Value	Initial Predicted Value	Revised Predicted Value
MD Tear	136	550	152	167	625	185

12% Difference

17% Difference

Optimized Structure

- ✓ Lowest MSI cost
- ✓ Meets barrier specs
- ✓ Good balance of physical properties

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Case Study #3: Environmental Effects:

Relative Humidity Effects on Properties of Polyamide Coex Films

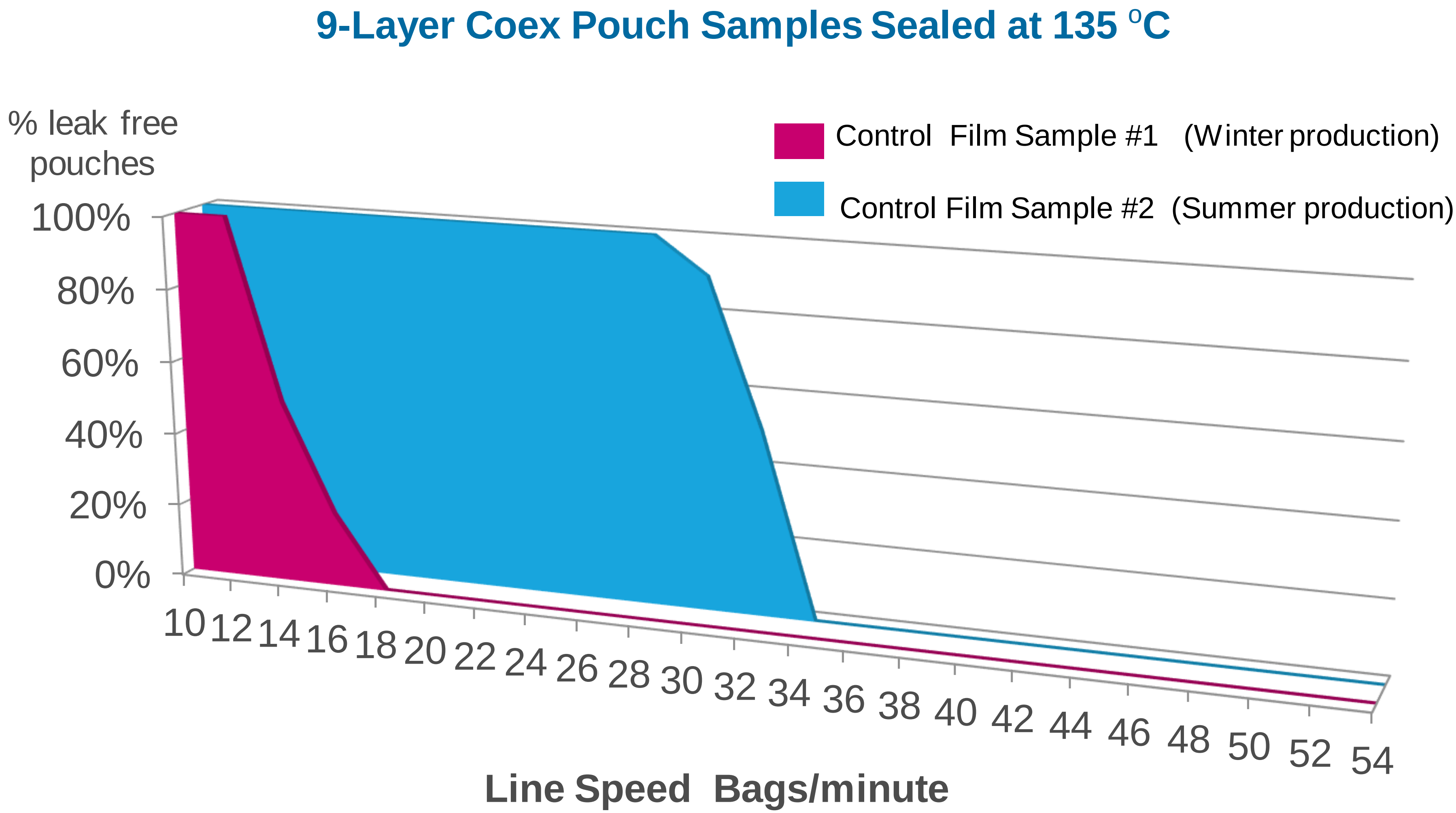
Test Film for Liquid Packaging Application

