Determination of Accurate Material Parameters using LS-OPT Based Optimization Techniques

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1 Abstract

Material models for high-performance thermoplastic polymers need to capture highly complex material characteristics accurately to enable lightweight and sustainable designs. ULTEM™ 1000 Polyetherimide Resin from SABIC's Specialties business display different behavior under impact loading under multi-axial loading compared to uniaxial tensile testing. This necessitates modelling the tri-axial state of stress and damage characteristics with sufficient detail rather than only relying on the uniaxial tensile data. This paper deals with predicting this complex state of stress and damage behavior using *MAT_187 and GISSMO in LS-DYNA® software respectively. *MAT_187 predicts behavior of the resin under complex stress states by considering the stress-strain curves generated from uniaxial tension, uniaxial compression and pure shear tests. GISSMO model is adopted to predict damage and failure. Four key damage parameters namely "critical plastic strain", "damage exponent", "fading exponent" and "biaxial plastic strain to failure" which are hard to determine through experiments are optimized using meta-model-based optimization technique in LS-OPT®. The finalized material card with optimized parameters was validated against physical test results providing confidence to use the cards in real-life application designs.

2 Introduction

Polymers find their applications in aircrafts, automobiles, spacecraft etc. and are extensively used in many other critical structures. As thermoplastics are used in many critical applications, understanding their mechanical properties are becoming increasingly significant. These mechanical properties are dependent on the strain rate, temperature, and pressure. They exhibit a complex behavior whose understanding is essential for analyzing and predicting its behavior.

1. **Failure dependency on strain rate:** The mechanical behavior of most of the polymers are time dependent. They exhibit rate dependent modulus of elasticity, yielding, post-yielding behavior. For a range of strain rates and temperatures, the mechanical response of the thermoplastics changes from rubbery state to ductile plastics to brittle. Lower strain rate corresponds to longer times while higher strain rate corresponds to shorter times. Hence, lower strain rates reflect the behavior observed at higher temperature while high strain rates mimic the behavior at lower temperatures. Strain rate dependent failure is one of the major properties which needs to be considered while studying the behavior of the polymer material under study.

2. **Failure dependency on strain rate for different stress state:** Stress triaxiality is defined as the ratio of hydrostatic stress to the Von Mises stress which quantifies the stress state of the material. It is a very important factor that influences the fracture strain. At different states of stress, i.e., at tension, compression and shear states of stress, the material behaves differently. The failure strain of the material is dependent on the state of stress.

3. **Volume dilation post yielding:** The macroscopic volume change can be studied during uniaxial tension test using digital image correlation technique (DIC). The assumption of incompressibility is more suitable for metals but does not hold good for polymers in order to characterize the true stress-strain. Polymers exhibit significant dilation in volume post yielding. This property of polymers has to be captured to determine the true stress-strain data.

Toughness of the material can be measured by quantifying the energy required to break a sample of definite geometry. Toughness tests are usually done at high rates of loading and are called impact tests. Typical impact tests include the Izod test, Charpy test and dart impact test. These standard tests play a major role in ranking of materials in the order of increasing toughness. These tests should be used to validate material cards even before the application level use.

During impact tests, failure behaviour of the specimen is significantly influenced by strain rate and temperature. All un-oriented plastics show brittle behaviour at high strain rates and low temperatures. The force–deflection curves obtained from mechanical measurements of various dart impact or puncture test standards give different transitions from ductile to brittle fracture.

Failure and damage behaviour of polymers is predicted using CAE simulations. LS-DYNA® software is one of the most common industry-standard CAE simulation tool to model thermoplastic materials. A large number of material models for polymers have been implemented in this tool. These material cards have shown excellent performance in modelling the material and failure behaviour of polymers under specific conditions. However, modelling of high end polymers under complex stress states still remains a challenge.

The current work deals with the establishment of high fidelity material model in LS-DYNA® software to predict the brittle behaviour exhibited by ULTEM™ 1000 resin under multiaxial loads. The work involves understanding the *MAT_SAMP-1(Semi Analytical Model for Polymers) material model available in LS-DYNA® software for modelling the complex plastic behaviour. In order to generate *MAT_187 card, detailed characterization tests were performed such as uniaxial tension, compression and pure shear tests. The experimental curves were processed to generate the input to the material card. Single element and specimen level simulations were carried out for the standard tests and the established material card was verified. Next the material card was validated against a dynatup test that subjects the material to dynamic multiaxial stress condition. Finally the material card was validated against a part level test under static multiaxial loading. The current validation gives confidence to use the material card for different real-life application designs.

2.1 ULTEM™ resin

The SABIC product under the study is material from a family of amorphous thermoplastic polyetherimide (PEI) resins offering outstanding elevated thermal resistance, high strength and stiffness, and broad chemical resistance. The PEI resins are available in transparent and opaque custom colors, as well as glass filled grades.

Properties of ULTEM™ 1000 resin are

1. High mechanical strength: ULTEM™ 1000 resin offers outstanding strength and stiffness at higher temperature.
2. Long term heat resistance: The material offers excellent mechanical and physical stability at elevated temperatures.
3. Dimensional stability: ULTEM™ 1000 resin product has outstanding ability to retain its original dimension under the varying environment conditions or change in temperature and humidity. It offers predictability over wide temperature range
4. Environmental stress and Cracking resistance: The material has the ability to retain strength and resist stress cracking when exposed to aggressive chemical agents like aircrafts fluids, acids, alcohols, hydrocarbons
5. Flammability, smoke generation and toxicity: Most of the ULTEM™ resin products offer inherent flame resistance. These materials are exceptionally difficult to ignite and generate less smoke with byproducts of combustion no more than that of wood.
6. Processability: ULTEM™ resins can be easily extruded, thermoformed, extrusion blow molded and injection molded.

