



Validation of a SAMP-1 Material Card for Polypropylene-based Materials

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Basell Poliolefine Italia srl,
A LyondellBasell Company

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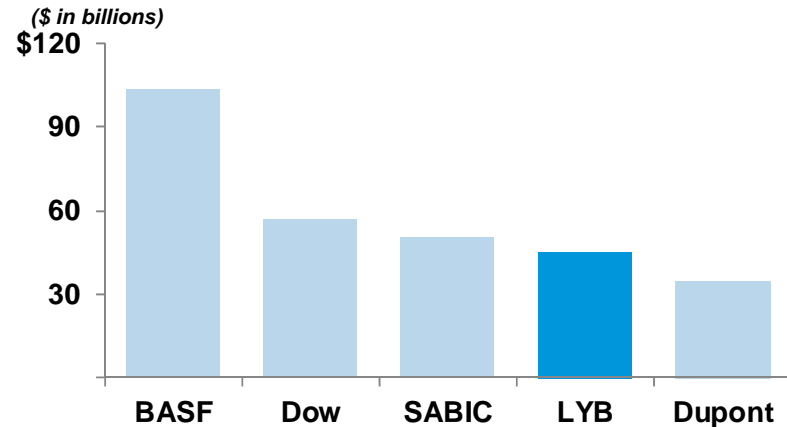
lyondellbasell
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Scheme of the Presentation

- LyondellBasell is...
- SAMP1- is...(brief history from literature)
- Basic SAMP-1 inputs.
- Advanced modeling with SAMP-1: damage
- Validation on a prototypal part

World-Class Scale With Leading Market Positions

2012 Revenues



Source: Capital IQ, LYB

Products

Global Position

Chemicals	
Ethylene	#5
Propylene	#5
Propylene Oxide	#2
Polymers	
Polyolefins (PE + PP)	#1
Polypropylene	#1
Polyethylene	#4
Polypropylene Compounds	#1
Fuel	
Oxyfuels	#1
Technology and R&D	
Polyolefins Licensing	#2

Note: Positions based on LyondellBasell wholly owned capacity and pro rata share of JV capacities as of December 31, 2012.

LyondellBasell Fast Facts

- One of the world's largest plastics, chemicals and refining companies with revenues of \$45 billion (2012)
- Global reach that addresses worldwide customer needs
- 58 manufacturing sites in 18 countries on five continents
- Sales in more than 100 countries
- Vertically integrated facilities enable conversion of crude hydrocarbons to materials for advanced applications
- Participation in 16 significant manufacturing joint ventures, 11 of which are outside of Western Europe and the United States, primarily in regions that have cost-advantaged raw materials or high growth rates

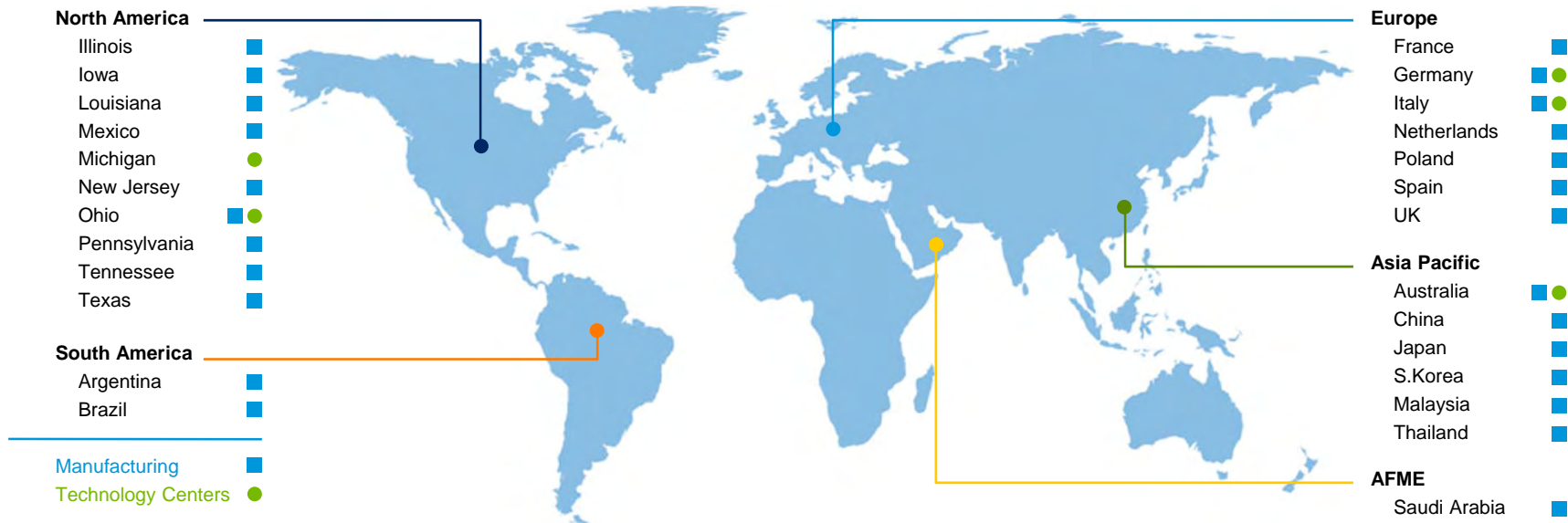


Global Reach

**58 plants in
18 countries**

**More than
13,000 employees
worldwide**

**Sales in
more than
100 countries**



Owned and operated by LyondellBasell, its subsidiaries and/or joint ventures.

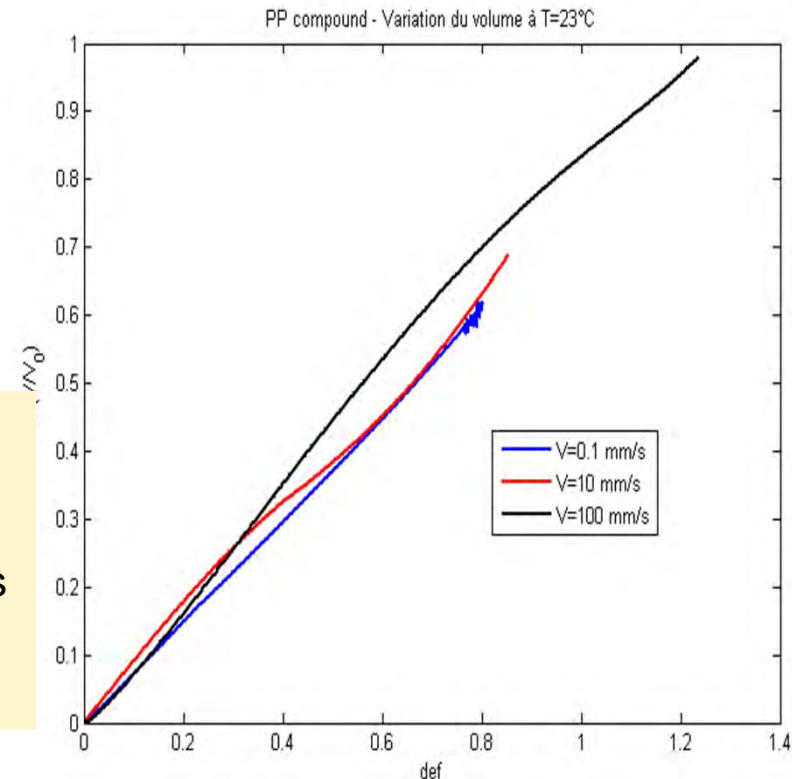
Our Product Lines and End Markets We Serve

