MODELING AND SIMULATION IN BONE TISSUE ENGINEERING

SCAFFOLD DEGRADATION

Scaffold plays an important role in tissue engineering and an optimum degradation rate and enough mechanical strength are required during the regeneration of tissue.

The objective of the work is to present an optimal 3D structure of scaffold by developing mathematical model combines scaffold degradation, mechanical stimuli and bone regeneration using computational methods.

The degradation of polymer occurs due to diffusion and hydrolysis reaction which results monomers with low molecular weight and low mechanical strength. The reduction in molecular weight over the time was modeled by understanding the concentration of functional groups remain inside the polymer matrix. The degradation behavior of bio degradable polymer described by the following reaction – diffusion equation.

$$\frac{dR}{dt} = C_{e0}\left[1 - \alpha\left(\frac{R}{C_{e0}}\right)^{\beta}\right]\left\{k_1 + k_2 C_{e0}^{n}\left[\frac{1}{m}\left(\frac{C_e}{C_{e0}}\right)\right]^{n}\right\}$$

$$\frac{dC_e}{dt} = \alpha\,\beta\left(\frac{R}{C_{e0}}\right)^{\beta-1}\frac{dR}{dt} + \frac{\partial}{\partial x}D\frac{\partial C_e}{\partial x}$$

R –Mole concentration of polymer chain scission

C_e - Mole concentration of ester bonds in polymer chains

C_{e0} – Initial mole concentration of ester bonds

k_1& k_2 – Rate constants of non-catalytic and auto-catalytic hydrolysis

m – Average degree of polymerization

α & β - Production rate of short chains by polymer chain scission

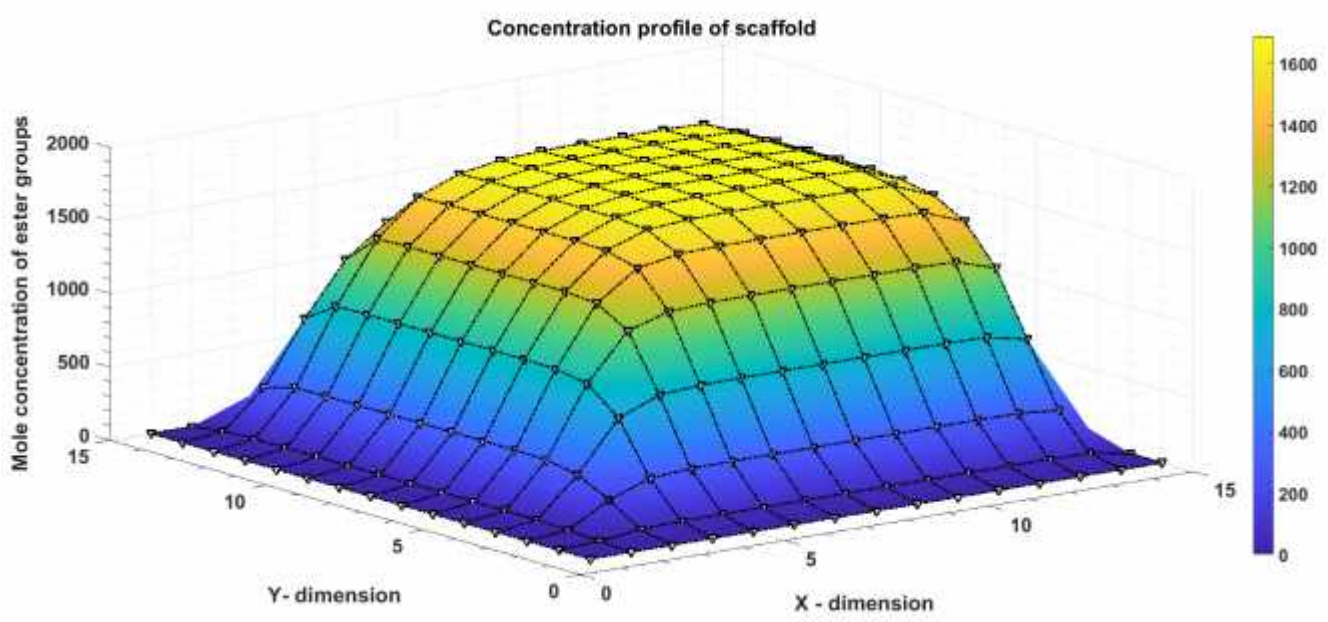
n – Acid dissociation constant

D – Effective diffusivity