2.2 Understanding of *MAT_187 material model in LS-DYNA® Software

Modelling of structures made from thermoplastic materials subjected to static abusive loads or transient-dynamic loads such as crash loads necessitates modeling of large deformations and failure. Hence, it is a challenge to model these structures using the simple material models available in commercial solvers. *MAT_187 material model in LS-DYNA, which is the semi analytical model for polymers was developed to consider the complex behaviour of plastics. *MAT_187, also known as *MAT_SAMP-1, is a complex material model that is able to capture many of the characteristics exhibited by thermoplastics.

The current study uses *MAT_187 material model in LS-DYNA® software to predict the multiaxial impact behavior of ULTEM™ 1000 resin. The material model applies a yield criteria based on an isotropic C-1 smooth yield surface. The model takes into account the pressure dependency by taking a yield function which incorporates pressure state. The softening and volumetric change is accounted by incorporating a parameter which is a function of plastic Possion's ratio in the plastic potential function. In *MAT_187, the tension, compression, shear and biaxial curves can be defined.

H.Y. Kim *et al.* [1] worked on improving the crash performance of plastic materials considering strain rate and fracture characteristics. A Dyna tup impact model was constructed to perform fracture analysis using *MAT_187 material model. A 100mm*100mm square shaped sample was used with the thickness of 2.9mm. Impact shaft load was 22.43kg, diameter was set at 12.7mm and fall speed at 3270mm/sec. *MAT_187 and *MAT_24 material models were used and results were compared to evaluate the differences. The results showed that, in case of *MAT_ 24 there was large error in time point of fracture but in *MAT_187 model, the load and fracture time tended to be similar to that of the actual test. P. Reithofer *et al.* [2] in his work studied and compared the various material models in LS-DYNA® software for thermoplastics. The author stated that in crash simulations, the material and failure models dealing with Von Mises visco-plasticity and equivalent strain failure criteria which is *MAT_24 material model simply cannot describe the complex behaviour of plastics. But, a complex material model like *MAT_187 incorporates yield behaviour under different loading conditions like tension, compression and shear thus able to describe the detailed behaviour of plastics.

2.3 Failure and damage modeling in LS-DYNA® software

LS-DYNA® software offers material models for materials having an implemented damage failure modeling. These models include simple failure models like plastic strain in *MAT_24, damage failure models like plastic failure strain with damage in *MAT_81 or the highly complex damage/failure models like *MAT_ADD_EROSION which incorporates failure in dependence of strain rate and triaxiality [18]. Generalized incremental stress-state dependent model (GISSMO) is a failure model that allows an incremental description of damage accumulation which includes the softening and failure. The governing equation to determine the damage accumulation is given in equation (1). D is initialized to a value of 10^{-20} for all the damage types in the first time steps.

$$\Delta D = \frac{DMGEXP \ x \ D^{\left(1-\frac{1}{DMGEXP}\right)}}{\varepsilon_f} \Delta\varepsilon_p \tag{1}$$

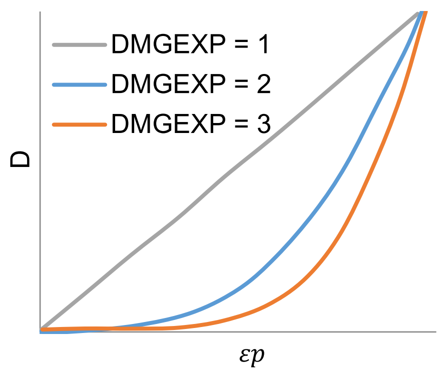

Fig. 1: Accumulation of damage with varying damage exponent

GISSMO model allows softening. This happens by decreasing the stress, by invoking it to be coupled with damage. Stress fadeout initiates when either critical plastic strain or critical damage value is reached and damage coupling flag is set to unity, as shown in figure 2, which is given as an input by the user and specific to the material under study. The equation which couples stress to damage and the critical values is given by equation (2).

$$\sigma = \tilde{\sigma}\left(\frac{D-DCRIT}{1-DCRIT}\right)^{FADEXP} \quad (2)$$

