Zach Swain 11/5/19

MSEG608-HW8

1.

$$M = 100\ g \quad , \quad M_0 = 54\ \frac{g}{mol}$$

$$\frac{(100\ g)}{\left(54\ \frac{g}{mol}\right)} = 1.85\ mol$$

$$(1.85\ mol) * \left(6.022E23\ \frac{monomers}{mol}\right) = 1.11E24\ monomers$$

A crosslinked system will have all monomers covalently bonded together (networked) via their crosslinks

$$\mathbf{1.11E24\ monomers\ covalently\ bonded}$$

2.

M_n: Number average molecular weight
M_w: Weight or mass average molecular weight
M_z: Z-average molecular weight
Mz+1: Z+1-average molecular weight
M_v: Viscosity average: a from Mark-Houwink equation $[\eta] = KM^a$

$M_w/M_n > 1$ is a measure of dispersity, *Đ*
0.5 <-a<-0.8

$$M = \frac{\Sigma N_i M_i^{n+1}}{\Sigma N_i M_i^n}$$

1.00-1.10: very narrow;
1.10-1.25: narrow;
1.25-2.5: broad;
2.5-10.0: very broad

[1]

where: n = 1 gives M = Mw
n = 2 gives M = Mz
n = 3 gives M = Mz+1
n=0 gives M=M_n

$$\left(\frac{\sum_i n_i M_i^{1+a}}{\sum_i n_i M_i}\right)^{1/a}$$ Intrinsic viscosity

MW	#	n*M	n*M^2	n*M^3	n*M^4	n*M^{1+a}
5.50E+03	1.09E+19	6.02E+22	3.31E+26	1.82E+30	1.00E+34	2.50E+25
2.00E+04	3.01E+18	6.02E+22	1.20E+27	2.41E+31	4.82E+35	6.17E+25
5.00E+04	1.20E+18	6.02E+22	3.01E+27	1.51E+32	7.53E+36	1.17E+26
1.00E+05	6.02E+17	6.02E+22	6.02E+27	6.02E+32	6.02E+37	1.90E+26
2.00E+05	3.01E+17	6.02E+22	1.20E+28	2.41E+33	4.82E+38	3.09E+26
4.00E+05	1.51E+17	6.02E+22	2.41E+28	9.64E+33	3.85E+39	5.03E+26
4.13E+05	1.46E+17	6.02E+22	2.49E+28	1.03E+34	4.24E+39	5.14E+26
5.00E+05	1.20E+17	6.02E+22	3.01E+28	1.51E+34	7.53E+39	5.88E+26
6.50E+05	9.26E+16	6.02E+22	3.91E+28	2.54E+34	1.65E+40	7.06E+26
7.00E+05	8.60E+16	6.02E+22	4.22E+28	2.95E+34	2.07E+40	7.44E+26
8.00E+05	7.53E+16	6.02E+22	4.82E+28	3.85E+34	3.08E+40	8.16E+26
Sum	1.67E+19	6.62E+23	2.31E+29	1.32E+35	8.42E+40	4.57E+27

Mn	**3.96E+04**
Mw	**3.49E+05**
Mz	**5.69E+05**
Mz+1	**6.40E+05**
Mv	**3.05E+05**
Đ	**8.82**

3.

Weight fraction $w_x = \dfrac{\text{Total mass of molecules with degree of polymerization x}}{\text{Total mass of all the molecules}}$

Neglecting end groups

$$w_x = \frac{N_x(x\overline{M_0})}{N_0\overline{M_0}} = \frac{xN_x}{N_0}$$

$$\overline{M_0} = \frac{\text{Molar mass of the repeat unit}}{\text{Number of monomer unit in the repeat}}$$

Average molecular weight of the repeating units

Replacing N_x $\quad N_x = N_0(1-p)^2 p^{x-1}$

$$\boxed{w_x = x(1-p)^2 p^{x-1}}$$

[2]