<p>Olefins & Polyolefins</p> <ul style="list-style-type: none"> Americas Europe, Asia & Int'l (EAI) 	<p>Intermediates & Derivatives</p>	<p>Refining</p>	<p>Technology</p>
			
<p>Ethylene Propylene Polyethylene Polypropylene <i>Catalloy</i> process resins PP Compounds Polybutene-1</p>	<p>Propylene Oxide Styrene Monomer PG and PGE Acetyls C₄ Chemicals Ethylene Oxide and Derivatives Oxyfuels</p>	<p>Gasoline Diesel Olefins Feed</p>	<p>Process Licensing Catalyst Sales Technology Services</p>
<p>End Uses</p> <ul style="list-style-type: none"> • Food Packaging • Textiles • Automotive • Appliances • Films • Flexible Piping 	<p>End Uses</p> <ul style="list-style-type: none"> • Insulation • Home Furnishings • Adhesives • Consumer Products • Coatings 	<p>End Uses</p> <ul style="list-style-type: none"> • Automotive Fuels • Aviation Fuels • Heating Oil • Industrial Engine Lube Oils 	<p>End Uses</p> <ul style="list-style-type: none"> • Polyolefin and Chemical Manufacturers

Before SAMP-1: Needs for a SAMP-1 like material

- N.Temini, N.Billon, “Plasticité et incompressibilité des polymers solides – Etude expérimentale à moyennes et hautes vitesses”, 16ème Congrès Français de Mécanique, Nice, Septembre 2003
- C. G’Sell C., Shu-Lin Bai, J.M.Hiver, “Polypropylene/polyamide 6/polyethylene-octene elastomer blends. Part 2: volume dilatation during plastic deformation under uniaxial tension”, Polymer 45, 2004, p- 5785-5792
- M.Nutini, M.Vitali, “Mesure de “déformation vraie”/”contrainte vraie” sur matériaux polypropylène et polyéthylène”, Congress « Mise en ouvre et comportement des polymères et des élastomères: quels progrès?», SFIP Congress, Sophia Antipolis, 2007

New experimental techniques allowed detailed measurement of volume variation in polymers subjected to tensile tests, not compatible with Von Mises plasticity



Source: LyondellBasell SFIP 2007

SAMP-1 is...

- [1] S.Koelling, A.Haufe, M.Feucht, P.DuBois, "SAMP-1: a Semi-analytical Model for the Simulation of Polymers", 4th Ls-dyna Anwenderforum, Bamberg, 2005

4. LS-DYNA Anwenderforum, Bamberg 2005 Keynote - Vorträge

**SAMP-1: A Semi-Analytical Model
for the Simulation of Polymers**

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1 Introduction

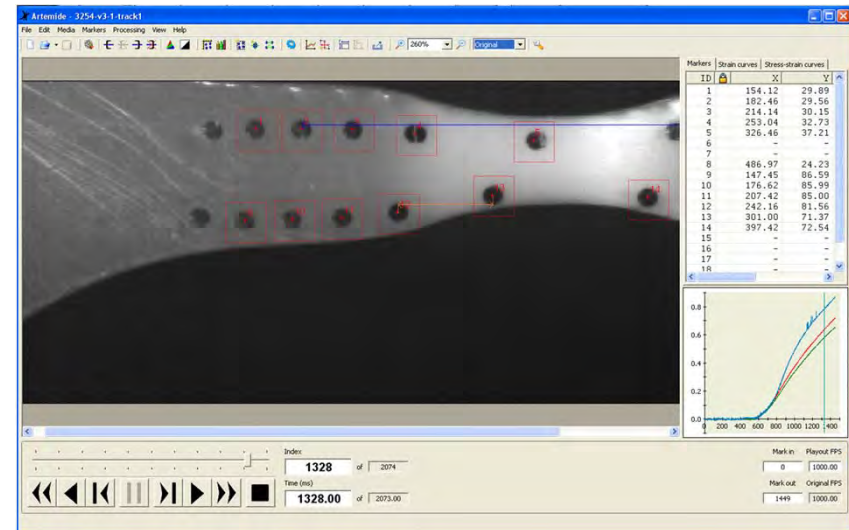
The numerical simulation of structural parts made from plastics is becoming increasingly important nowadays. The fact that almost any structural requirement can be combined in a lightweight, durable and cost effective structure is the driving force behind its widespread application. More and more structural relevant parts are being constructed and manufactured from plastics. This on the other hand drives the demand for reliable and robust methods to design these parts and to predict their structural behaviour. The key ingredients that need to be available are verified, calibrated and validated constitutive models for any family of plastic material. This holds not only true for crashworthiness applications but for any other application field.

Under high velocity impact loading, thermoplastic components undergo large plastic deformations and will most likely fail. Consequently, the unloading behaviour is irrelevant and thermoplastics can be modelled with a sufficiently good approximation as pseudo-metallic elastic-plastic bodies. This is, however, not always the case – even in crashworthiness applications. Nowadays important applications in crash simulation that demand a more accurate modelling of thermoplastics are simulation problems in pedestrian protection, e.g. head and leg impact (see [6], [10], [11], [12]) and passenger protection. Although highly sophisticated material laws are available in commercial finite element programs, there are still open questions, especially in the aforementioned field of application. In this pa-

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SAMP-1 Users: Initial Concerns

- [7] H. Lobo, B. Croop, D. Roy , “Applying Digital image Correlation Methods to SAMP-1 characterization”, 9th European Ls-dyna Users Conference, Manchester, 2013
- [8] H. Daiyan , F. Grytten, A. Andreassen, H.Osnes, O.V. Lyngstad, “Numerical Simulation of low-velocity impact loading of a ductile polymer material”, Materials and Design 42 (2012), p.450-458



LyondellBasell Contribution

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

SAMP-1 Users: Initial Concerns

How to characterize the materials for providing input data to SAMP-1?

Which tests?