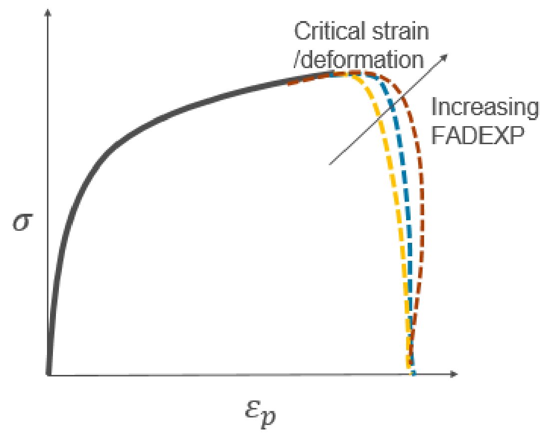

Fig. 2: Influence of fading exponent

4 Input data processing

4.1 Single point and multipoint data generation for input in *MAT_187

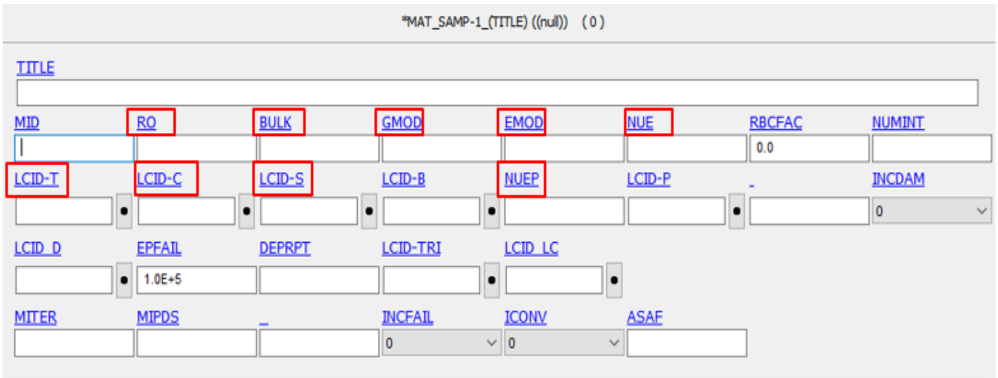

*Fig. 3: *MAT_187 card in LS-DYNA® Software*

The single point data which is defined in *MAT_187 card is directly obtained from the testing, as well as data that is computed using the appropriate mathematical relations. Density, tensile modulus, shear modulus, bulk modulus, Poisson's ratio, and plastic Poisson's ratio are the single point values defined in the *MAT_187 card. The multipoint data in *MAT_187 is defined as True stress vs Plastic strain curves. In the current study, multi-point values are processed and the data sets generated for tensile, compression, shear and Poisson's ratio.

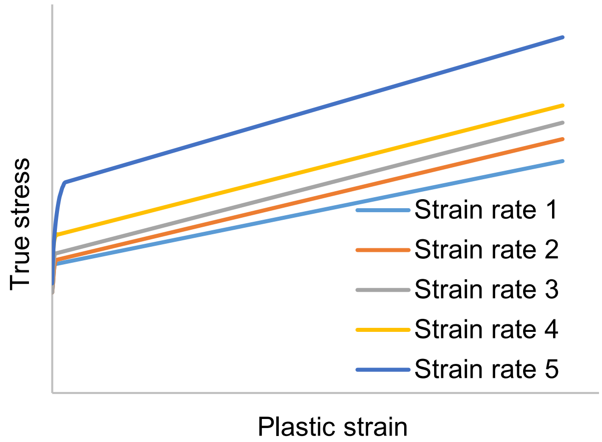

Fig. 4: True stress vs Plastic strain curves for tension

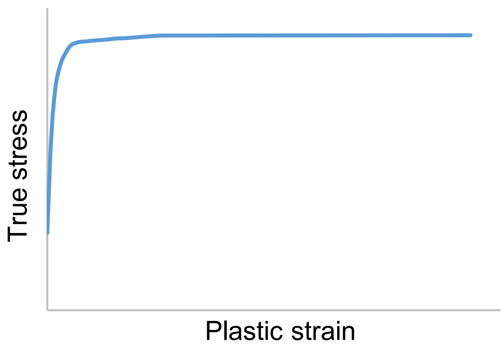

Fig. 5: True stress vs Plastic strain curve for compression

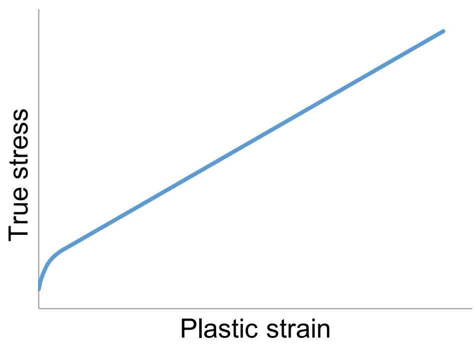

Fig. 6: True stress vs Plastic strain curve for shear

4.2 Single point and multipoint data generation for GISSMO card

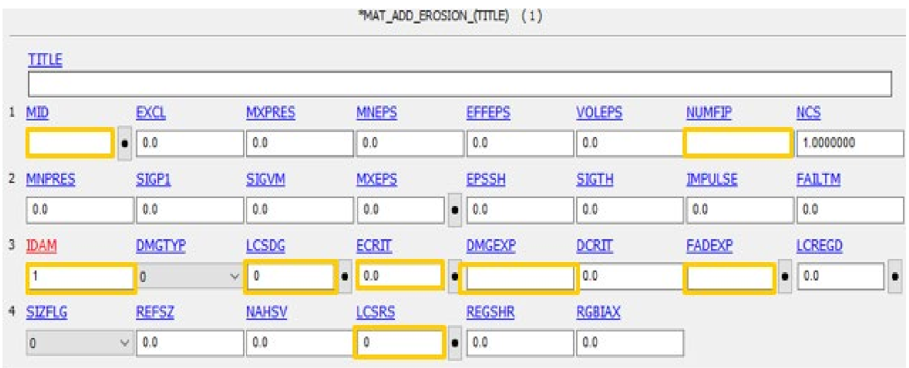

*Fig. 7: *MAT_ADD EROSION card in LS-DYNA® Software*

To consider the damage and failure, *MAT_ADD_EROSION card was used. The highlighted variables in figure 7 are the single point data and multipoint data input in the card. IDAM is used to invoke the GISSMO model. ECRIT, DMGEXP AND FADEXP are the damage parameters which determine the softening behavior of the material. These damage parameters are material specific and was determined using an optimization tool called LS-OPT®. A detailed study on determining these parameters using optimization technique is discussed in the paper. NUMFIP represents the number of failed integration points prior to element deletion. It determines the percentage of layers which must fail for the shell element deletion. The layers represent the thickness of the shell element. The failure is captured by

NUMFIP, LCSDG and LCSRS in *MAT_ADD_EROSION card. Failure is the product of the plastic strain to failure considered at a particular stress triaxiality and plastic strain rate. When this particular plastic strain value gets exceeded the element is deleted.

4.2.1 Equivalent plastic strain to failure v/s stress triaxiality

A curve is defined in the LCSDG of the GISSMO card which gives the equivalent plastic strain to failure corresponding to respective stress triaxiality.