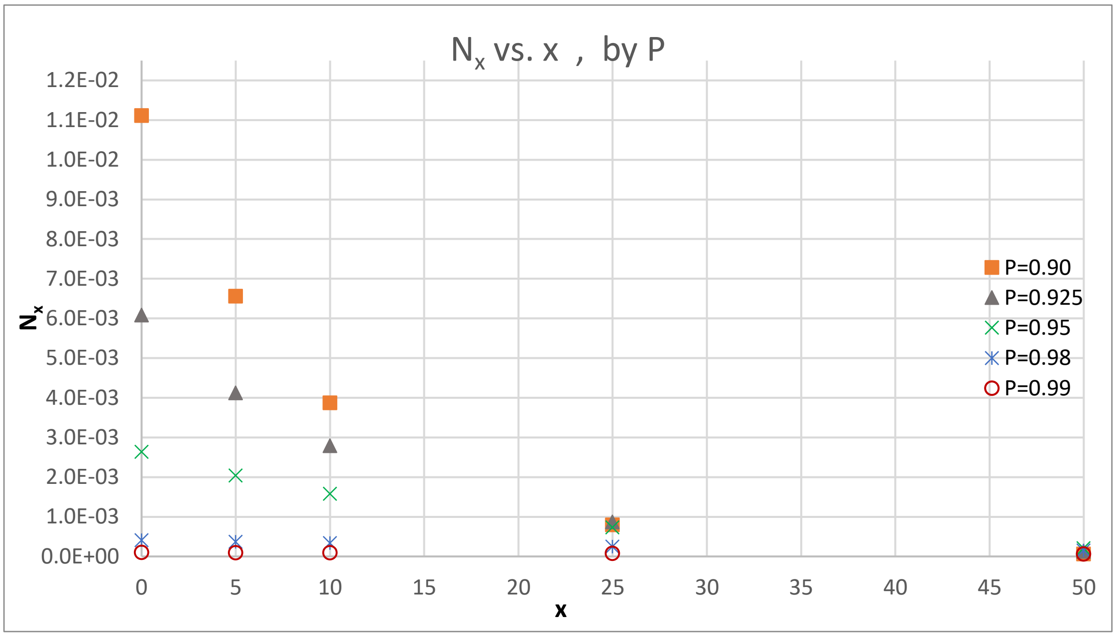

FIG. 1. Statistically derived mole fraction for a step-growth polymerization is plotted as a function of x, and varied by extent of reaction.

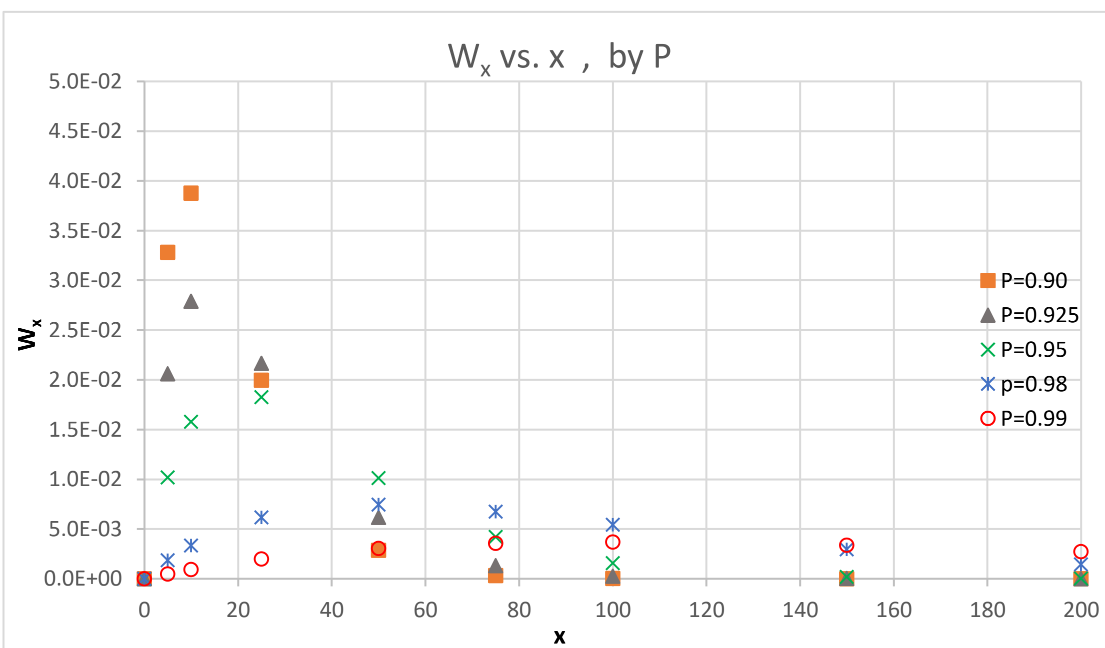

FIG. 2. Statistically derived weight fraction for a step-growth polymerization is plotted as a function of x, varied by extent of reaction.

References

[1] Korley, Wang. (2019). *MSEG608 – Structures and Properties of Materials*. University of Delaware. Lecture 16, Slide 17.

[2] Korley, Wang. (2019). *MSEG608 – Structures and Properties of Materials*. University of Delaware. Lecture 17, Slide 23.

Supplementary

2. If there is question about the calculations used, the full excel file can be found here:

https://github.com/zswain/MSEG608 as "ZachSwain_MSEG608-HW8.xlsx"

3. These calculations were done in the same excel worksheet as detailed above.

Mol frac

P\X	0	5	10	25	50	75	100	150	200	300	400	500
0.9	1.11E-02	6.56E-03	3.87E-03	7.98E-04	5.73E-05	4.11E-06	2.95E-07	1.52E-09	7.84E-12	2.08E-16	5.53E-21	1.47E-25
0.925	6.08E-03	4.12E-03	2.79E-03	8.66E-04	1.23E-04	1.76E-05	2.50E-06	5.07E-08	1.03E-09	4.23E-13	1.74E-16	7.16E-20
0.95	2.63E-03	2.04E-03	1.58E-03	7.30E-04	2.02E-04	5.62E-05	1.56E-05	1.20E-06	9.22E-08	5.46E-10	3.23E-12	1.91E-14
0.98	4.08E-04	3.69E-04	3.33E-04	2.46E-04	1.49E-04	8.97E-05	5.41E-05	1.97E-05	7.18E-06	9.52E-07	1.26E-07	1.67E-08
0.99	1.01E-04	9.61E-05	9.14E-05	7.86E-05	6.11E-05	4.75E-05	3.70E-05	2.24E-05	1.35E-05	4.95E-06	1.81E-06	6.64E-07