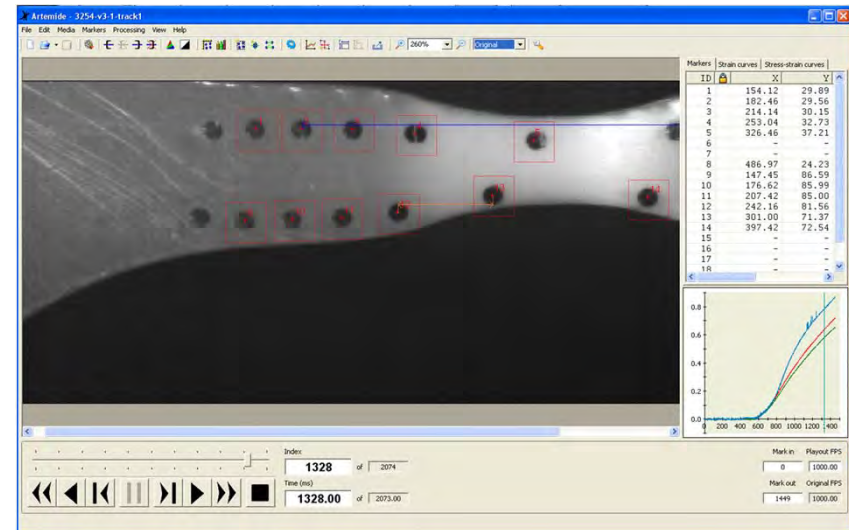
- Tension, compression, shear
- Testing speeds?
- Material orientation?

Which testing methodologies?

- Engineering data?
- True stress/Strain?
- Local measurement?
- Optical methods, e.g. Digital Image Correlation (DIC)?

Data elaboration?

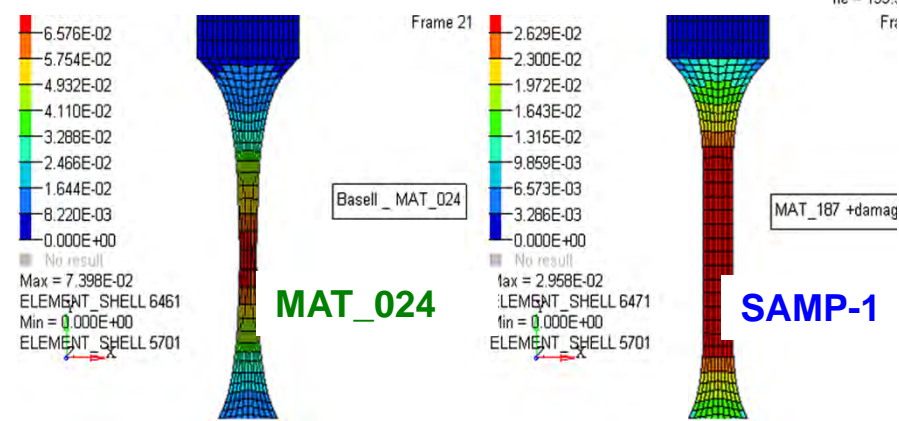
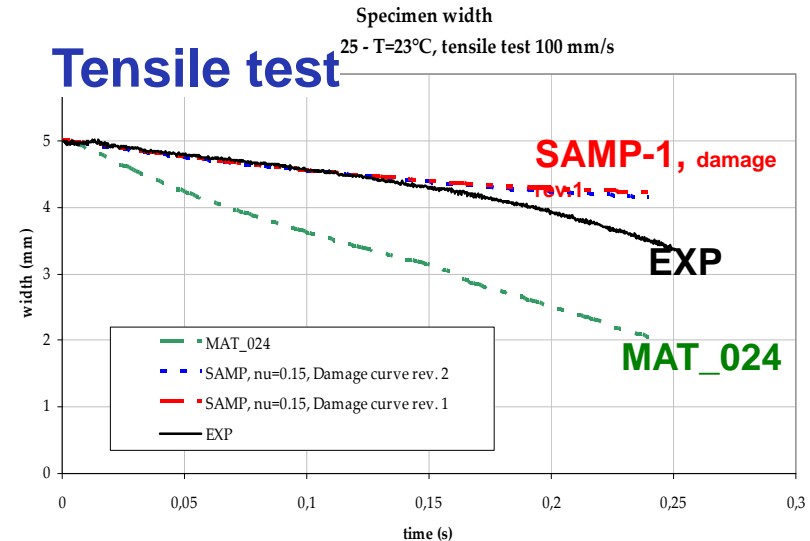
- Optimization techniques (based on what outputs)?
- Data filtering?



SAMP-1 Users: Initial Concerns

How to validate a SAMP-1 material card?

- First studies based on simple tensile / bending tests (reverse engineering)
- Additional studies on selected benchmark tests

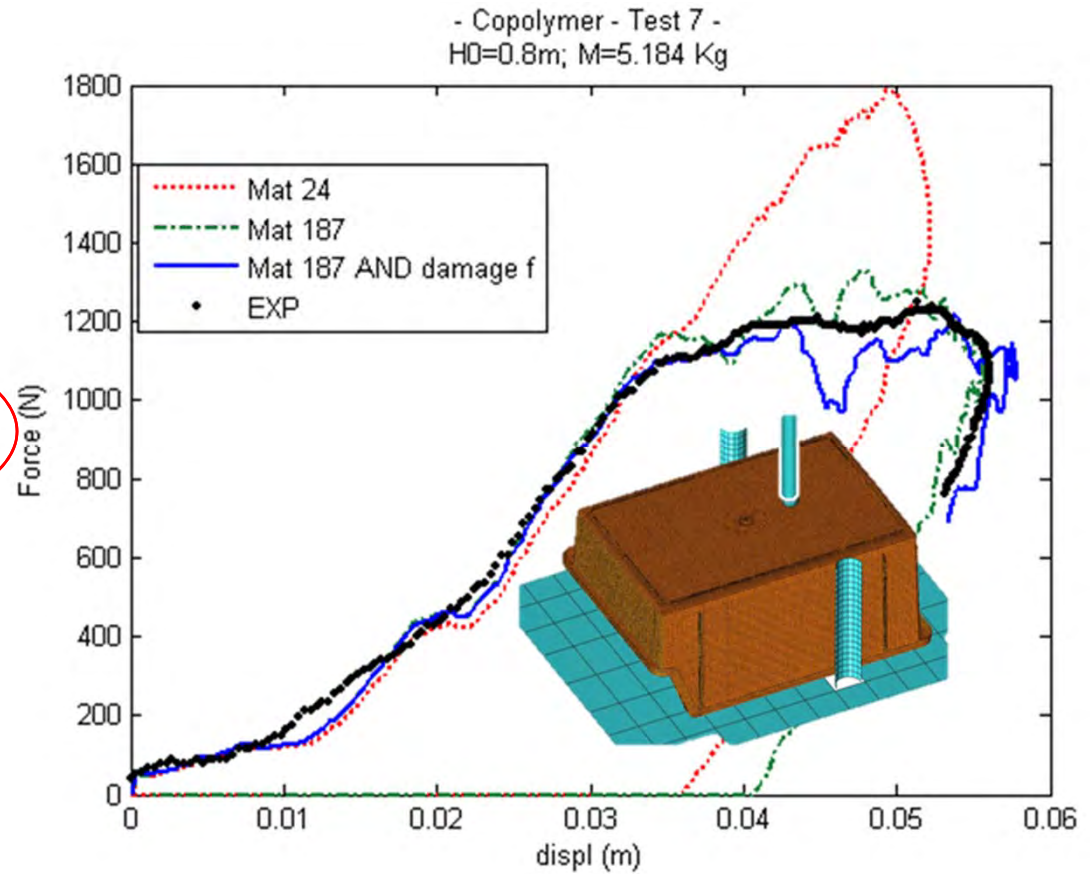


Source: M. Nutini, M. Vitali, "Characterization of polyolefins for design under impact: from true stress/ local strain measurement to the F.E. simulation with Ls-dyna Mat. SAMP-1", 7th Ls-dyna German forum, Bamberg 2008