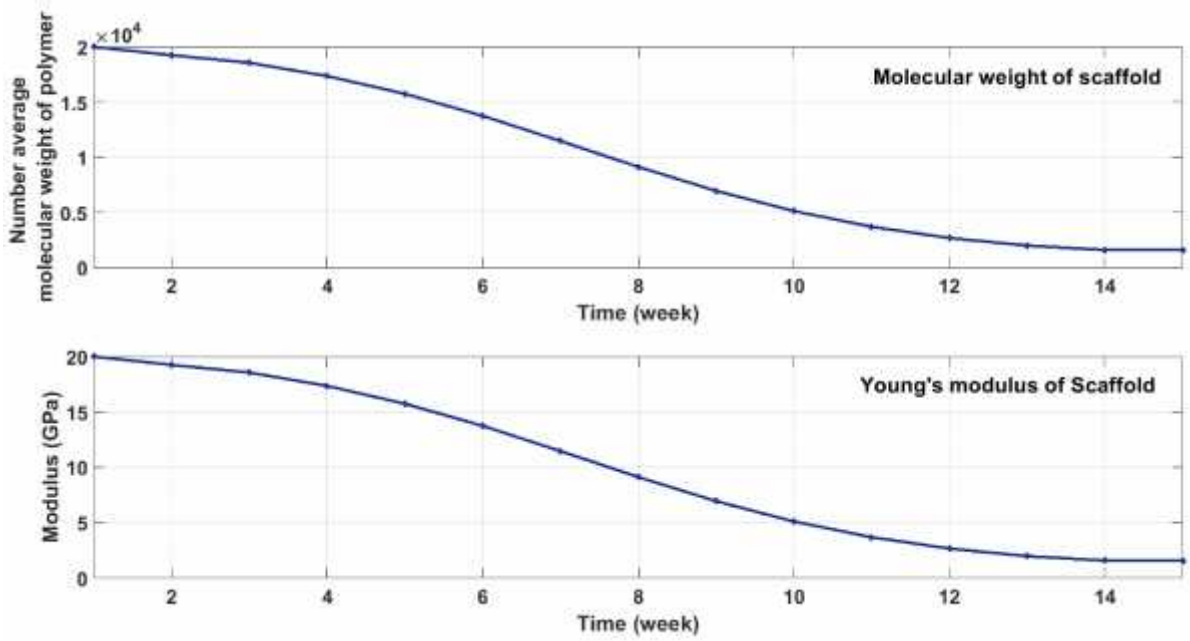
A linear model between the number average molecular weight and Young's modulus was developed by knowing the Young's modulus at zero porosity.The equations were simultaneously solved to get molecular weight and Young's modulus over the time using finite difference method.

Athree-dimensional scaffold mesh was constructed and concentration of functional group in polymer matrix was obtained. The following figure shows the distribution of mole concentration of ester in a polymer matrix.

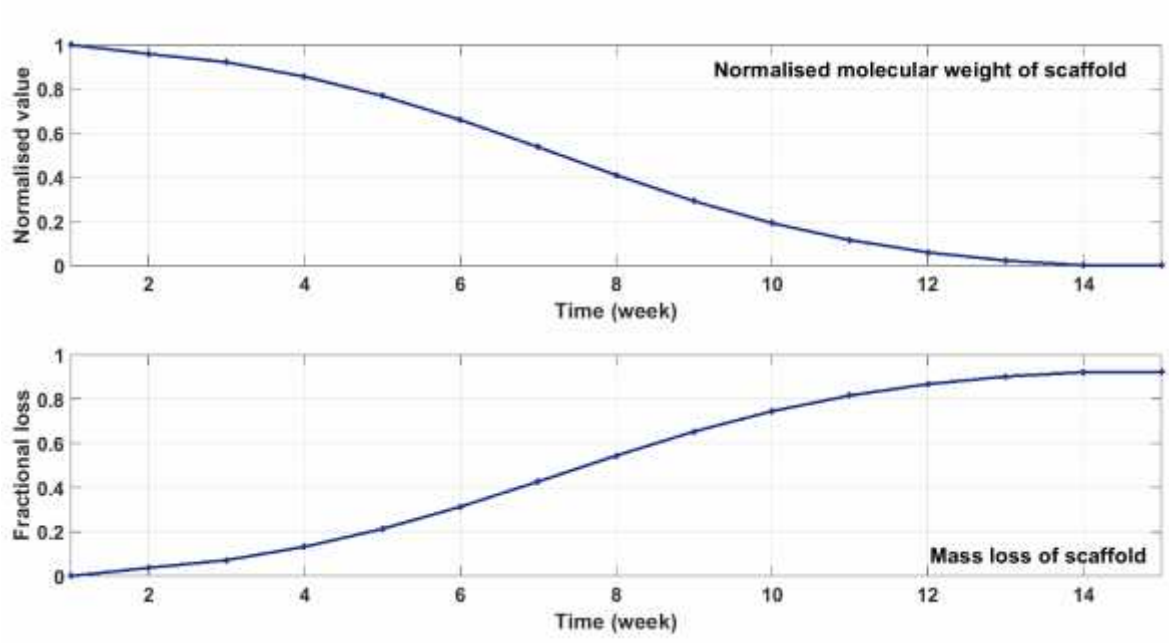
Model parameters used for the finite difference analysis of data from Grizzi et al.,



The following graph shows change in the molecular weight and mechanical property of polymer during the degradation. The molecular weight and Young's modulus follows the similar linear relation over the time; up to 15-week time period simulation was performed. From the normalized value of molecular weight, we could confirm that the entire polymer matrix degraded in 14 weeks.



Graph showing the percentage of mass loss of polymer from the initial molar mass indicates that 80 percent of polymer gets degraded at the end of 14 week. Young's modulus calculated using the porosity of scaffold reveals that, up to 4 week the degradation rate is slower and after which undergoes faster degradation and the modulus value reaches lower value in next 10 weeks.



It is planned to validate the model by performing *invivo* experiment using various aliphatic polymers used in bone regeneration applications.

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