9-layer Coextruded Film Structure

Layer	A	B	C	D	E	F	G	H	I
Layer ratio	11	11	11	11	12	11	11	11	11
Material	**Sealant**	sLL	sLL	sLL + 20 % tie	Nylon	sLL + 20 % tie	sLL	sLL + 20 % tie	Nylon
Layer Designation	Seal			Tie layer	Core	Tie layer		Tie layer	Skin

- 89.9 um film gauge, equal layer ratios
- Blown film, 160 mm Brampton die, 113 kg/hour production rate
- Nylon core and skin layers = Nylon 6/6,6
- Tie concentrate = DuPont BYNEL® 41E710
- sLL interior layers = NOVA Chemicals SURPASS® FPs016 resin

Pouch Pass Rate for Coex Films vs. Line Speed



Primary Mode of Bag Failure:	Channel Leakers at Edge Fold

Effect of Relative Humidity on Physical Properties of Polyamide Coex Films

Key Difference:

Control Film #1 was stored at tested under low ambient RH conditions

- Mean (Winter) Storage Relative Humidity = 55%

Control Film #2 was stored and tested under high ambient RH conditions

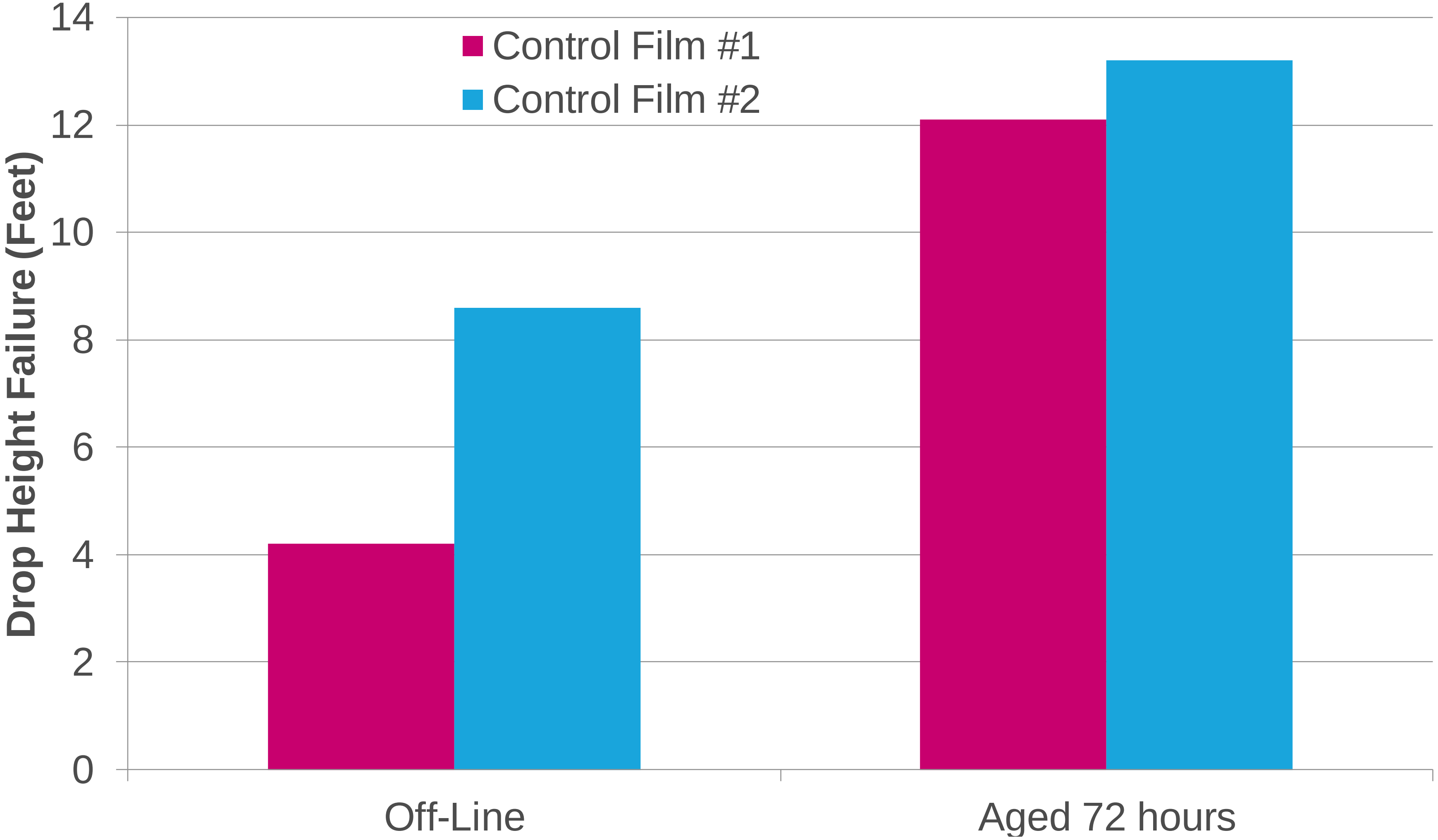
- Mean (Summer) Storage Relative Humidity = 74%