Weight frac

P\X	0	5	10	25	50	75	100	150	200	300	400	500
0.9	0	3.28E-02	3.87E-02	1.99E-02	2.86E-03	3.08E-04	2.95E-05	2.28E-07	1.57E-09	6.25E-14	2.21E-18	7.34E-23
0.925	0	2.06E-02	2.79E-02	2.17E-02	6.17E-03	1.32E-03	2.50E-04	7.61E-06	2.06E-07	1.27E-10	6.96E-14	3.58E-17
0.95	0	1.02E-02	1.58E-02	1.82E-02	1.01E-02	4.21E-03	1.56E-03	1.80E-04	1.84E-05	1.64E-07	1.29E-09	9.57E-12
0.98	0	1.84E-03	3.33E-03	6.16E-03	7.43E-03	6.73E-03	5.41E-03	2.96E-03	1.44E-03	2.86E-04	5.05E-05	8.37E-06
0.99	0	4.80E-04	9.14E-04	1.96E-03	3.06E-03	3.57E-03	3.70E-03	3.36E-03	2.71E-03	1.49E-03	7.25E-04	3.32E-04

Mole Fraction

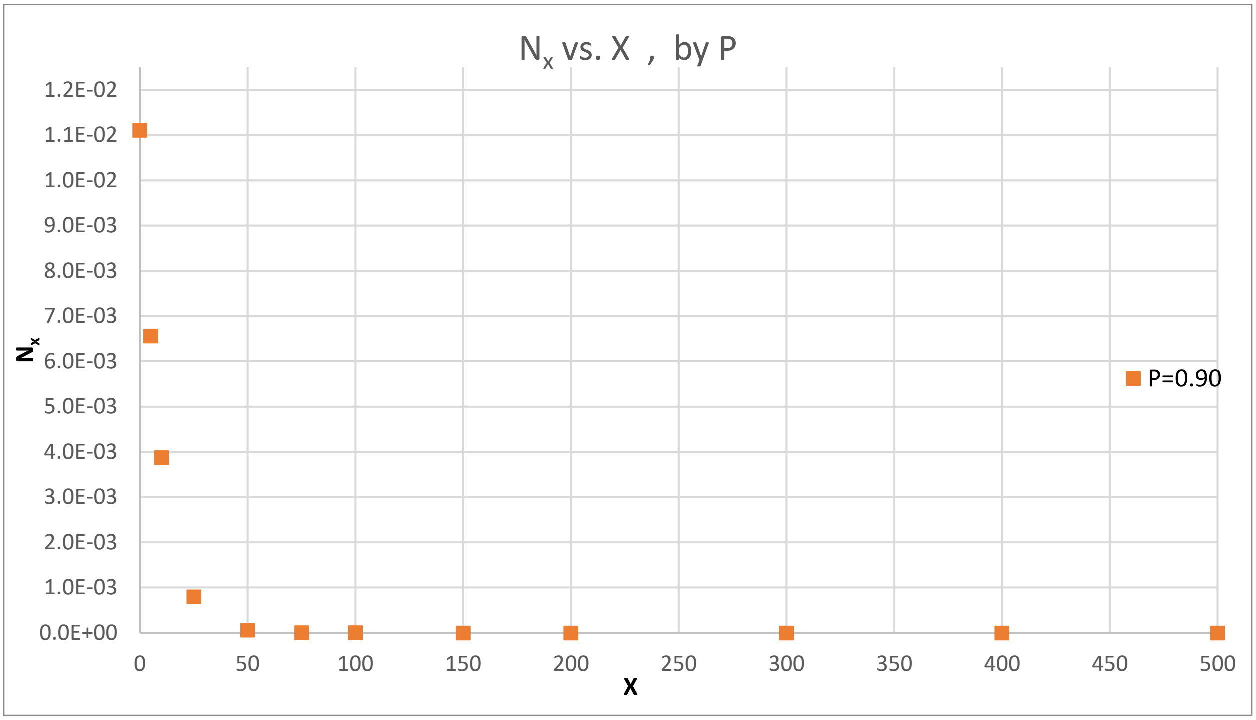

FIG. 3. Statistically derived mole fraction for a step-growth polymerization is plotted as a function of x, for P=0.9