4.2.2 Scaling factor for equivalent failure strain v/s plastic strain rates

A curve is defined in the LCSRS of the GISSMO card which gives a scaling factor for failure value with respect to plastic strain rate.

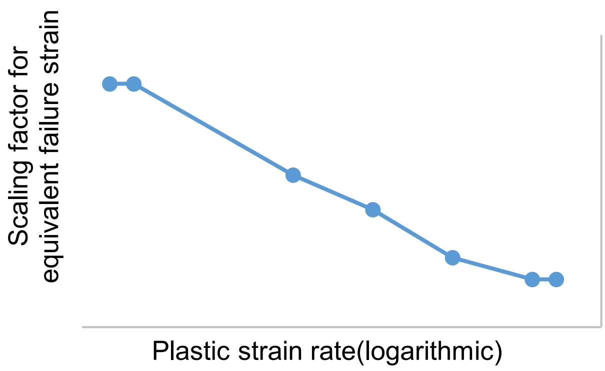

Fig. 8: Scaling factor for equivalent failure strain vs plastic strain rates

5 *MAT_187 validations for different stress states

5.1 Tension

Tensile test was performed as per ISO 527 standard using ISO 8256 Type 3 specimen of gauge length 10mm. Here the plaques are injection molded and specimen geometry as per ISO 8256 Type 3 were machined longitudinally out of plaques. The test is carried out at 23ºC and at five different strain rates. The experimental results were obtained as engineering stress-strain and force-displacement curves. The simulations were carried out using full integration shell elements. Figure 9 shows the FEA model of tensile specimen. Element size of 1mm was considered. The left fixed nodes were constrained in all 6 degrees of freedom and right moving nodes were pulled in the positive x direction at a particular velocity, corresponding to the strain rate for which the test was carried out. The simulation was performed at three different strain rates and the simulation results correlated well with the experimental data for all the three strain rates.

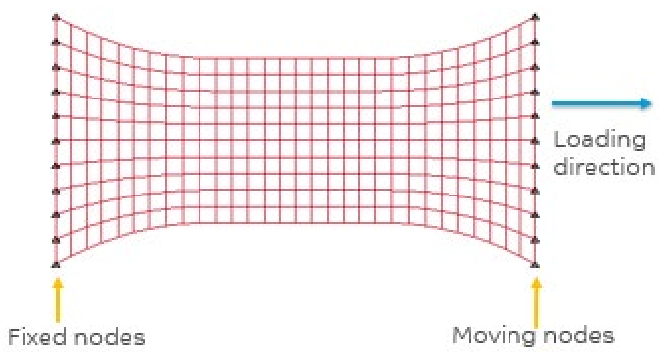

Fig. 9: Shell model of tensile specimen

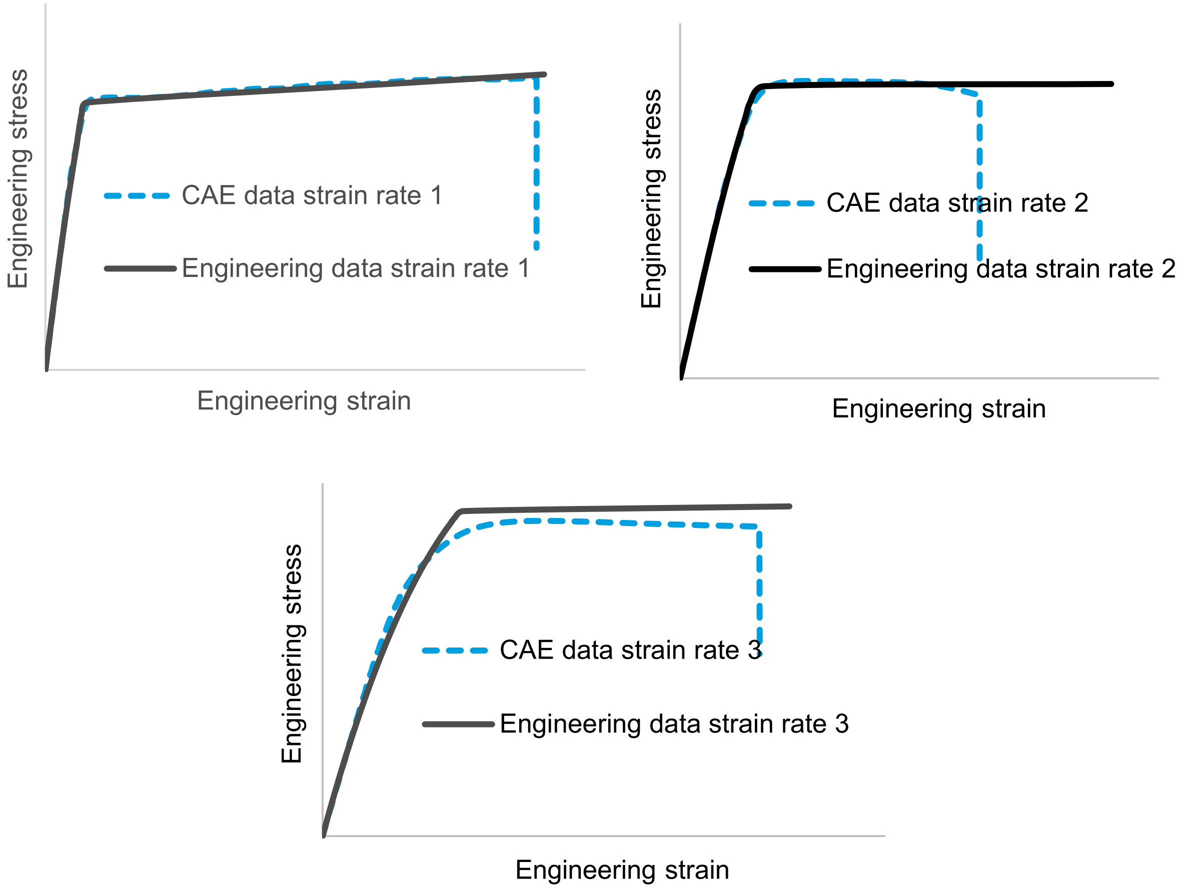

Fig. 10: Correlation of experimental and simulation engineering stress vs engineering strain curves at three strain rates

