Greek Letters

α = complementary apex angle
$\dot{\gamma}$ = shear rate
ω = angular velocity
η = viscosity
η_a = apparent viscosity
η_o = zero-shear viscosity
η_{oM}, η_{oL} = zero-shear viscosity of the more and less viscous components, respectively
λ = characteristic time
σ_1 = primary normal stress coefficient
θ_M = mixing time
θ_B = blending time
ρ = density

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Probability Models in Reaction Path Synthesis

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A significant contribution has been made in the field of reaction path synthesis by Powers and his associates (1975). In employing their approach, we need to know the probability of failure in each step of the reaction path and the number of trials required to obtain the first success at each step. This note introduces a general probability model for the reaction path synthesis which can be used to predict the number of trials required to obtain the first success for sequential trials and at least one success for simultaneous tests.

FORMULATION

As shown in Figure 1, n sequential trials are conducted in the horizontal direction in synthesizing a reaction path. At the i^{th} trial the reagent is divided into l_i portions, M_{i1}, M_{i2}, ..., M_{il_i}, distributed in the vertical direction, which can be used either simultaneously or sequentially. Several specific cases can be considered.

Case 1. Sequential both in the horizontal and vertical directions. The probability for the first success to occur at the M_{ij}th test (the j^{th} test at the i^{th} trial) can be expressed as (Parzen, 1960)

$$Pr\ \{\text{the first success to occur at the } M_{ij}\text{th test}\}$$
$$= (1-P_s)^{l_1}(1-P_s)^{l_2}\cdots\cdots(1-P_s)^{l_{i-1}}(1-P_s)^{j-1}P_s$$
$$= (1-P_s)^{\sum_{r=1}^{i-1}(l_r)+j-1}\ P_s \qquad (1)$$

where P_s is the probability of success in a single test. Equation (1) is the geometrical probability density function. The expected number of tests to obtain the first success, according to this probability density function, is (Parzen, 1962; Appendix 1)*:

$$E\left[\sum_{r=1}^{i-1}(l_r)+j\right]=\frac{1}{P_s} \qquad (2)$$

If we have

$$l_1 = l_2 = \ldots = l_i = 1$$

and consequently $j = 1$, we have from Equation (1)

$$Pr\ \{\text{the first success to occur at the } i^{th} \text{ trial}\}$$
$$= (1-P_s)^{i-1}P_s$$

which is the geometrical probability density function in a simple form (Parzen, 1960). Of course, the expected number of trials to obtain the first success can still be calculated by Equation (2).

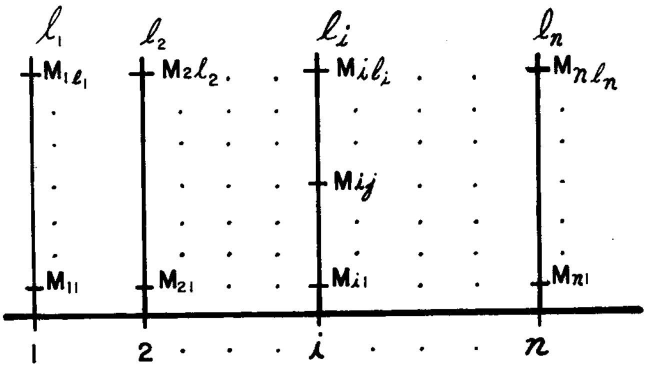

Fig. 1. A probability model for the reaction path synthesis.

Case 2. Sequential in the horizontal direction and simultaneous in the vertical direction. For this case, we may have more than one success at any given trial because l_i tests are carried out simultaneously at the i^{th} trial. The probability for at least one success to occur at the i^{th} trial can be expressed as (Feller, 1950; Parzen, 1962)

$$Pr\ \{\text{at least one success in } l_i \text{ simultaneous tests to occur at the } i^{th} \text{ trial}\}$$
$$= (1-P_s)^{\sum_{r=0}^{i-1} l_r}\{1-(1-P_s)^{l_i}\} \qquad (3)$$

where

$$i \geq 1$$
$$l_0 \equiv 0$$

Let

$$Q_i \equiv (1-P_s)^{l_i} \quad \text{where} \quad Q_0 \equiv (1-P_s)^{l_0} \equiv 1$$

Q_i is the probability that the i^{th} trial is a failure. Thus

$$R_i = 1 - Q_i$$

is the probability that the i^{th} trial is a success. Then Equation (3) can be rewritten as

$$Pr\ \{\text{at least one success to occur at the } i^{th} \text{ trial}\}$$
$$= \left(\prod_{r=0}^{i-1} Q_r\right)\cdot R_i \quad i \geq 1 \quad Q_0 \equiv 1 \qquad (4)$$