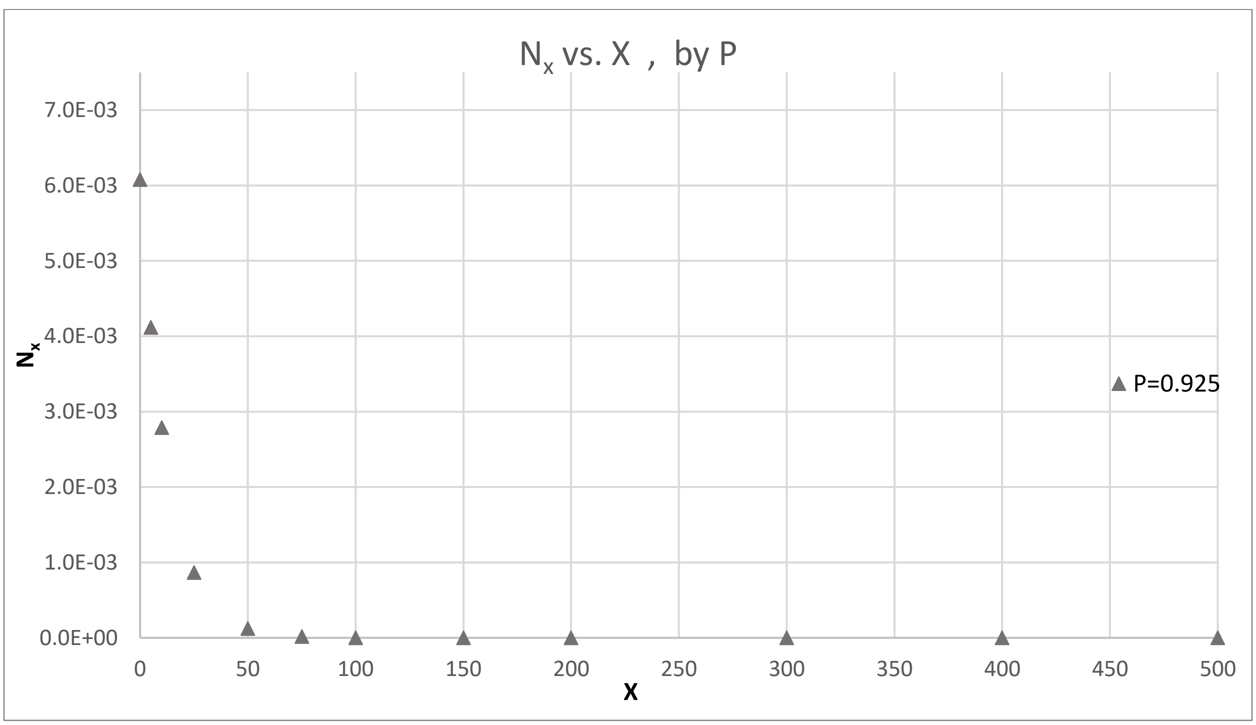

FIG. 4. Statistically derived mole fraction for a step-growth polymerization is plotted as a function of x, for P=0.925

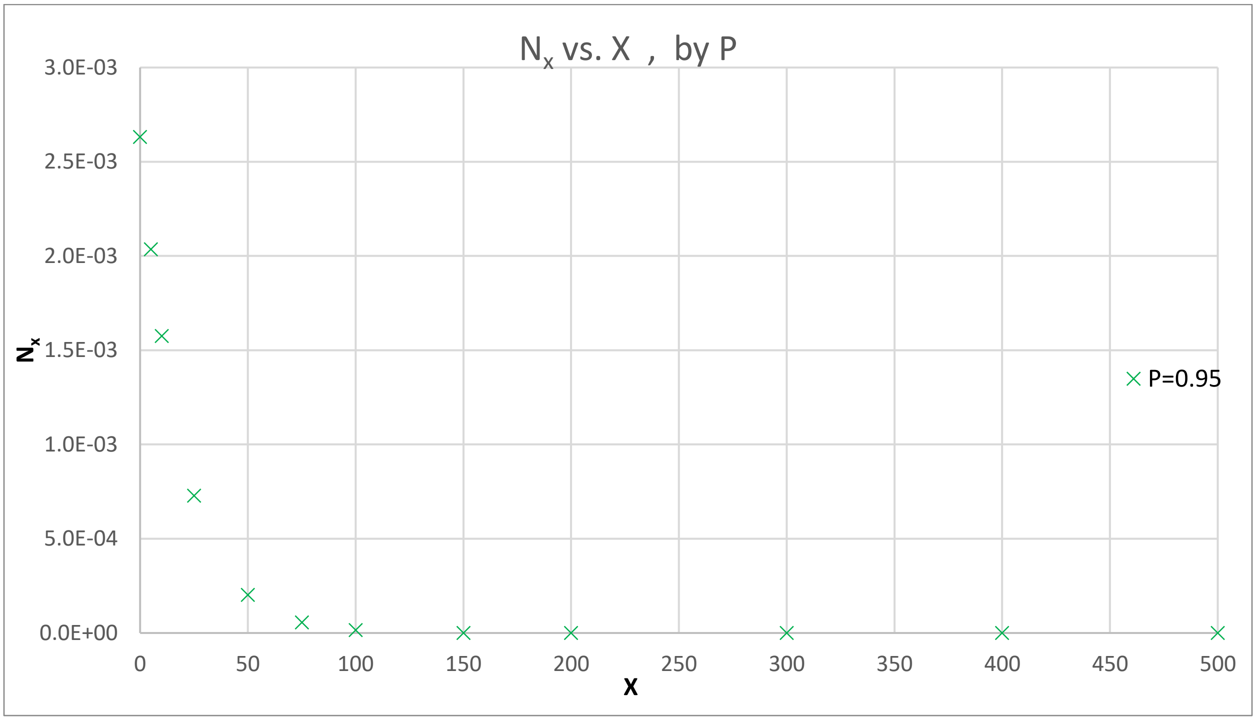

FIG. 5. Statistically derived mole fraction for a step-growth polymerization is plotted as a function of x, for P=0.95

