

Notes:  
Incorporating Loops into Initial Model

Spyros Koumarianos

February 5, 2020

# 1 Model Description

We assume a full coverage scenario for n-mer chains being attached to the spherical surface. We also let the original spherical lattice surface be approximated by a rectangular surface lattice with an initial distribution of sites that will be a mesh of rectangles with area 1 Mer.

The next step, will be to gradually remove lattice sites and calculate what effect that has on the contribution to the number of available configurations (cardinality of configurations) for that specific number of sites. the ulterior goal is to

Long	Arbitrary Midlength	Short	Largest Contribution
$n_L$	$n_M$	$n_S$	L?, M?, S?
$n_L - 1$	$n_M - 1$	$n_S - 1$	$\vdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$n_L - k$	$n_M - k$	$n_S - k$	$\vdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$n_L - (n_L - 1)$	$n_M - (n_M - 1)$	$n_S - (n_S - 1)$	$\vdots$

*\*The last row may vary as they may be hard to calculate or may have no physical or chemical significance*

## 2 Parameter Calculations

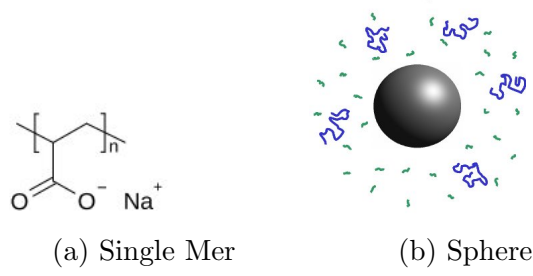


Figure 1

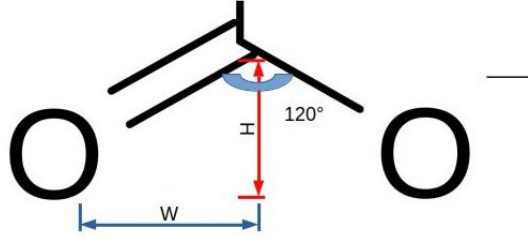


Figure 2: Single Mer

(1)  $N_{Short} \approx 27 \text{ Mers}$

(3)  $N_{Long} \approx 6200 \text{ Mers}$

(4)  $E[2 \cdot r_{sphere}] \approx 85 \text{ nm}$

(5)  $\mathbb{L}_{C-C} = .154 \text{ nm}$

(6)  $\mathbb{L}_{C=O} = .745 \text{ nm}$

(7)  $\mathbb{L}_{C-H} = .109 \text{ nm}$

(8)  $\phi_{C-O, C=O} = \frac{2\pi}{3} \Rightarrow \text{Orth. Triangle has, } \theta = \frac{\pi}{3}$

(9)  $\mathbb{L}_{Short} \approx 8.3 \text{ nm}$

(10)  $\mathbb{L}_{Long} \approx 1910 \text{ nm}$

(11)  $\text{Area}_{Sphere} \approx 2300 \text{ nm}^2$

(12)  $H_{Figure2} = \cos\theta \cdot (\mathbb{L}_{C=O}) = \cos(\frac{\pi}{3}) \cdot (.745) = .373 \text{ nm}$

$$(13) \text{ TotalHeight}_{SingleMer} = H + \mathbb{L}_C \text{---} \mathbb{H} = (.373) + (.109) = .482 \text{ nm}$$

$$(14) \text{ TotalLength}_{SingleMer} = 2 \cdot \mathbb{L}_C \text{---} \mathbb{C} = .308 \text{ nm}$$

$$(15) \text{ Area}_{SingleMer} = (.482) \cdot (.308) = .148 \text{ nm}^2$$

$$(16) \text{ Area}_{ShortMer} = \text{Area}_{SingleMer} \cdot N_{Short} = (.148) \cdot 27 \approx 3.99 \text{ nm}^2$$

$$(17) \text{ Area}_{LongMer} = \text{Area}_{SingleMer} \cdot N_{Long} = (.148) \cdot 6200 \approx 918 \text{ nm}^2$$