NEW CONTROL TEST FILM - IDENTICAL ROLLS STORED IN CONTROLLED RH CHAMBER FOR 72 HOURS BEFORE TESTING

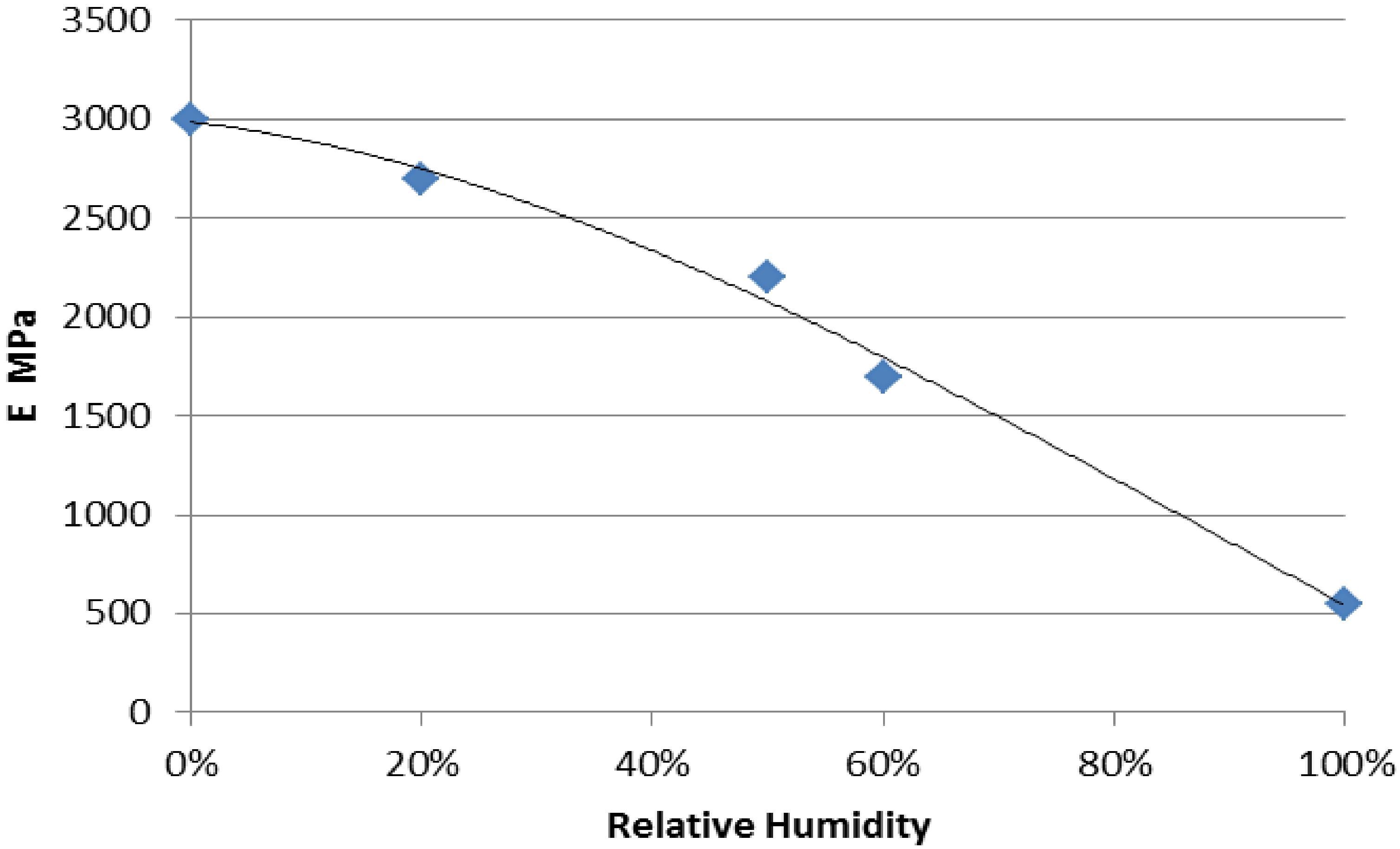
Test	Units	Film Conditioned at 30% RH	Film Conditioned at 50% RH	Difference
Impact Energy	Ft-Lb	1.17	1.93	65%
Secant Modulus MD 1%	MPa	730	304	-58%
Secant Modulus TD 1%	MPa	669	332	-50%
Film Tensile at Yield MD	MPa	28	22.5	-20%
Film Elongation at Yield MD	%	6	9	50%