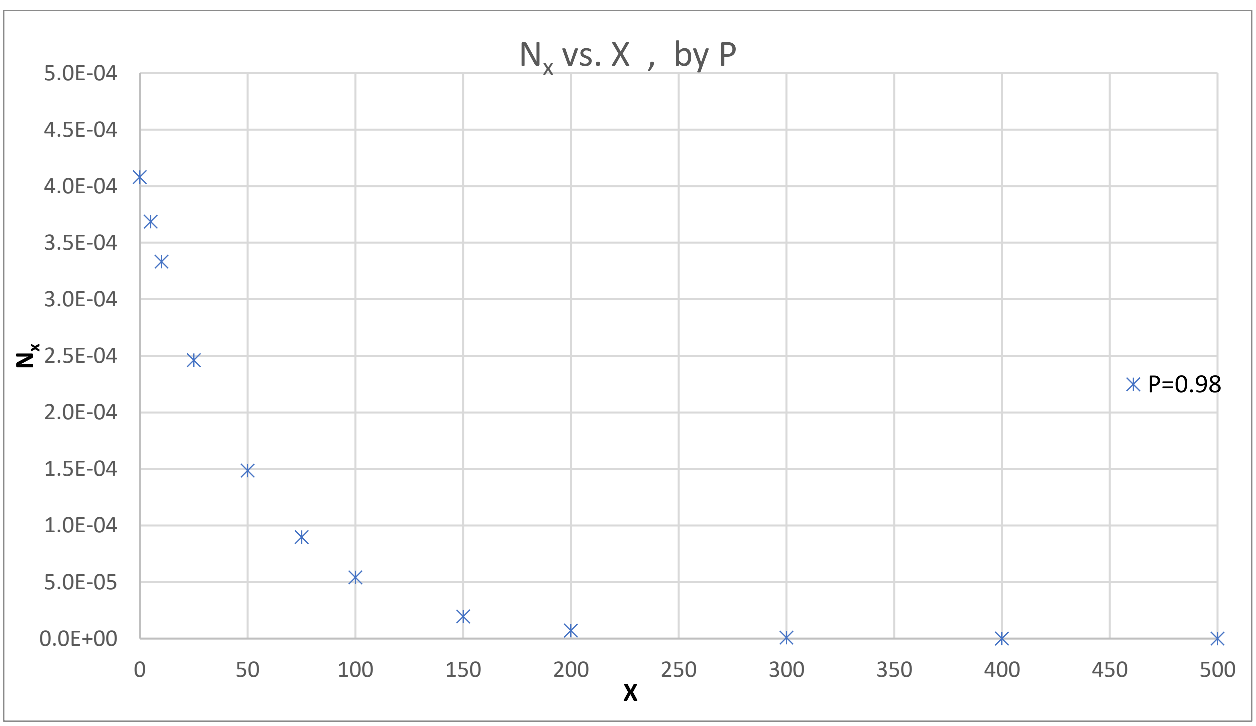

FIG. 6. Statistically derived mole fraction for a step-growth polymerization is plotted as a function of x, for P=0.98

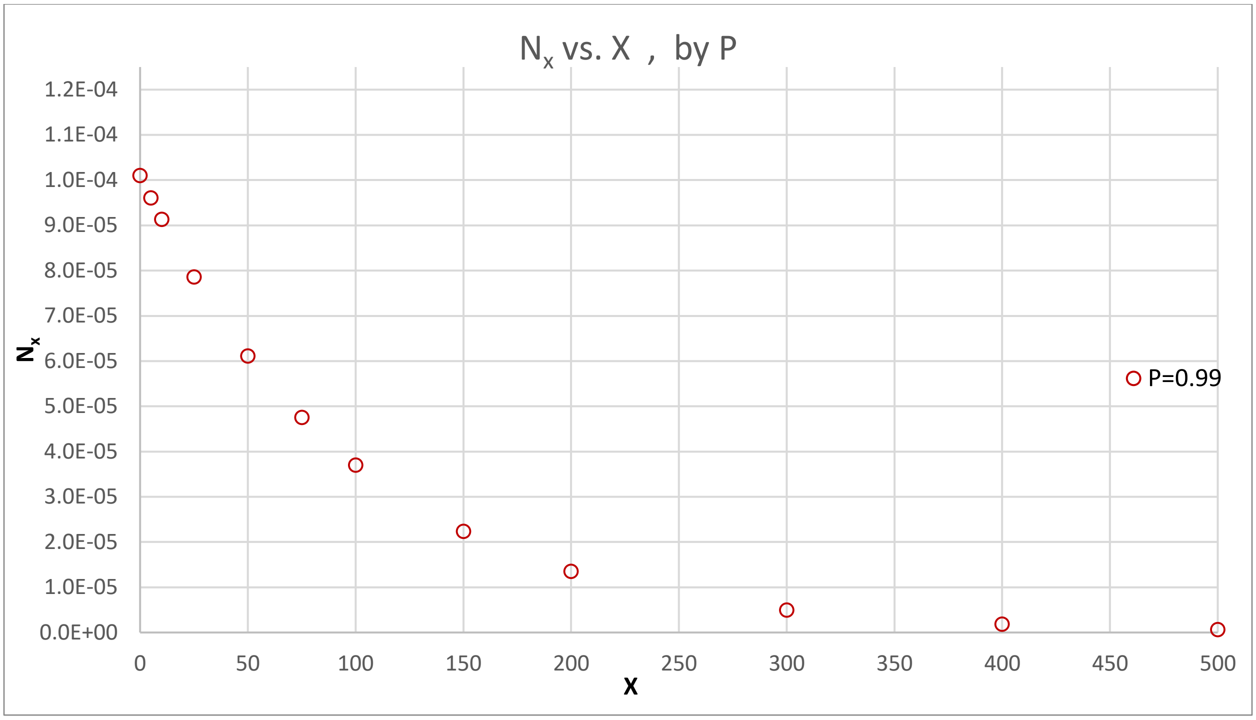

FIG. 7. Statistically derived mole fraction for a step-growth polymerization is plotted as a function of x, for P=0.99