5.2 Compression

For compression testing, ISO 8256 Type-3 specimen geometry was considered. Similar to tension test, the specimen was machined longitudinally out of plaques. The gauge length of the specimen was 10mm. Compression test was performed as per ISO 6641 standard using a combined loading compression test fixture. The test was performed at 23ºC and at a single speed. The compression test simulation was carried out using shell elements of same type as in tensile test. In the model, the left fixed nodes were constrained in all degrees of freedom and moving nodes were given a velocity, corresponding to the test strain rate in negative x direction. Figure 11 shows the shell model of compression test specimen. It was observed that the experimental data correlated well with the engineering stress – strain curve obtained from simulation.

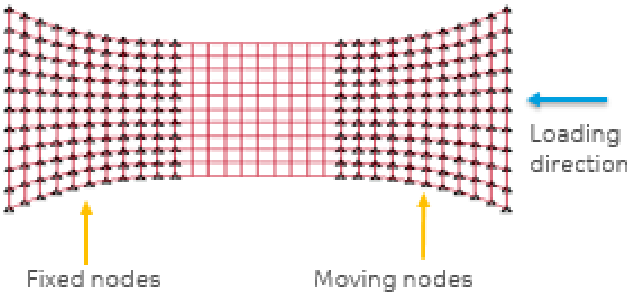

Fig. 11: Shell model of compression test specimen

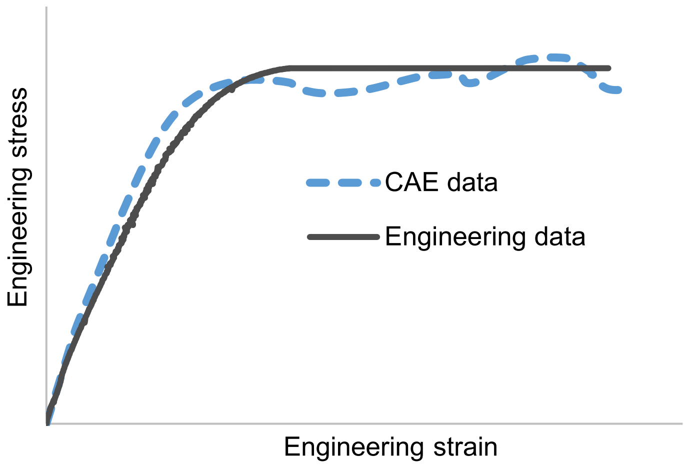

Fig. 12: Comparison of engineering stress-strain curves of compression test with the simulation results

5.3 Shear

Shear test was conducted as per ASTM 5379 standard using a notched specimen. The test was conducted at 23ºC at a single speed. FEA model used for simulation is shown in figure 13. Shear test simulation was carried out using the same type of shell elements as in other tests, ELFORM 16. The element size considered was 1mm. The fixed nodes were constrained in all degrees of freedom, whereas the moving nodes were moving with a constant velocity. The simulation was performed using an implicit solver. The results correlated reasonably well with the input curve.

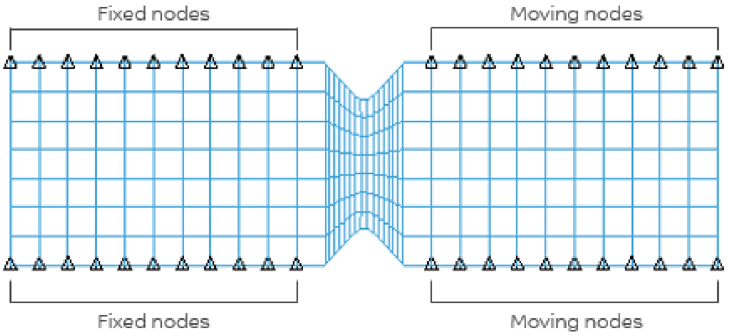

Figure 13: Shell model of shear test specimen

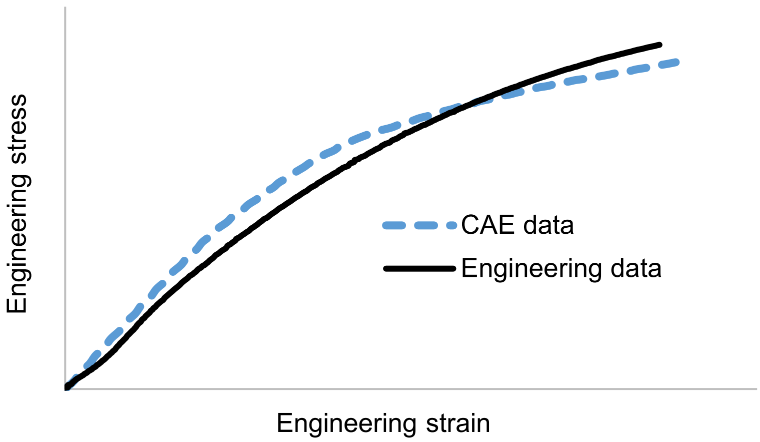

Fig. 14: Comparison of engineering stress-strain curves of shear test with the simulation results

5.4 Dynatup or Falling Dirt Test

Dynatup or falling dirt test was conducted as per ASTM D3763 standard where a hemispherical steel impactor having a diameter of 12.7 mm impacts a clamped disc with an initial velocity. An injection molded disc shaped specimen of 102mm diameter was considered for the test. Figure 11 shows the schematic model of dynatup test.