SAMP-1 Users: Initial Concerns

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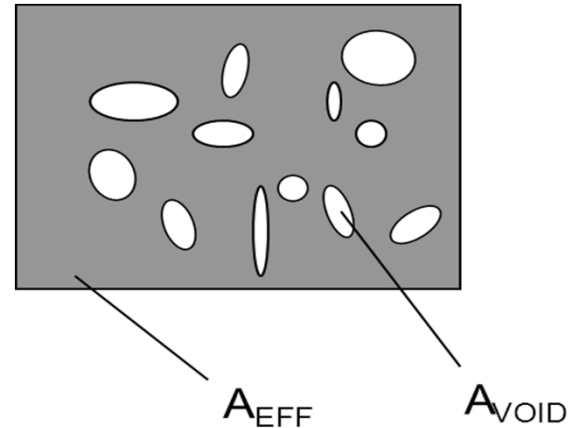


Source: M. Nutini, M. Vitali, "Characterization of polyolefins for design under impact: from true stress/ local strain measurement to the F.E. simulation with Ls-dyna Mat. SAMP-1", 7th Ls-dyna German forum, Bamberg 2008

SAMP-1 Advanced Input: Damage

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

- P.DuBois, M.Feucht, A.Haufe, S.Koelling, “An Overview of Ductile Damage Models in LS-DYNA”, Ls-dyna Anwenderforum, Frankenthal, 2007
- J.Lemaitre, J.L.Chaboche, “Mechanics of solid materials”, Cambridge Univ. press, 2002



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

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

Damage Parameters Identification

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 Ls-dyna Mat. SAMP-1”, 7th Ls-dyna German forum, Bamberg 2008

Damage function associated to the volume strain, experimentally accessible

$$\tilde{m} := \ln \frac{V}{V_0} = (\varepsilon_1 + \varepsilon_2 + \varepsilon_3)$$

$$D = 1 - \frac{V_0}{V} = 1 - e^{-\tilde{m}}$$

Effective stress identified as the stress at constant volume

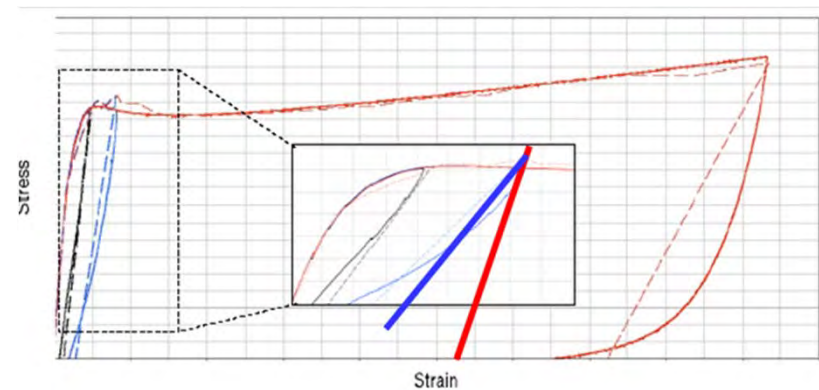
$$\sigma_{EFF} = \sigma_{CV}$$

Damage Parameters Identification

Alternative approaches

- J.Lemaitre, J.L.Chaboche, “Mechanics of solid materials”, Cambridge Univ. press, 2002
- M.Xu, I.Wang, “A new method for studying the dynamic response and damage evolution of polymers at high strain rates”, Mechanics of Materials 38 (2006), p. 68-75
- 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

Damage function through elastic modulus measurement from uniaxial tensile tests with repeated unloading



Damage Parameters Identification

LyondellBasell Method and Alternative approaches Comparative assessments:

- 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), <http://dx.doi.org/10.1016/j.ijplas.2013.05.002> (article in press)
- 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!

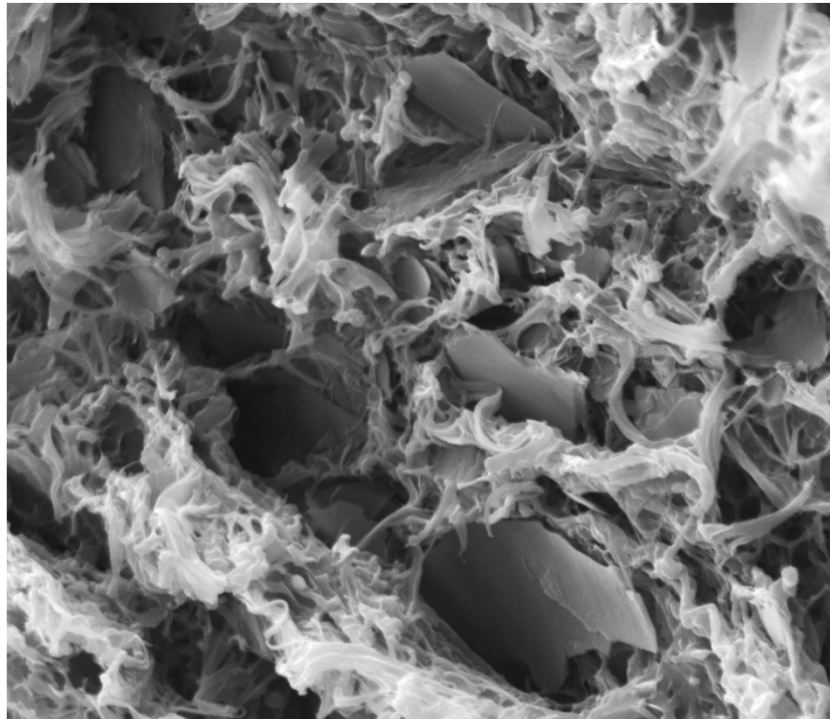
- *Results overlapping (Balieu et al.)*
- *Results are different (Gu et al.): Damage underestimated when volume strain is used rather than elastic modulus ($D=0.4$ vs. $D=0.9$)*