Weight Fraction

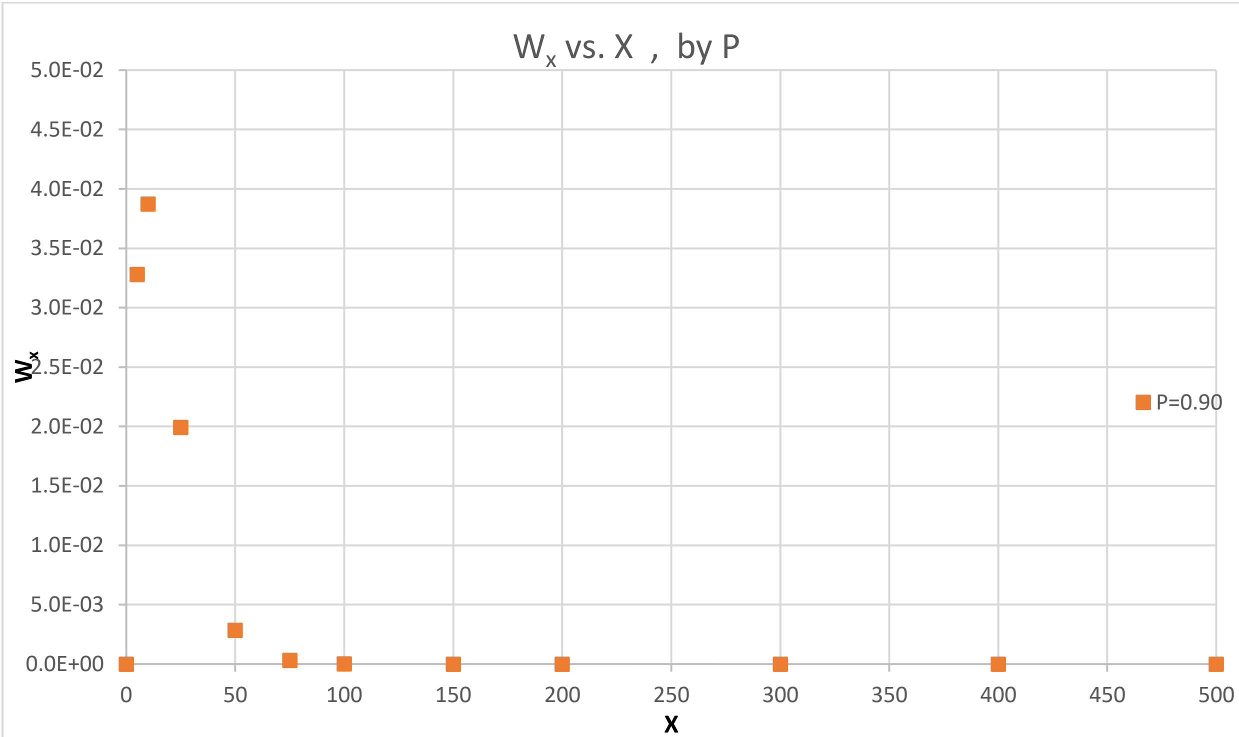

FIG. 8. Statistically derived weight fraction for a step-growth polymerization is plotted as a function of x, for P=0.9