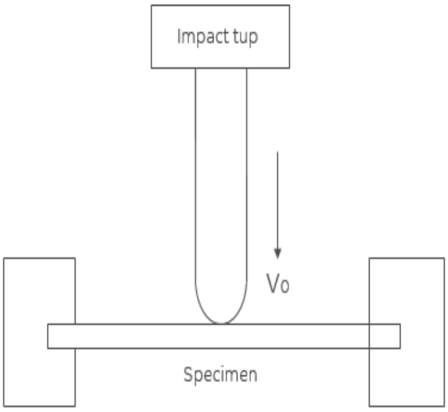

Fig. 15: Schematic model of dynatup test setup

The simulation was carried out by applying the load in two phases, initialization and transient phase. In the initialization phase, a clamping force of 5KN was applied on the top surface of the clamp and then the specimen, clamp and support were made to stabilize. The clamping force is given as a time-dependent force curve. The defined load curve is applied to both initialization and transient phase. Once the model is stabilized in the initialization phase, the impactor starts moving toward the specimen in the second phase which is the transient phase. The figure below shows the FEA model of the dart impact test.

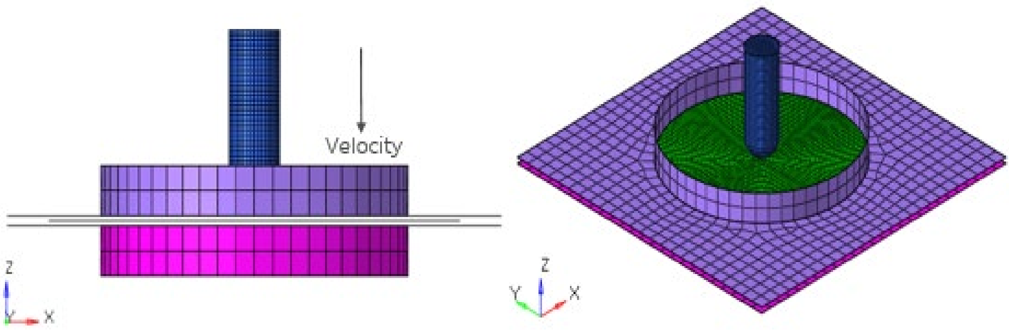

Fig. 16: FEA model of dynatup test

Force between the impactor and specimen as well as the displacement of the specimen when the impactor penetrates the specimen were captured and plotted as force vs. displacements curves. These force vs. displacement results from the test are used to compare with the simulations results. Figure below shows the dynatup simulation at different time intervals.

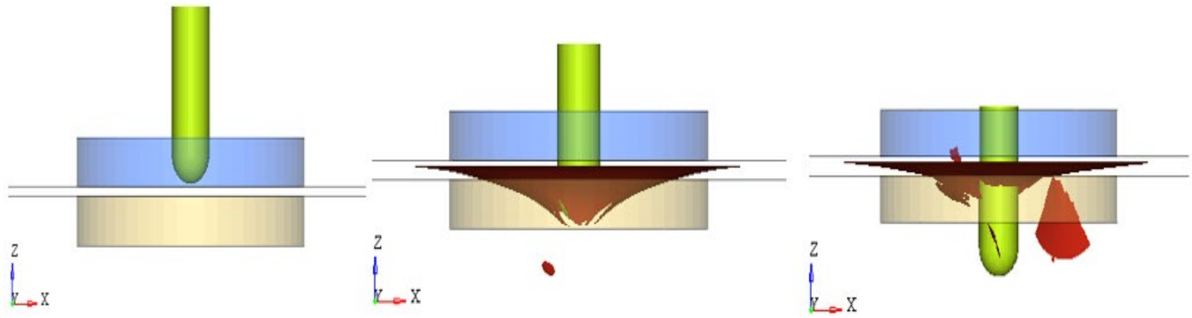

Fig 17: Dynatup simulation at three different time intervals

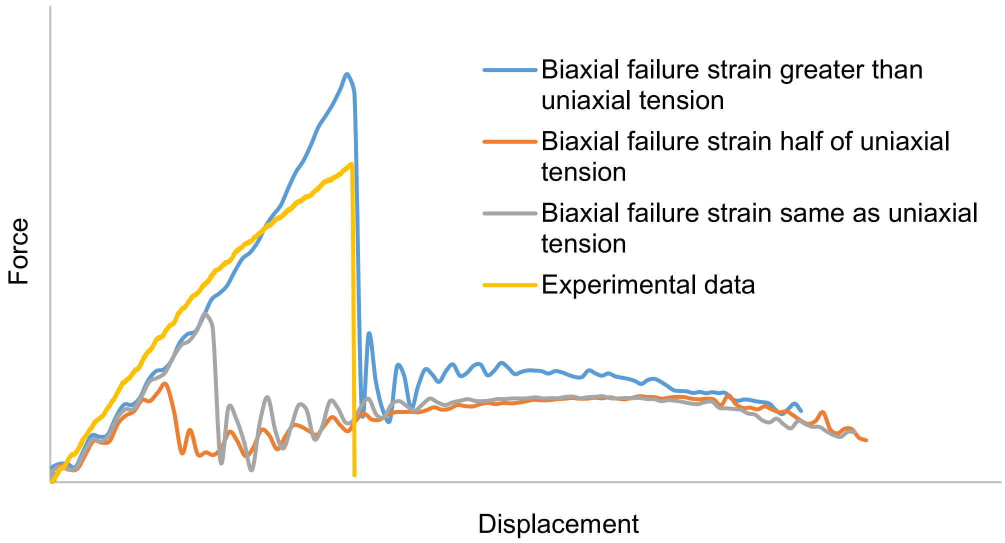

Fig. 18: Correlation of experimental data with simulation results without damage parameters and manually iterated biaxial failure strain in GISSMO model

For the first cut run, the biaxial failure strain was arrived at by manually iterating the values to correlate with the experimental curve. It was observed that the biaxial failure strain was greater than failure strain at uniaxial tension. Also, a difference in stiffness was observed between the experimental and simulation results. To better model damage in the material and improve correlation, the damage parameters in the GISSMO model were next included in the model.