Drop-Tower Failure Height for VFFS Water Filled Pouches Made with PA Coex Films

Pouches converted at 10 Bags/minute

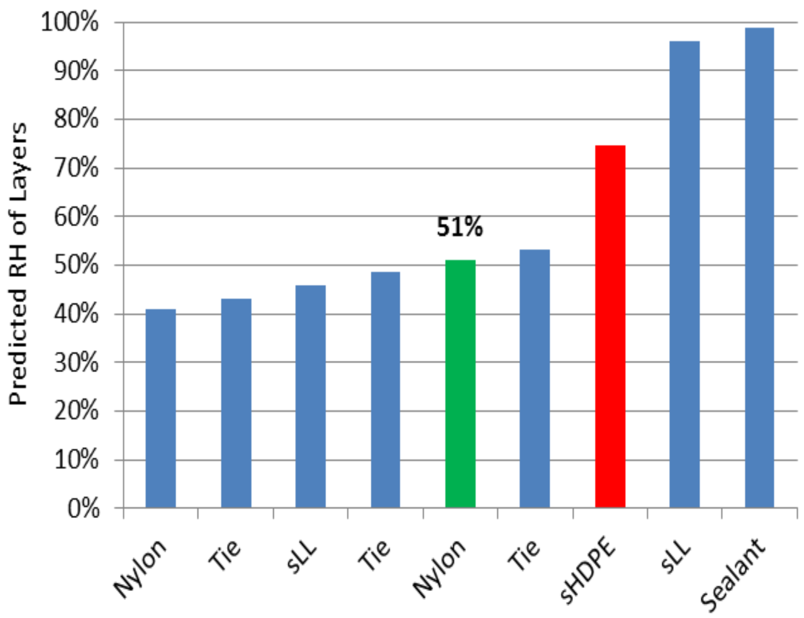


Polyamide 6, 6-6 Secant Modulus vs. RH
1 mil blown film



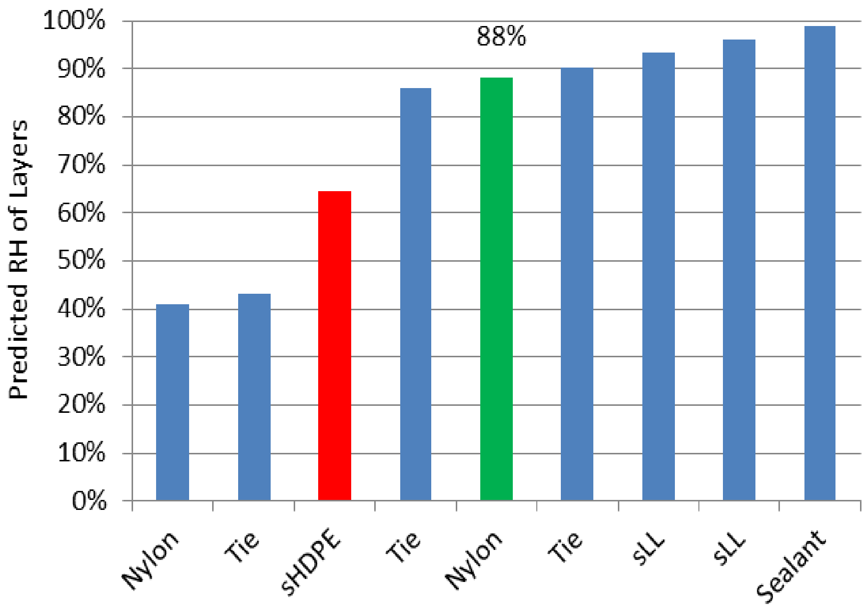
Predicted RH of Coex Layers
100% RH inside package, 40% RH outside

Test Film 1 – HDPE in interior coex layer



Predicted Film Modulus = 688 MPa
Predicted Film OTR = 2.97 cc/100in2-day atm

Test Film 2 – HDPE in exterior coex layer



Predicted Film Modulus = 610 MPa
Predicted Film OTR = 3.63

Properties of Films Used in Water-Filled Pouches

Testing completed on water-filled VFFS pouches aged for 72 hours
Inside RH = 100%, Outside RH @ 40% RH

Structure	Film Puncture (J/mm)	2% MD Secant Modulus (MPa)	Oxygen Permeability (cc/100in^2-day-atm)	Drop height failure – F50 (feet)	
				Off-line	Aged
Control (no HDPE) PA/tie/LLDPE//PA/tie/LLDPE/seal	57	450	4.2	9.4	18.3
Test Film 1 PA/tie/LLDPE/tie/**PA**/tie/**sHDPE**/seal	48	684	3.37	10.7	13.0