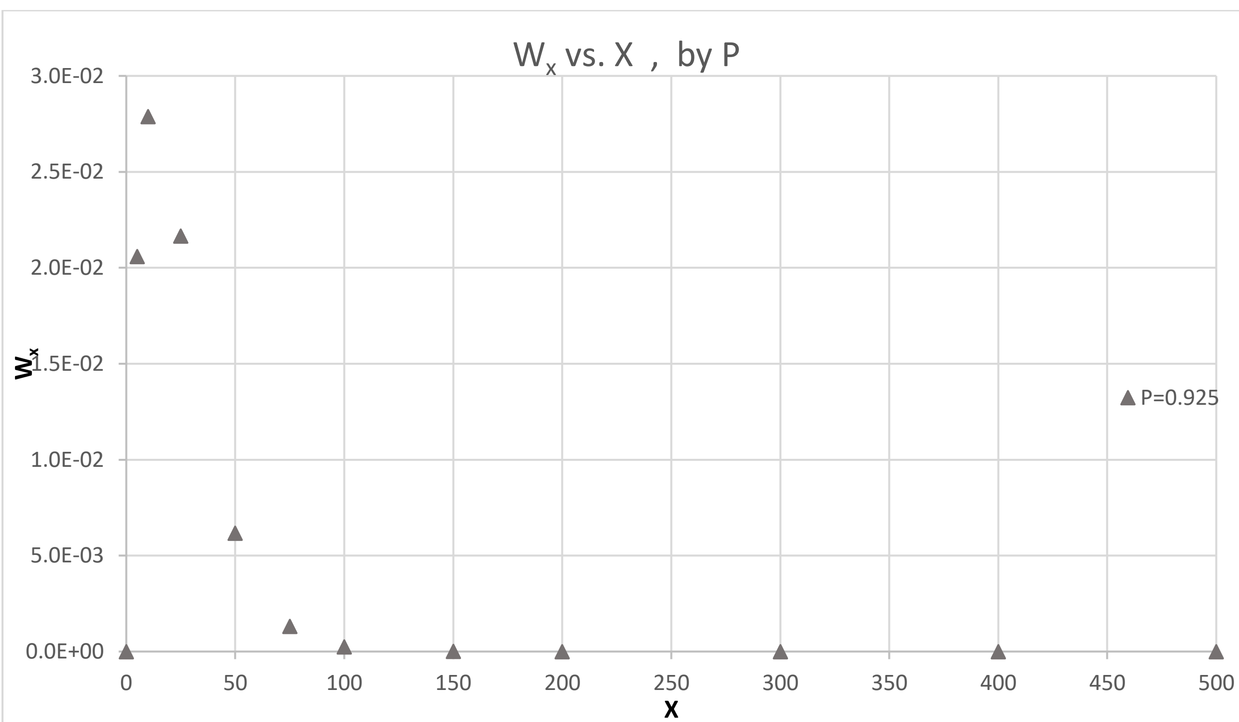

FIG. 9. Statistically derived weight fraction for a step-growth polymerization is plotted as a function of x, for P=0.925

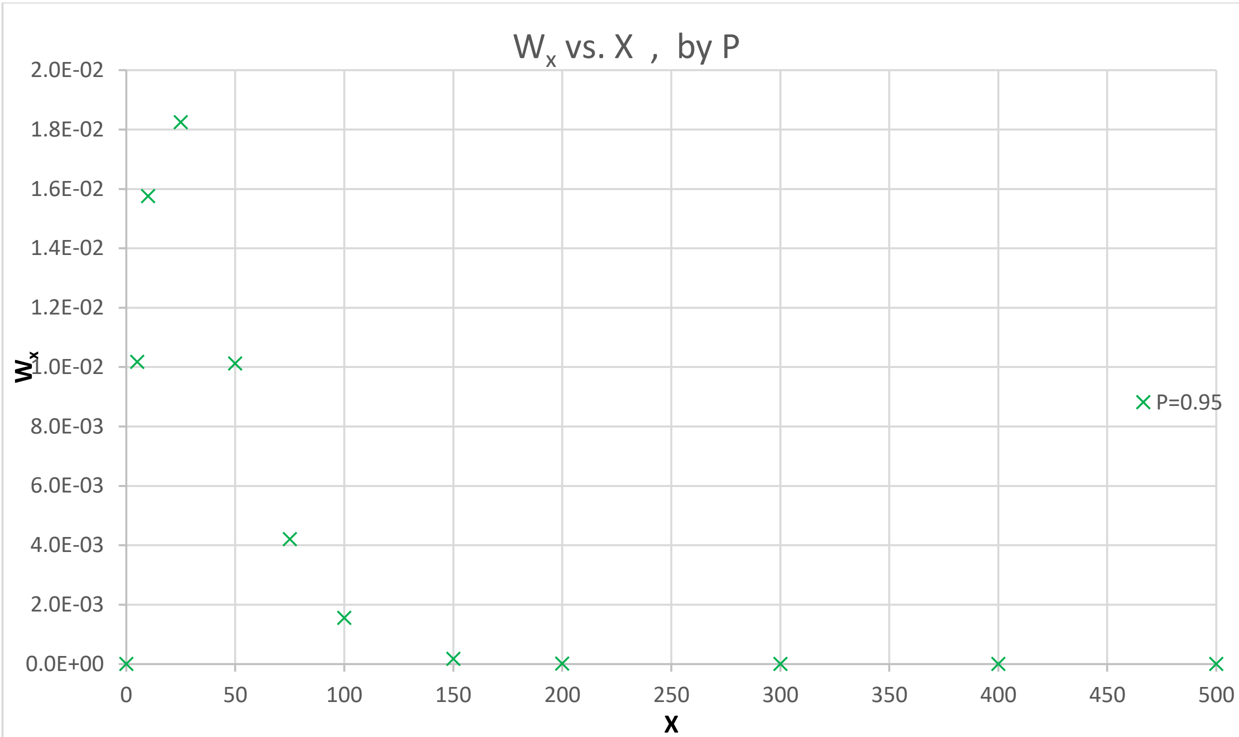

FIG. 10. Statistically derived weight fraction for a step-growth polymerization is plotted as a function of x, for P=0.95