Damage: deeper investigations of the Damage Physics

- V.Delhaye, A.H. Clausen, F.Moussy, R.Othman, O.S. Hopperstad, “Influence of stress state and strain rate on the behavior of a rubber-particle reinforced polypropylene”, International Journal of Impact Engineering 38 (2011), p. 208-218
- E.M. Parsons, M.C.Boyce, D.M.Parks, M.Weinberg, “Three-dimensional large-strain tensile deformation of neat and calcium carbonate-filled high density polyethylene”, Polymer 46(2005), p. 2257-2265
- A.F. Epee, F.Lauro, B.Bennani, B.Bourel, “Constitutive model for a semi-crystalline polymer under dynamic loading”, International Journal of Solids and Structures, 48 (2011), p. 1500-1599

Debonding of (talc) particles from the polymer matrix leads to micro cavities initiation and to the damage of the matrix

Damage: deeper investigations of the Damage Physics



Source: LyondellBasell

*LyondellBasell Contribution
(study in progress)*

*Debonding of (talc) particles from the
polymer matrix leads to micro cavities
initiation and to the damage of the
matrix*

Damage modeling

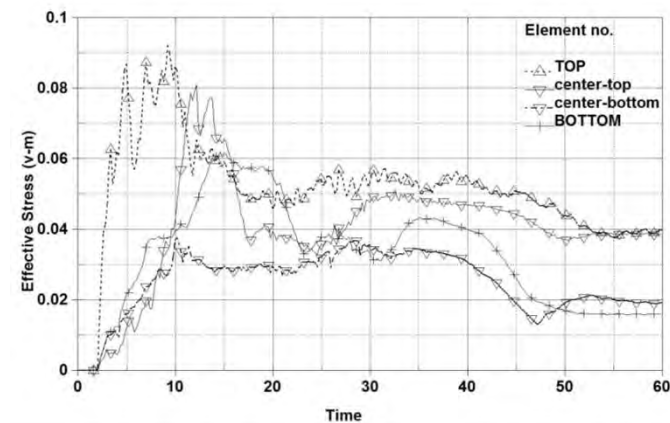
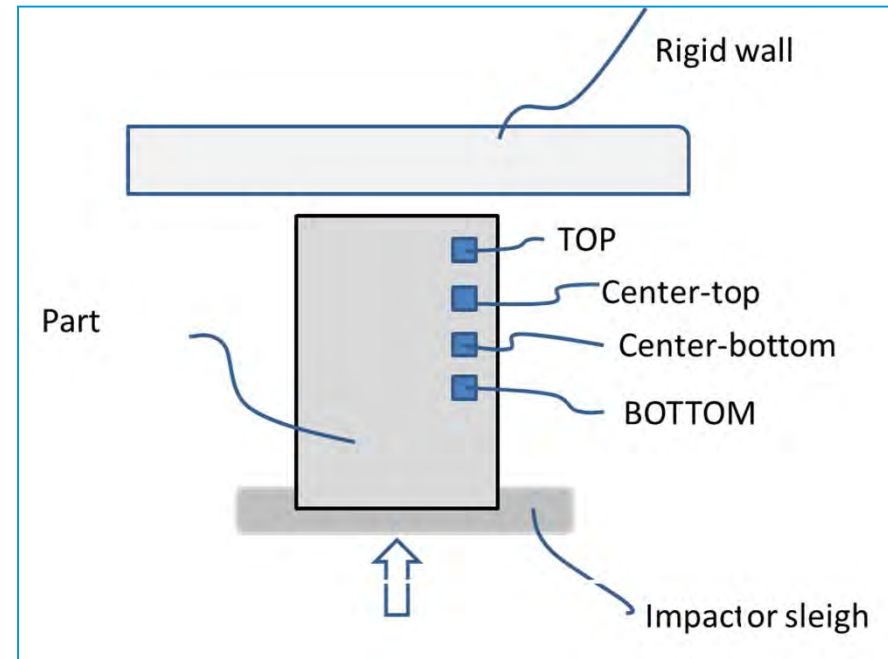
- Considering how damage originates and evolves in talc-filled materials, and also the uncertainties in the current debate as emerging from the references:
 - The Chaboche-Lemaitre model coupled with volume-strain based parameter identification is the preferred choice for this class of materials
 - A dedicated test will be used for its validation

Choice of a further validation test

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

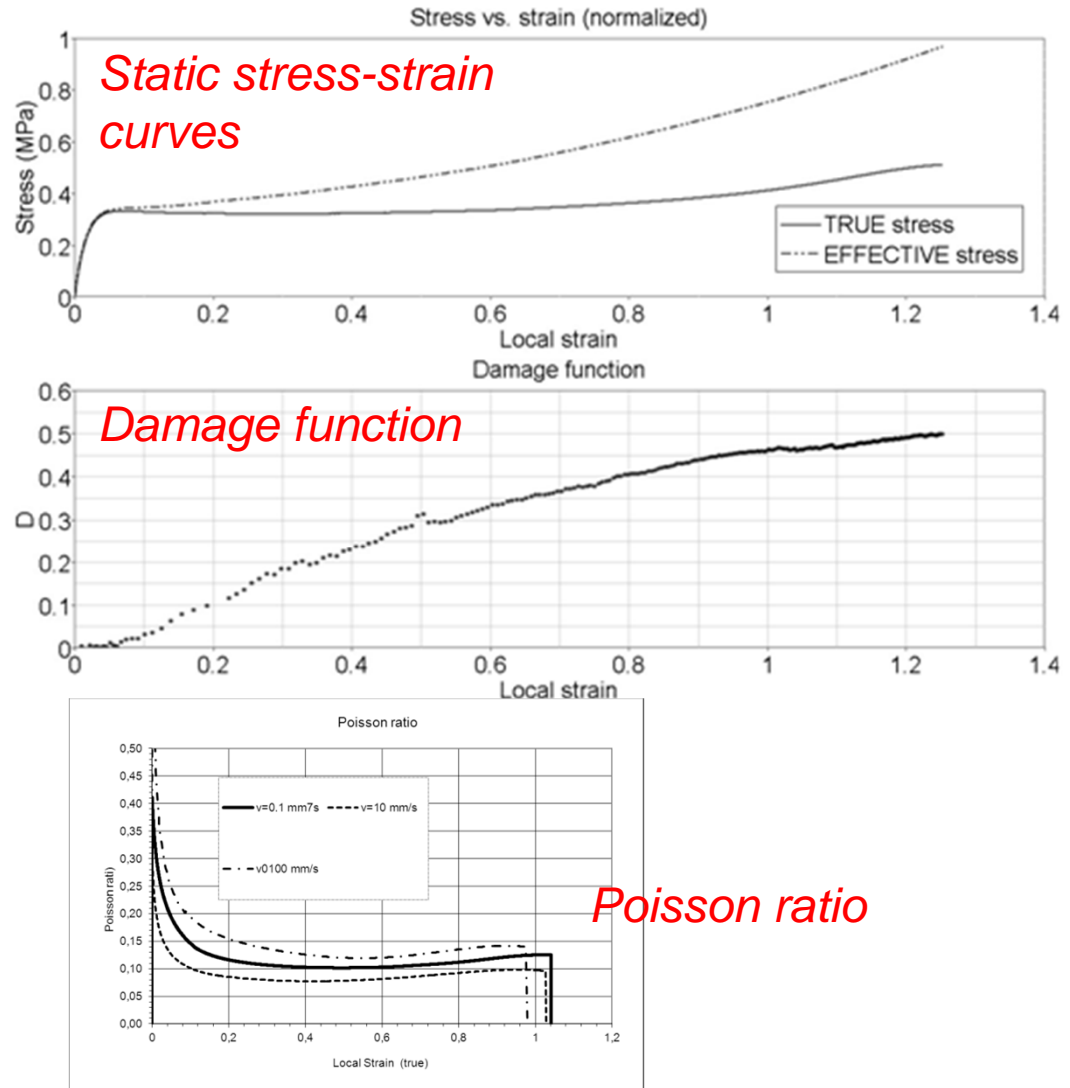
Testing several SAMP-1 features as:

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



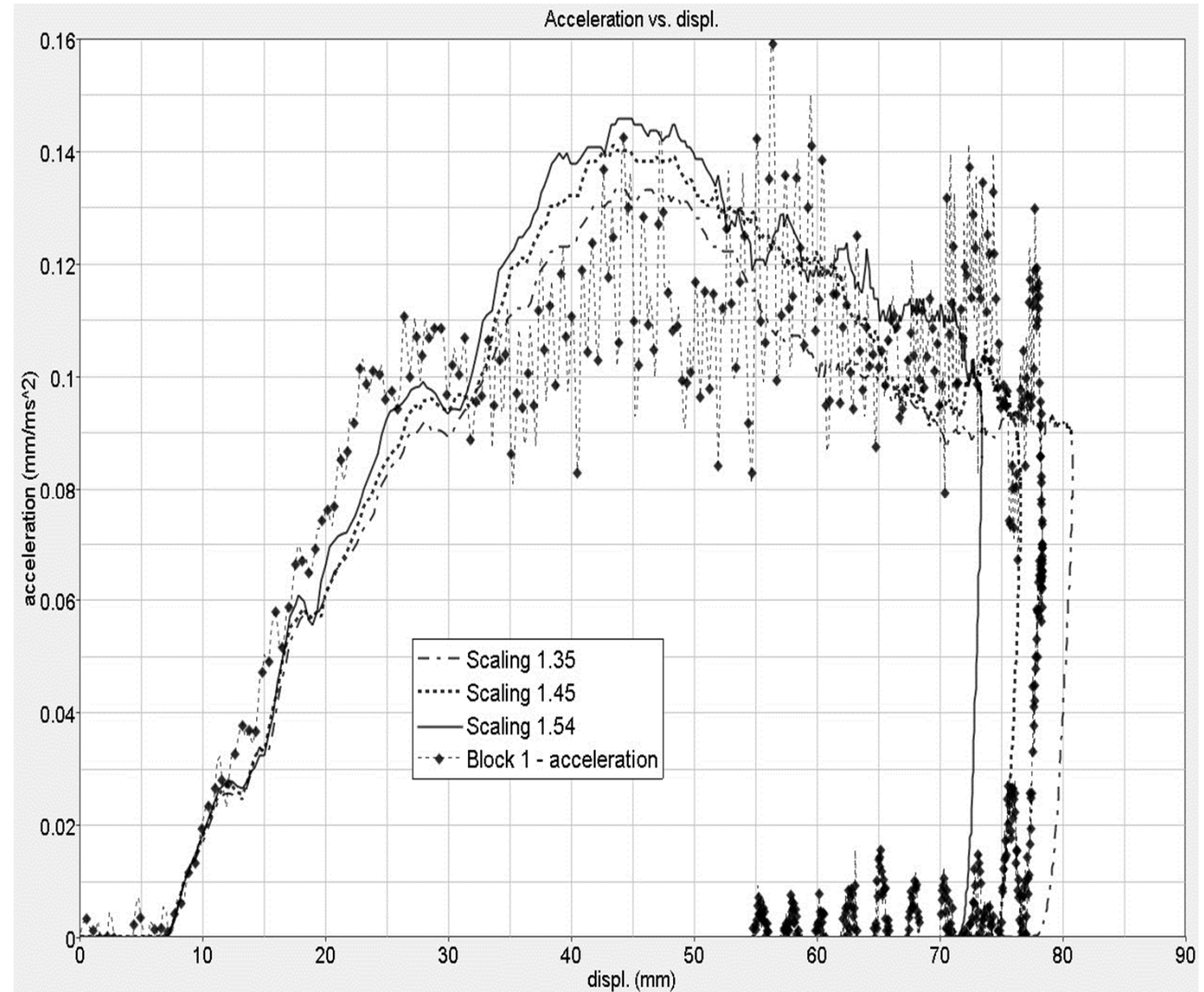
Material card preparation

- Data from tensile test at different speeds, using DIC/Optical strain measurement, measured on specimens cut from injection molded plaques
- Compression / Shear data: through scaling tensile stress-strain curves. Scaling Coefficient: 1.3 to 1.5 for compression, 0.7 for shear
- Poisson ratio: function of the strain
- Average (Long/Transv) material properties are used



