Biodegradable Polymers: An Introduction

Aoife Hill

William Ronan and Michel Destrade

Postgraduate Modelling Research Group

National University of Ireland, Galway

03 November 2017

Research Objective

Develop a modelling framework for biodegradable polymers;
For use in the medical device industry.

“In-silico” testing

- reduces costs
- speeds up development of new devices
- reduces reliance on animal trials

Motivation

Biodegradable Polymers:

Uses:

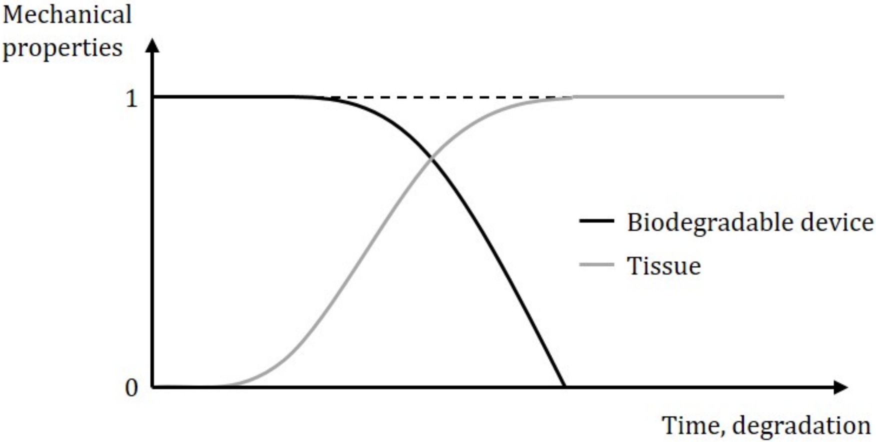
- Drug delivery
- Tissue engineering
- **Cardiovascular stents**

Click!

Advantages:
Overcome issues associated with current stents.

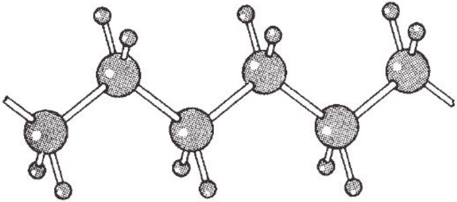
Why accurate modelling is vital

Insufficiently stiff $\Longrightarrow$ healing not supported
Too stiff $\Longrightarrow$ stress-shielding effect
Optimal stiffness:

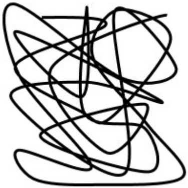


Polymers

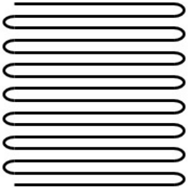
- Long macromolecular chains
- Monomers + chemical bonds



Structure types:



Amorphous

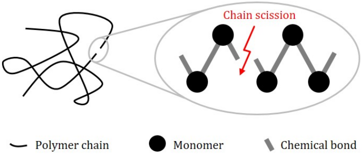


Crystalline

Semi-crystalline

Degradation

Material is placed in aqueous medium $\Longrightarrow$ chain scissions occur

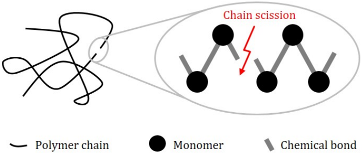


Terminology:

- end scissions
- random scissions

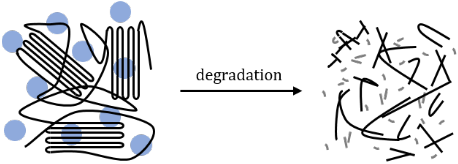
Degradation

Material is placed in aqueous medium $\Longrightarrow$ chain scissions occur



Terminology:

- end scissions
- random scissions
- autocatalysis
- bulk degradation



Degradation Model (Molecular Weight Model)

Developed by Wang *et al.* (2008).

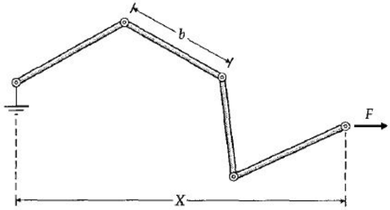
$$\frac{\partial C_m}{\partial t} = k_1 C_e + k_2 C_e C_m^{\beta} + \nabla \cdot (D \nabla C_m)$$
$$\frac{\partial C_e}{\partial t} = -(k_1 C_e + k_2 C_e C_m^{\beta})$$

- C_m = monomer concentration
- C_e = ester concentration
- k_1 = rate of non-catalytic degration
- k_2 = rate of autocatalytic degration
- β accounts for dissociation of acid end groups
- D = diffusion coeffiecient

Entropy Spring Model

Freely jointed chain:

- Behaves as entropic spring
- Good model for rubber-like elasticity



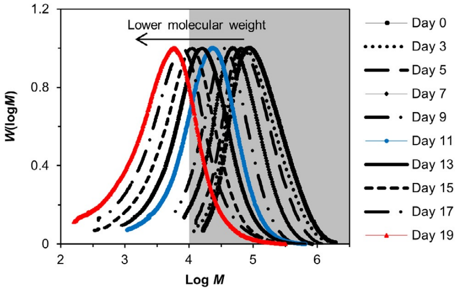
$$F = \frac{3kT}{nb^2}X$$

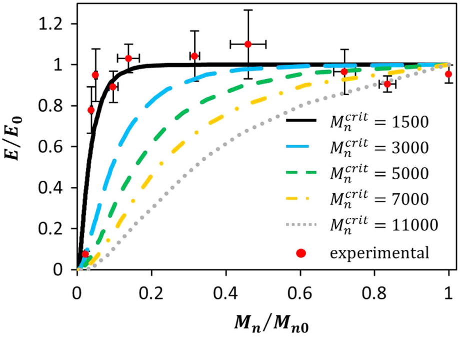
$$\implies E = 3NkT$$

- k = Boltzmann's constant
- T = absolute temperature
- n = number of segments
- b = length of each segment
- N = number of chains per unit volume

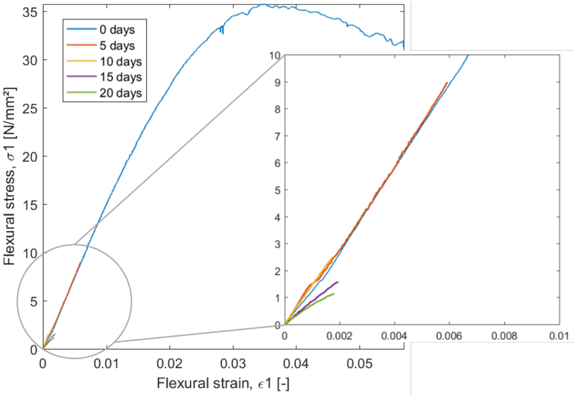
From the literature

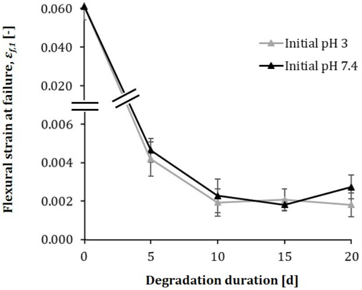
Degradation model coupled with entropy spring model (Shirazi *et al.*, 2016):



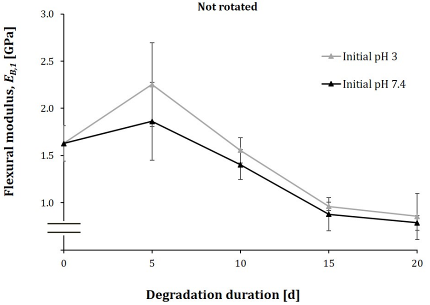


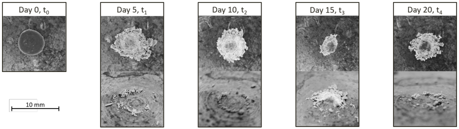
Existing data

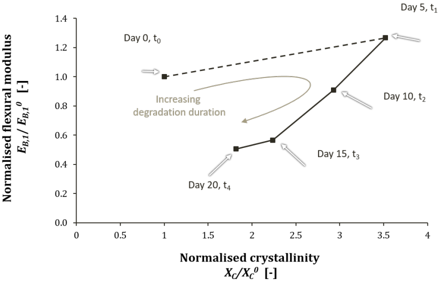




Existing data







Future work

- Develop a more robust model of degradation: $E \neq 3NkT$
- Investigate experimentally observed significant decrease in ductility
- Establish criteria describing failure under loading

$$\left.\begin{array}{l} \text{Develop a more robust model of degradation} \\ \text{Investigate experimentally observed significant decrease in ductility} \\ \text{Establish criteria describing failure under loading} \end{array}\right\} \quad \varepsilon_f = f(X_c, M_w)?$$

References

Y. Wang, J. Pan, X. Han, *et al.*.
A phenomenological model for the degradation of biodegradable polymers.
Biomaterials, **29**(23):3393-3401, 2008.

R. N. Shirazi, W. Ronan, Y. Rochev, P. E. McHugh.
Modelling the degradation and elastic properties of poly(lactic-co-glycolic acid) films and regular open-cell tissue engineering scaffolds.
Journal of the Mechanical Behavior of Biomedical Materials, **54**:48-59, 2016.

K. S. Bezela.
Examination of biodegradable materials for medical devices.
Unplublished ME thesis. RWTH Aachen University; National University of Ireland, Galway, 2017.