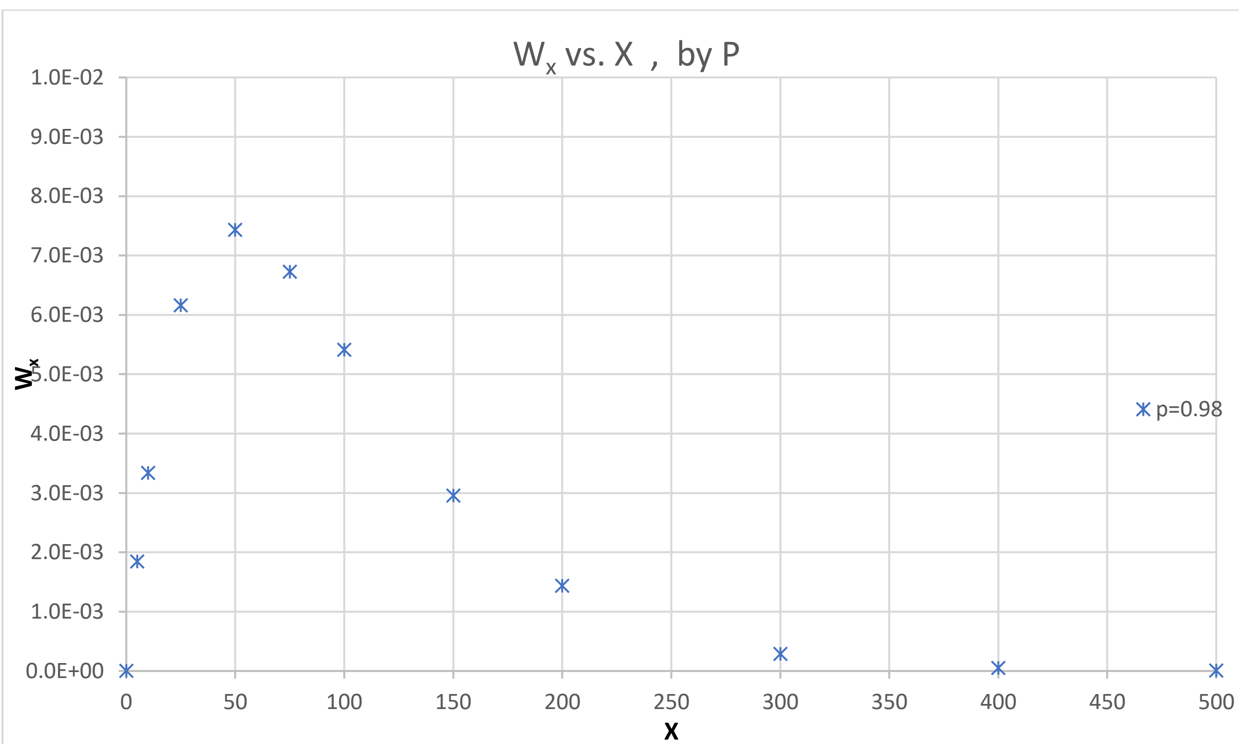

FIG. 11. Statistically derived weight fraction for a step-growth polymerization is plotted as a function of x, for P=0.98

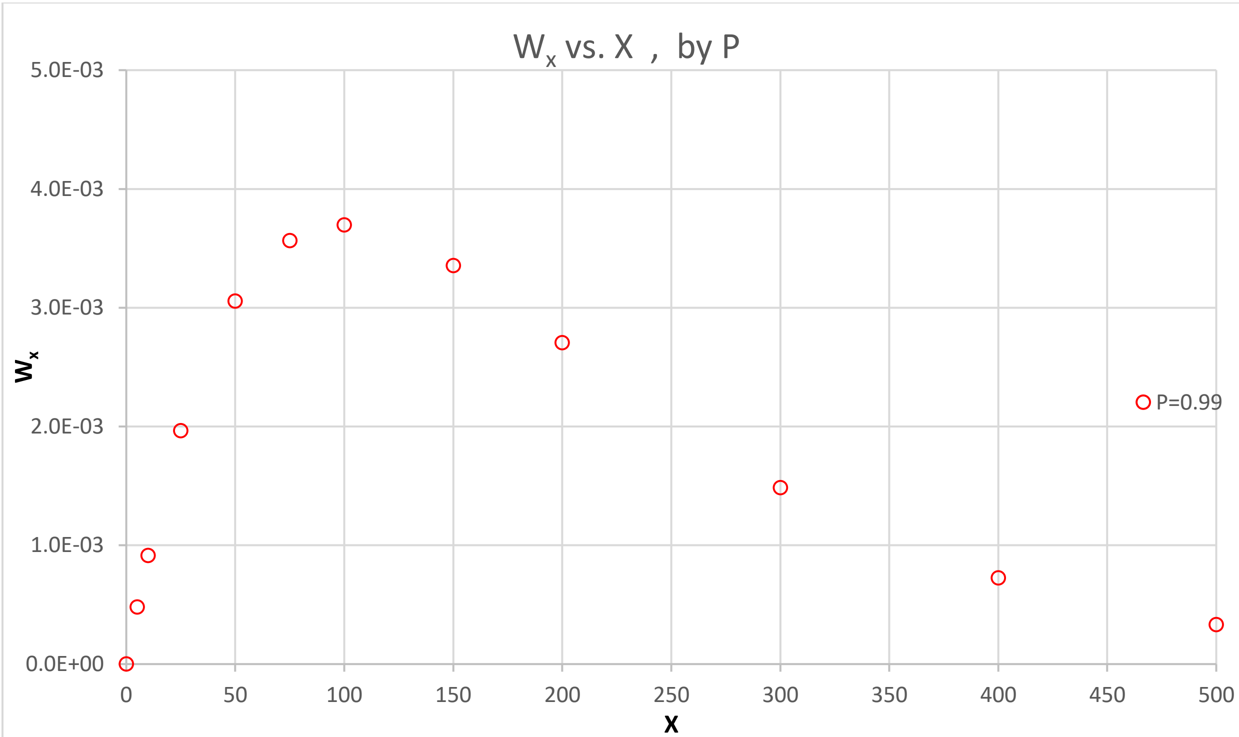

FIG. 12. Statistically derived weight fraction for a step-growth polymerization is plotted as a function of x, for P=0.99