

Damage Modeling under Impact Loading in Talc-Filled Polypropylene Compounds

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Scheme of the presentation

- LyondellBasell: Company at a Glance
- Damage in mineral filled Polypropylene under impact conditions
- Damage modeling and parameter identification: prior art, LyondellBasell contributions, debate in the CAE community
- Experimental and numerical validation
- Next steps

LyondellBasell At A Glance

- One of the largest plastics, chemical and refining companies
- Annual revenues of \$44 billion
- 13,300 employees worldwide

	2011	2012	2013
Revenues (USD millions)	\$48,183	\$45,352	\$44,062
EBITDA (USD millions)	\$5,469	\$5,808	\$6,311
Income from Continuing Operations (USD millions)	\$2,472	\$2,858	\$3,860
Diluted EPS from Continuing Operations	\$4.32 per share	\$4.96 per share	\$6.76 per share
Cash from Operating Activities (USD millions)	\$2,860	\$4,787	\$4,835
Cash and Cash Equivalents ⁽¹⁾ (USD millions)	\$1,065	\$2,732	\$4,450
EBITDA Margins	11%	13%	14%
Regular Dividend	\$0.55 per share	\$1.45 per share	\$2.00 per share
Special Dividend	\$4.50 share	\$2.75 share	
Total Debt/EBITDA ⁽¹⁾	0.74x	0.76x	0.92x
Total Debt/Book Capital ⁽¹⁾	27%	28%	32%



1. Balance sheet items represent end of year data.



What We Make Shapes Tomorrow



We Make Chemicals the World Counts On

Olefins & Polyolefins	Intermediates & Derivatives	Refining	Technology	
Ethylene	Propylene Oxide			
Propylene	Styrene Monomer			
Polyethylene	PG and PGE	Gasoline	Process Licensing	
Polypropylene	Acetyls	Diesel	Catalyst Sales	
Catalloy process resins	Oxyfuels	Olefins Feed	Technology Services	
PP Compounds	Ethylene Oxide			
Polybutene-1	EG and EOD			
	BDO & Derivatives			
End Uses	End Uses	End Uses	End Uses	
 Food Packaging 	•Insulation	•Automotive Fuels	 Polyolefins and Chemical Manufacturers 	
•Textiles	•Home Furnishings	•Aviation Fuels		
•Automotive	•Adhesives	•Heating Oil		
•Appliances	•Consumer Products	 Industrial Engine Lube Oils 		
•Films	•Coatings			
•Flexible Piping				



Global Capacity Positions



Note: Capacities and worldwide capacity positions are as of December 31, 2012, and include our pro rata share of joint ventures.

Damage in Mineral Filled Polypropylene under Impact Conditions



Damage in Mineral Filled Polypropylene under Impact Conditions

- How can we detect it?
- How can we measure it?
- How can we model it?
- How can we proof it?

Damage in Mineral Filled Polypropylene under Impact Conditions



Source: LyondellBasell

Debonding of (talc) particles from the polymer matrix leads to micro cavities initiation and to the damage of the matrix Damage is associated to the volume strain, which is experimentally accessible

 LyondellBasell Contribution :Proposal for a method based on Local Strain Measurement

M. Nutini, M. Vitali, "Characterization of polyolefins for design under impact: from true stress/ local strain measurement to the F.E. simulation with Lsdyna Mat. SAMP-1", 7th Ls-dyna German forum, Bamberg 2008

$$\frac{dV}{V} = (\varepsilon_X + \varepsilon_Y + \varepsilon_Z)$$



Damage: how can we detect it?



Source: LyondellBasell

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Damage: how can we measure it?

Damage function implemented according to Chaboche-Lemaitre model: Continuum Damage Mechanics (CDM) approach

Damage variable D: 0 (virgin mat.) $\leq D \leq 1$ (failure)

$$D = \frac{A_{VOID}}{A_{TOT}} \quad Damage function$$

$$\sigma_{EFF} = \frac{F}{A_{EFF}} \quad Effective stress$$

$$\sigma_{TRUE} = \frac{F}{A_{TOT}} \quad True stress$$



$$D = 1 - \frac{\sigma_{TRUE}}{\sigma_{EFF}}$$

Damage: how can we measure it?



