

## Micro-mechanical Modelling

Viscoplastic model

$$\dot{\epsilon} = \dot{\epsilon}_0 \left( \frac{\tau}{\tau_0} \right)^n$$

Model with damage

$$\dot{\epsilon} = \dot{\epsilon}_0 \left( \frac{\tau}{(1-\Omega)\tau_0} \right)^n$$

No. atomic bonds  
Initial No. atomic bonds  
Damage variable

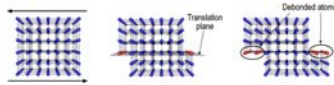
$$\frac{d\Omega}{dt} = \frac{d\Omega}{dt} \left( \frac{\tau}{\tau_0} \right)^m$$

Damage evolution law

$$\dot{\epsilon} = h \sum_i \dot{\epsilon}_i$$

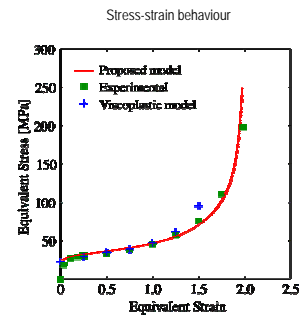
Hardening law

$$h = h_0 \operatorname{sech}^2(h_0 \tau / C)$$

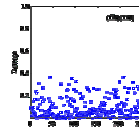


Idealized damage mechanisms for crystal slip systems

### Uniaxial tension case



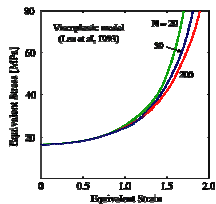
Planes damage



- Model including damage gives better simulation of material response
- Unique model development with time evolution of damage

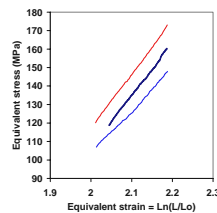
## Strain Hardening Behaviour

Simulation Results



N – number of C-C unit between entanglements

Test Results

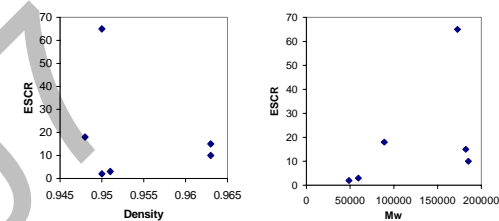


	Gp (MPa)	ESCR (hours)
PE N	300.08	1000
PE 100	292.73	1000
PE 80	235.10	500

- Higher values of relative strain hardening modulus correlate with higher ESCR values
- Model predicts higher strain hardening response with more entanglements

The prediction of mechanical properties of a polymer based on its chemical composition has always been a challenge for material science. This is especially true for ESCR (environmental stress cracking resistance) of polyethylene.

## Single Factor Correlations



- Not reliable!
- Too many exceptions

## Entanglement of chains

- According to reptation theory, entanglements detected should be result of long chain branching
- Resin with more entanglements should have better ESCR

Average entanglement per chain

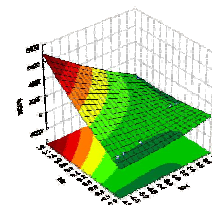
	Mn	Mw	Mz	ESCR
PE1	0.57	6.61	96.4	65
PE3	1.15	10.12	138.1	15
PE4	0.87	3.79	20.4	18
PE5	0.04	0.12	0.3	2
PE6	0.24	1.01	3.9	3

$$1/J_e^0 = N_e = \frac{\rho RT}{M_e}$$

Calculation for Me

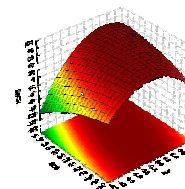
## Multi Factor Correlations

Effect of MWs

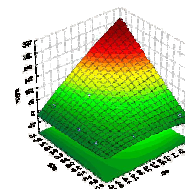


Effect of SCB and MWs

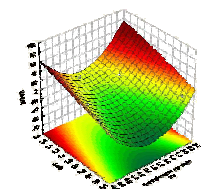
SCB and Mw



SCB and Mz



Effect of SCB and number of entanglements



- More complete picture of ESCR behaviour; avoids previous pitfalls
- Combined influence of micromolecular properties can be seen