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A Nomograph for Copolymer Composition and Sequence Distribution

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Many hundreds of reactivity ratios have been tabulated for copolymer systems which obey the Mayo-Lewis composition equation[1]

$$F_1 = (r_1f_1^2 + f_1f_2)/(r_1f_2^2 + 2f_1f_2 + r_2f_2^2) \tag{1}$$

where F_1 is the mole fraction of monomer 1 contained in a copolymer formed instantaneously from a feed having mole fractions f_1 and f_2 of monomers 1 and 2, respectively; and r_1 and r_2 are the reactivity ratios. Calculations with eq. (1) are straightforward but slightly time consuming. Therefore we present in this communication a nomograph which simplifies the calculation of copolymer composition from the monomer feed and reactivity ratios. Because of the approach we use, this nomograph also simplifies the calculation of sequence distributions in copolymers.[2]

The nomograph, Figure 1, was constructed on the basis of the following equations:

$$\epsilon/(1 - \epsilon) = r_1f_1/(1 - f_1) \tag{2}$$

$$\eta/(1 - \eta) = r_2f_2/(1 - f_2) \tag{3}$$

where ϵ and η are conditional probabilities and are equivalent, respectively, to P_{AA} and P_{BB} defined by Goldfinger and Kane.[3] The copolymer composition, in these terms, is

$$F_1/F_2 = (1 - \eta)/(1 - \epsilon) \tag{4}$$

which can be rearranged (since $F_1 + F_2 = 1$) to give

$$F_1 = (1 - \eta)/[(1 - \eta) + (1 - \epsilon)]. \tag{5}$$

The fraction of diads in the chain sequences formed is

$$\begin{aligned} f_{11} &= \epsilon(1 - \eta)/[(1 - \eta) + (1 - \epsilon)] \\ f_{12} = f_{21} &= (1 - \eta)(1 - \epsilon)/[(1 - \eta) + (1 - \epsilon)] \\ f_{22} &= \eta(1 - \epsilon)/[(1 - \eta) + (1 - \epsilon)]. \end{aligned} \tag{6}$$

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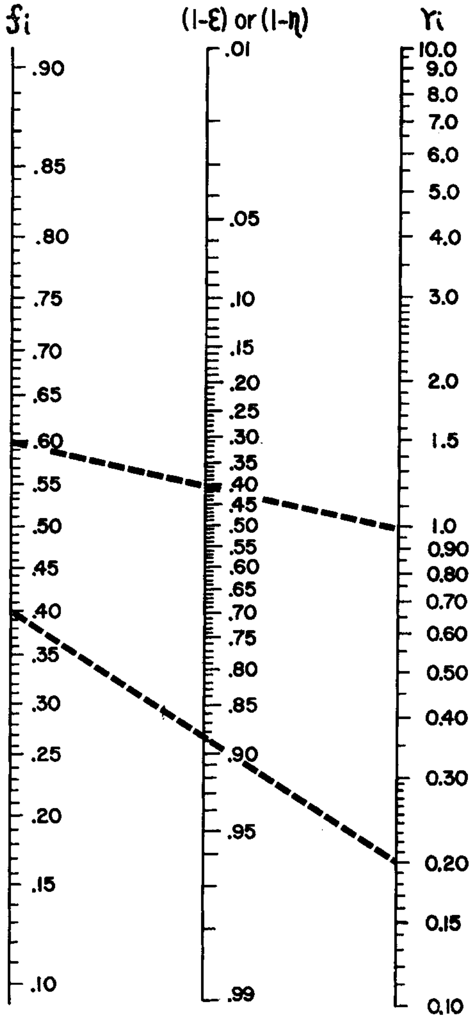

Fig. 1. Nomograph.

Triad fractions are expressed as

$$
\begin{aligned}
f_{111} &= f_{11}\epsilon \\
f_{112} &= f_{11}(1 - \epsilon) \\
f_{121} &= f_{12}(1 - \eta) \\
f_{122} &= f_{12}(\eta) \\
&\text{etc.}
\end{aligned}
\tag{7}
$$

Use of the nomograph is best illustrated by an example. Assume the following values:

$$r_1 = 0.2,\ r_2 = 1.0,\ f_1 = 0.4,\ f_2 = 0.6.$$

Connect the values of r_1 and f_1 with a straight line to obtain the value of $1 - \epsilon = 0.885$. Connect the values of r_2 and f_2 with a straight line to obtain the value of $1 - \eta = 0.40$.

Use eq. (5) to obtain

$$F_1 = 0.4/(0.4 + 0.885) = 0.311.$$

The 121 triad fraction, for example, is calculated from the appropriate form of eqs. (6) and (7) as

$$f_{121} = \frac{0.4 \times 0.885}{0.4 + 0.885} \times 0.4 = 0.11.$$

References

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3. G. Goldfinger and T. Kane, *J. Polym. Sci.*, **3**, 462 (1948).

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