Test Film 2 PA/tie/**sHDPE**/tie/**PA**/tie/LLDPE/seal	62	634	3.62	10.0	9.2

Stiffness and OTR Predictions were accurate after incorporating RH correction in the model

Conclusions and Recommendations

- Many multilayer film properties are difficult to predict or model. They are affected by material and layer interactions, environmental, processing and many other factors that should be accounted for.
- However, the accuracy of basic models can be improved. Models should be built in a modular, flexible platform that allows designers to easily incorporate new discoveries, relationships and materials.
- Predictive models should not be used as a substitute for multilayer film trials, only as a general tool for identifying materials, optimizing layer and blend ratios, and predicting general trends.

Come Work With Us!

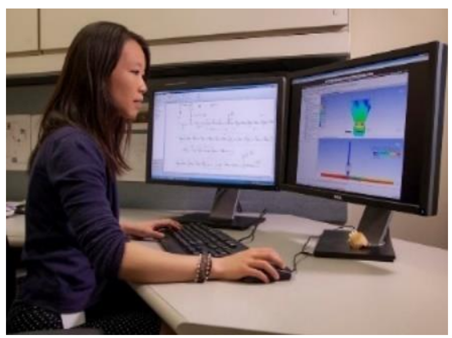
Shrink Tunnel

Horizontal FFS

Vertical FFS

9 Layer Blown Film Line

Physical Testing Lab



Virtual Design Tools

Adhesive Laminator

Thermoformer

novachemicals.com