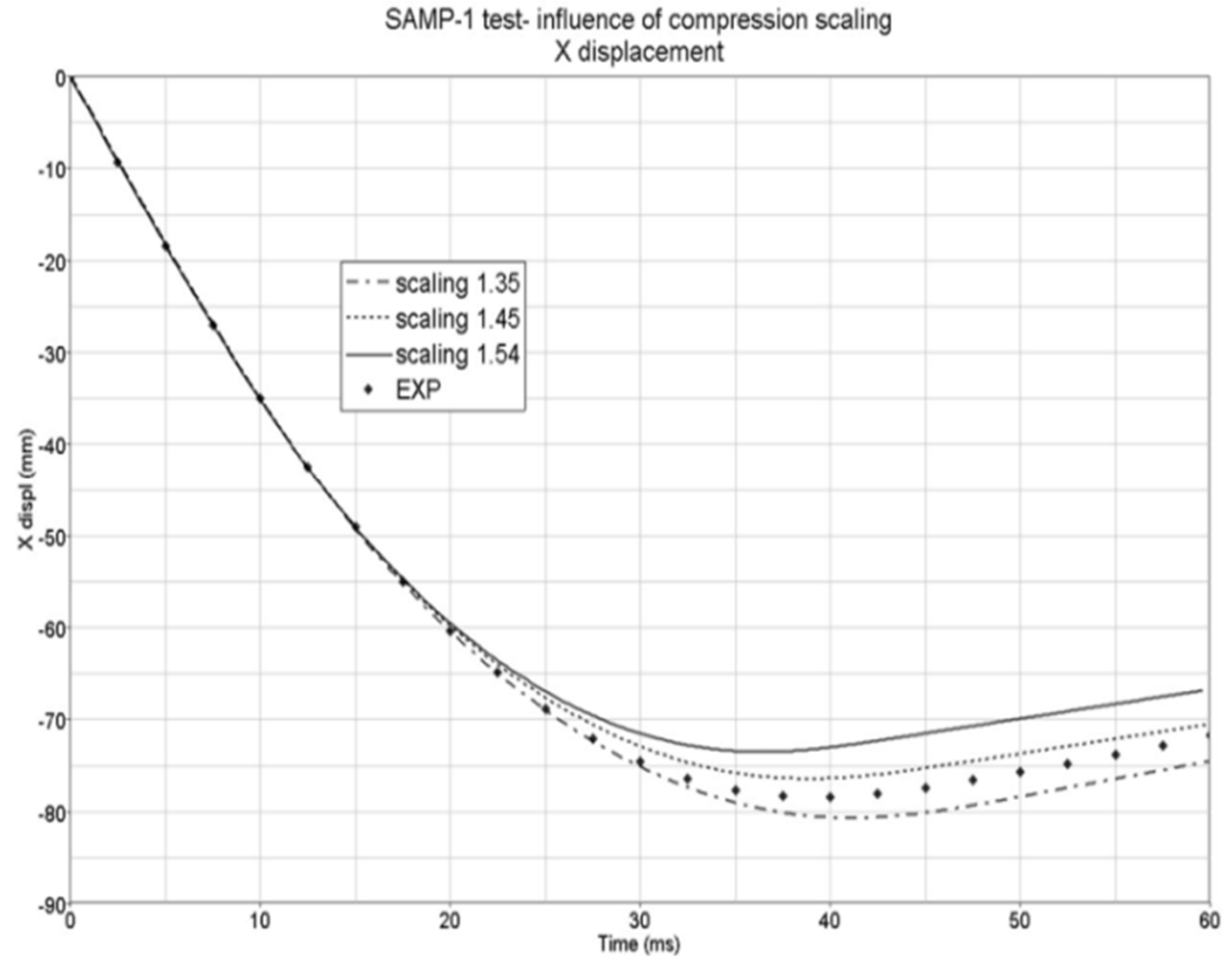
Result: Compression modeling

- Several scaling coefficients used.
- Comparison based on Force vs. displ. Curve (right)
- Definitely good agreement between experiment and simulation.
- Scaling coefficient for compression data from tensile data better around 1.4



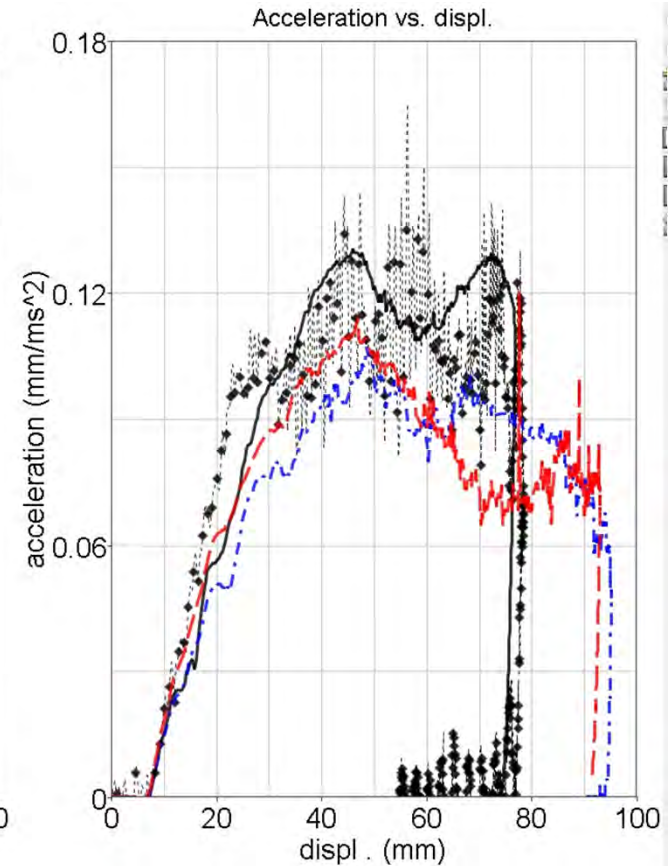
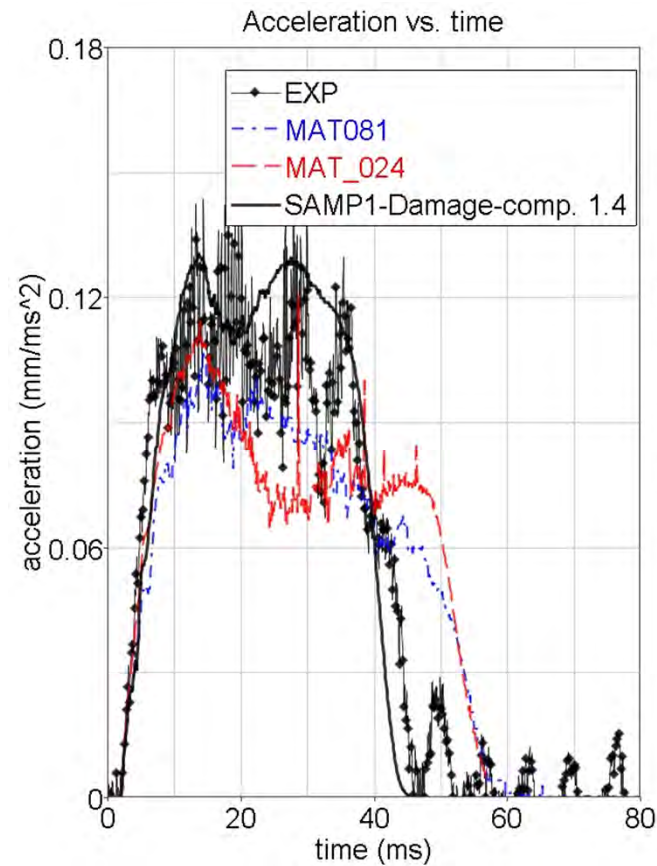
Result: Compression modeling

- Several scaling coefficients used.
- Comparison based on displ. vs. time (right)
- Note: the slope after velocity is reversed (t =35 ms about) is the same for all the simulations (Same damage parameters!)
- Best result: scaling coefficient around 1.4