6 Optimization of damage parameters using LS-OPT® tool

Optimization technique using LS-OPT® tool is used to optimize the damage parameters in the GISSMO model. Initially seven variables were considered for the optimization. These variables are those which are hard to obtain from the experiments. It includes the biaxial failure strain (biaxial), compression failure strain (cmpfail), shear failure strain (shfail), viscous damping coefficient (VDC), damage exponent (dmgexp), fade exponent (fadexp) and critical plastic strain (ECRIT). The first run in LS-OPT® tool included these seven parameters to optimize. By carrying out a sensitivity study after the first run, the variables which are not having a significant effect on the correlation were eliminated.

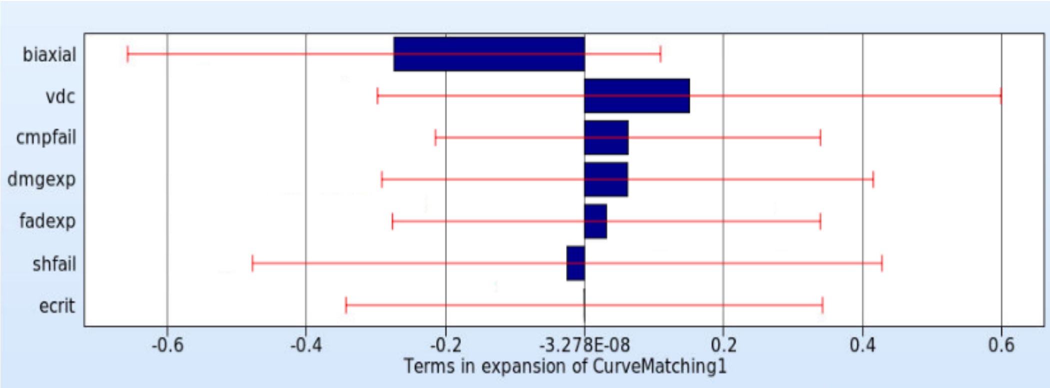

Fig. 19: Sensitivity study plot in LS-OPT® tool

From the plot in Figure 19, it can be seen that critical plastic strain (ECRIT) and shfail had least influence on the results compared to other variables. Hence these two variables were eliminated in the future runs. VDC was also removed as the simulation results looked unrealistic with higher values of viscous damping coefficient. So, the next run was performed considering only 4 parameters for optimization. Those are DMGEXP, FADEXP, biaxial and compression failure strain. Realistic limits were specified for each of these parameters and initial values were also defined. A total of 30 interactions were performed in LS-OPT® tool to optimize these parameters. The figure below shows the iteration results and their comaprison with the experimental curve which is represented as black dotted curve.

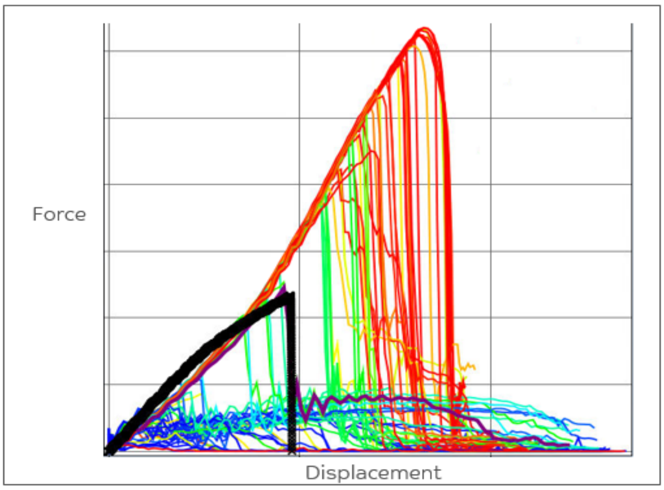

Fig. 20: Iteration results of Dynatup test in LS-OPT® tool for parameter identification

After obtaining the optimized damage parameters and failure strain values for shear and biaxial tension from LS-OPT® run, dynatup test was simulated with these optimized parameters. The experimental data correlated reasonalbly well with the simulation results except for a difference in initial stiffness. Figure 21 shows the comparison of the simulation results with optimized damage parameters and the experimental curve.