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3D local measurement and data elaboration

 $A_{TOT} = A_{Eff} + A_{Void}$

What is "true"? Notes on the Nomenclature

"Stat rosa pristina nomine, nomina nuda tenemus"



Nomenclature might be misleading



We are not running alone ...



Source: LyondellBasell Image Databank

Same approach can be found in other more recent publications, e.g.:

 R.Balieu, F.Lauro, B.Bennani, R.Delille, T.Matsumoto, E.Mottola, "A fully coupled elastoviscoplastic damage model at finite strains for mineral filled semi-crystalline polymer, Int. J. Plasticity, (2013)

Other approaches



Other – classical - approaches



 Gongyao Gu, Yong Xia, Chin-hsu Lin, Shaoting Lin, Yan Meng, Qing Zhou, "Experimental Study on characterizing damage behavior of thermoplastics", Materials and Design 33 (2013),p. 199-207

Comparison of the results from volume strain and Modulus variation: conflicting responses!

- Results are different (Gu et al.): Damage underestimated when volume strain is used rather than elastic modulus(D=0.4 vs. D=0.9)

Open Questions

- Methodologies for measuring the damage give different numerical values (Gu et al.), or similar values (Balieu et al.).
- Damage values reported to reach values of about 0.8-0.9 when based on stiffness assessment (Gu et al.)
- Damage values according to Chaboche-Lemaitre are supposed to range from 0 (virgin material) to 1 (failure).
- Experienced values from Volume Strain measurement not higher than 0.4-0.5

Questions /Answers

- Experimental answer, reprising the ideas of Delhaye et al. (Int. Journal Impact. Engineering, 2011):
 - SEM observation of fracture surface of tensile specimens
- Numerical answer:
 - Implementing Damage curves in the Finite Element simulation of an impact test

Experimental Answer



- Fracture surface of tensile specimens analyzed with SEM
- Specimens cut from an injection molded 3 mm thick plaque
- Specimens subjected to tensile test at 100mm/s
- Fracture surfaces cleaned through ultrasounds, then metallized
- Fracture surfaces compared with samples from virgin (= not tested) material
 - Material: mineral filled, impact modified Polypropylene

Analysis at SEM of a Compound Material: Specimen Fracture Surface (SE)



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Source: LyondellBasell

Analysis at SEM of a Compound Material: Specimen Fracture Surface (BS)

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Analysis at SEM of a Compound Material: Virgin Material

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Analysis at SEM of a compound material (CAE1164)

- Areas with different morphologies can be identified (cfr. Delhaye et al.)
- Area (a): "ductile" area: long stretched ligaments
- Area (c): "brittle" area
- Evidence of NOT UNIFORM damage condition oh the fracture surface.
- The Damage parameter measured with optical tools is then Averaged on the section, in agreement with Continuum approach.
- Higher Damage values could occur more locally but are not visible nor useful when coupled with a TRUE stress/ EFFECTIVE stress measurement

Numerical Answer

Numerical Answer

Industrial prototypal part (energy absorber), made of talc-filled, impact-modified PP

Material law uses (Ls-dyna SAMP-1):

- Pressure-sensitive plasticity
- Strain rate dependence
- Complex loading (Tension , Compression, Bending)
- Damage: portions of the part are subjected to unloading during the impact sequence

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1 111

29

Result: Alternative modeling

 Simulations with SAMP-1 have provided forcedispl-time curves in better agreement with the real test than MAT_024 and MAT_081.

Result: Deformation

Part deformation during the real test (left) and simulated with SAMP-1 t= 15 ms (top) and t=25 ms (bottom)

Result: Damage modeling

- For this class of materials the damage model combined with parameter identification through volume strain give good results (see the <u>slope</u> after motion reversal)
- Arbitrary scaling of damage curves to reach the value 0.9 at failure (to simulate Gu's results) does not give reasonable predictions
- Damage is better evaluated from 3-D strain measurement (curve DIC3D)

Conclusions and next steps

- The damage parameter assessed based on volume strain measurement seems reasonable taking into account the damage localization occurring in the test
- The proposed measurement methodology can be coupled with true stress/ effective stress measured from tensile test which are easily input in an input deck for Finite Element Analysis, in the frame of CDM (Continuum Damage Modeling)
- A further quantitative assessment of damage localization is ongoing
- Watch out! Nomenclature can be misleading, especially regarding "TRUE" variables.

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