Thus the expected number of trials to obtain at least one success at the i^{th} trial is (Appendix II)*

$$E(i) = \sum_{i=1}^{\infty} i \left(\underset{r=0}{\overset{i-1}{\pi}} Q_r \right) \cdot R_i$$

$$= 1 + Q_1 + Q_1Q_2 + Q_1Q_2Q_3 + \ldots + Q_1Q_2 \ldots Q_i + \ldots \quad (5)$$

This case can be resolved into the following subcases:

Case 2.1. If

$$l_1 = l_2 = \ldots = l_i = l$$

we have, according to Equation (3)

$$Pr \{\text{at least one success to occur at the } i^{th} \text{ trial}\}$$
$$= (1 - P_s)^{l(i-1)} - (1 - P_s)^{li} \quad (6)$$

and thus (Appendix III)*

$$E(i) = \frac{1}{1 - (1 - P_s)^l} \quad (7)$$

Case 2.2. If $i = 1$, according to Equation (3), we have

$$p_1 = Pr \{\text{at least one success in } l_1 \text{ simultaneous tests to occur at the first trial}\}$$
$$= 1 - (1 - P_s)^{l_1} \quad (8)$$

or

$$1 - p_1 = (1 - P_s)^{l_1} \quad (9)$$

Equation (8) can also be derived from the binomial probability density function which is (Parzen, 1962)

$$Pr \{\text{exactly } k \text{ successes to occur in } l_1 \text{ simultaneous tests at the first trial}\}$$
$$= \binom{l_1}{k} P_s^k (1 - P_s)^{l_1 - k}$$

Then

$$p_1 = Pr \{\text{at least one success in } l_1 \text{ simultaneous tests to occur at the first trial}\}$$
$$= 1 - Pr \{\text{exactly zero successes to occur in } l_1 \text{ simultaneously tests at the first trial}\}$$
$$= 1 - (1 - P_s)^{l_1}$$

which is Equation (8).

Let

$$p_0 = 1 - p_1$$

where p_0 is the probability of exactly zero successes to occur in l_1 simultaneous tests. Since the probability of failure is

$$P_F = 1 - P_s$$

Equation (9) can be rewritten as

$$p_0 = P_F^{l_1} \quad (10)$$

Then l_1 is given by solving Equation (10) as

$$l_1 = \frac{\ln p_0}{\ln P_F} \quad (11)$$

This is the number of tests required to achieve at least one success in simultaneous testing, provided that the probability of zero successes is known to be p_0 (Hadley, 1967). However, it should not be stated as the number of trials to the first success with probability of success of $(1 - p_0)$ (Powers et al., 1975).

ESTIMATION OF PROBABILITY OF ZERO SUCCESSES IN BINOMIAL TRIALS

The probability of exactly zero successes in n binomial trials is an important parameter in the synthesis of fault tolerant reaction paths (Powers et al., 1975). In this section, we consider the problem of obtaining a best point estimate of the probability of exactly zero successes in n binomial trials (simultaneous tests), p_0. An approach which is similar to that of Rutemiller (1967) is employed here.

If P_s is the probability of success in any test, the probability of exactly zero successes in n simultaneous tests is given by

$$p_0 = (1 - P_s)^n \quad (12)$$

Suppose that r successes have been observed in m simultaneous tests. Then the maximum likelihood estimator (mle) for p_0 is

$$\hat{p}_0 = \left(1 - \frac{r}{m} \right)^n \quad (13)$$

for all values of n and m (Rutemiller, 1967; Appendix IV).*

An alternative estimator of p_0, namely, the minimum variance unbiased estimator (mvue), may be obtained directly from a theorem of Patil (1963) for the generized power series distribution as shown below (Appendix V):*

$$n \leq m$$

$$\tilde{p}_0 = \frac{\binom{m-n}{r}}{\binom{m}{r}} \quad \text{if} \quad r \leq m - n \quad (14)$$

$$\tilde{p}_0 = 0 \quad \text{if} \quad r > m - n$$

The mvue, $\tilde{p}_0$, does not exist for $n > m$. Rutmiller (1967) concluded that the mle, $\hat{p}_0$ is generally preferable to the mvue, $\tilde{p}_0$, to estimate the probability of zero failures in binomial trials when this probability is anticipated to be greater than 0.50. This should also be true in estimating the probability of zero successes in binomial trials because Equations (13) and (14) are the same as those for estimating, respectively, the mle, $\hat{p}_0$, and the mvue, $\tilde{p}_0$, of the probability of zero failures.

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* See document No. 02691, National Auxiliary Publications (NAPS).