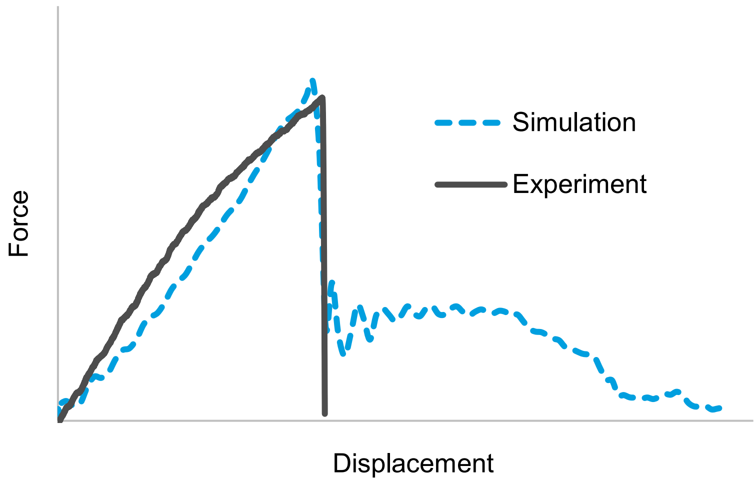

Fig. 21: Comparison of experimental and simulation force-displacement curve for Dynatup test considering the optimized parameters in GISSMO model

7 Static tray impact test

Since the material failure and damage parameters were optimized for the dynatup test, a static push test was performed on a healthcare tray to further validate these optimized damage variables. The geometry of the tray is shown in Figure 22 (a). The thickness of the tray is 2.5mm. The tray was placed on L-type supports and the load is applied by slowly pushing a load pin against the tray by giving a vertical displacement until the part fails.

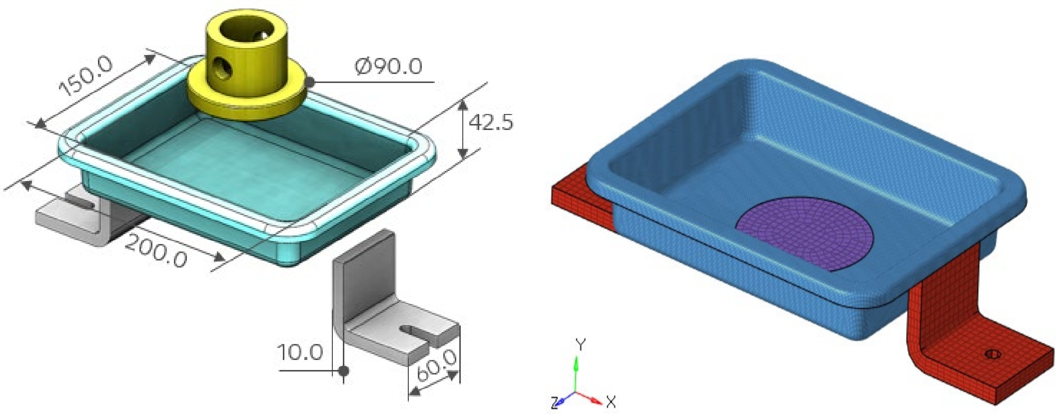

Fig. 22: (a) Part geomtery (b) FEA model of the tray

Figure 22(b) shows the FEA model of the tray where the tray is meshed using shell elements and the load is applied by a rigid loading pin pressing in vertically downward direction against the tray. The output is obtained in the form of reaction force vs. displacement and is plotted again the experimental result. By considering the same damage parameters obtained from dynatup test simulation, the strength, stiffness and failure behavior of the healthcare tray test was accurately predicted as shown in Figures 23 and 24.

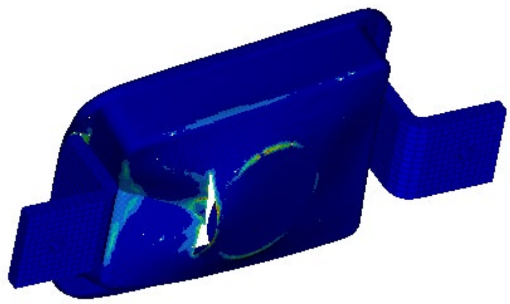

Fig 23: Simulation of static tray impact test

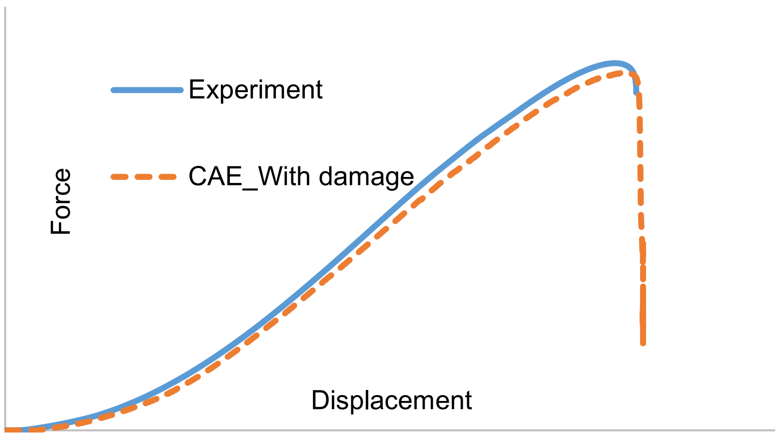

Fig. 24: Correlation of tray test simulation results with experimental curve considering the damage, failure without damage and no failure in the simulation

Hence the established *MAT_187 card with GISSMO model for ULTEM™ 1000 resin is now validated and can be used with high confidence for real life applications.

8 Conclusions

1. The generated material card was validated for standard uniaxial tests such as uniaxial tension, uniaxial compression and pure shear.
2. ULTEM™ 1000 resin product exhibited ductile behavior during the uniaxial tension test. A good elongation before failure was observed. But in the multiaxial static and impact tests, the specimen showed brittle behavior.
3. To capture the damage and failure in the material, GISSMO model was used. The damage parameters as well as biaxial and compressive failure strains were obtained by employing an optimization technique in LS-OPT® tool.
4. Using the optimized damage parameters and failure strain values, the experimental data of dynatup test correlated well with the simulation results.
5. The optimized damage parameters and failure strains were further validated for a static multiaxial tray test. The model was able to predict the stiffness, strength and failure very well.

9 References

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10 Definitions/Abbreviations

D	Damage
DMGEXP	Damage exponent
ε_p	Effective plastic strain
ε_f	Effective plastic strain at failure
FADEXP	Fade exponent