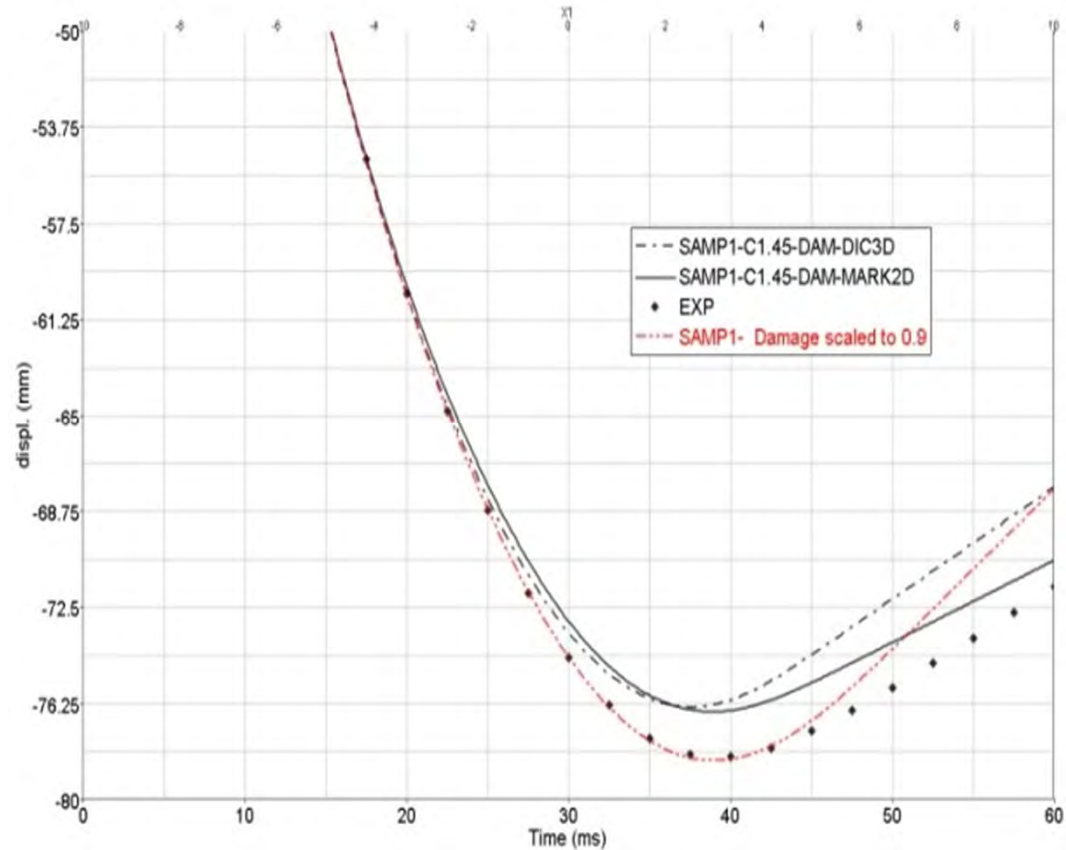
Result: Alternative modeling

- Simulations with SAMP-1 have provided force-displ-time curves in better agreement with the real test than MAT_024 and MAT_081.
- Taking into account the slight anisotropy in the material is believed to improved the prediction accuracy



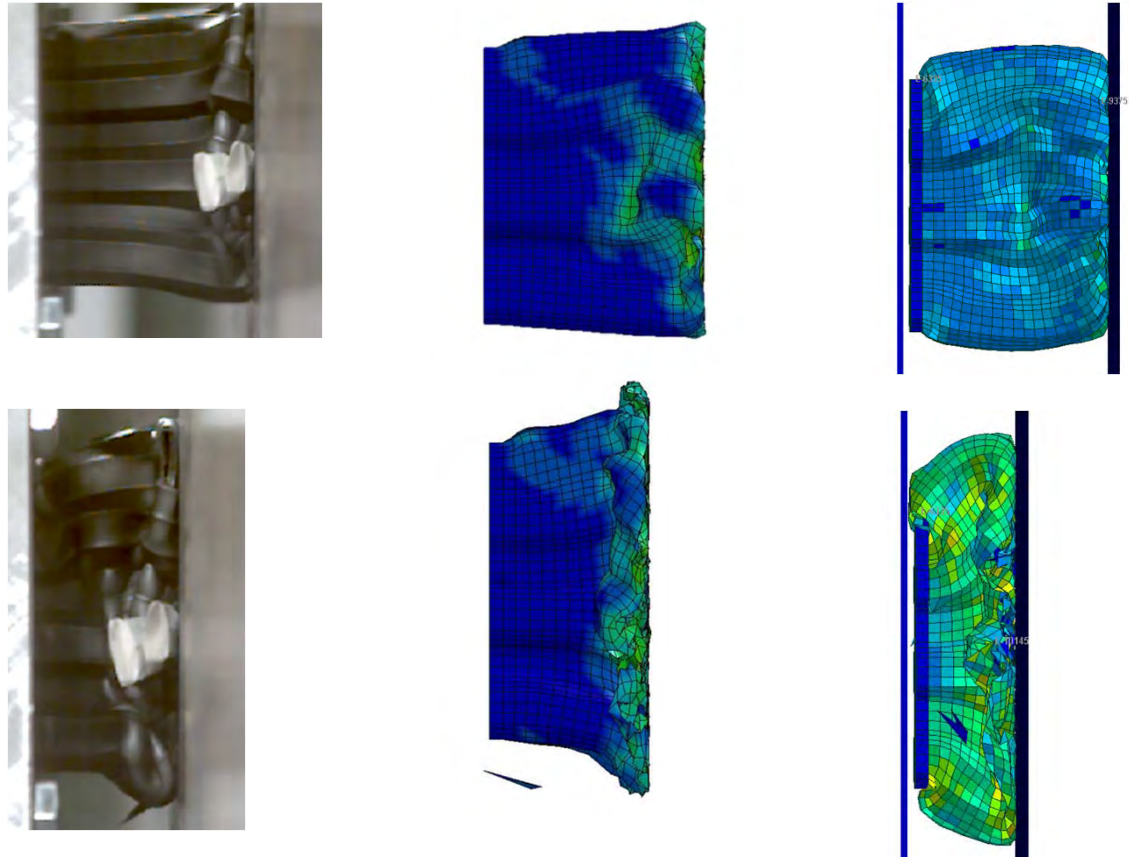
Result: Damage modeling

- For this class of materials the damage model combined with parameter identification through volume strain give good results (see the slope 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)



Result: Deformation

The deformation predicted using SAMP-1 is definitely closer to the real test than the one predicted by MAT_024



Part deformation during the real test (left) and simulated with SAMP-1 (center) and MAT_024 (right); $t = 15\text{ ms}$ (top) and $t = 25\text{ ms}$ (bottom)

Conclusions

The benchmark case here presented confirms that accurate local strain measurement using non contact optical-based methods are suitable to generate input data for impact analyses for advanced material laws, as SAMP-1, taking into account peculiar characteristics of polymeric materials, as viscoelasticity, viscoplasticity, pressure-dependent yield stress, plastic dilatation and damage.

In particular, the validity of the approach to damage modeling based on the measurement of volume strain has been experimentally verified for mineral-filled Polypropylene-based compounds.

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