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Technical Note

Simplification of a Molten Zone Refining Formula

by Keith S. Milliken

NORMAN W. Lord¹ has shown that the resultant impurity distribution after n zone passes is given by

$$C_n(a) = C_0 \left\{ 1 - (1-k)e^{-ka} \left[n - \sum_{t=1}^{n-1} \sum_{s=1}^t k^{s-1} e^{-sk} \sum_{r=0}^{s-1} f_r^{(s)} a^r (r+1-ka) \right] \right\}$$

in the ingot section $0 \leq a < N-n$, where a is the displacement in zone lengths, N is the ingot length in zone lengths, C_0 is the initial uniform impurity concentration, k is the segregation constant $= C_{solid}/C_{liquid}$ at equilibrium, and

$$f_r^{(s)} = \frac{s^{s-r-2}}{(s-r-1)!r!}.$$

The foregoing expression is formidable in respect to computational labor. However, the triple sum can be reduced as follows

$$\sum_{r=0}^{s-1} f_r^{(s)} a^r = \frac{s^{s-2}}{(s-1)!} \sum_{r=0}^{s-1} \frac{(s-1)!}{(s-r-1)!r!} \left(\frac{a}{s}\right)^r = \frac{(s+a)^{s-1}}{s!}$$

using the binomial theorem. Similarly

$$\sum_{r=0}^{s-1} f_r^{(s)} r a^r = a(s-1) \frac{(s+a)^{s-2}}{s!}$$

giving

$$\sum_{r=0}^{s-1} f_r^{(s)} a^r (r+1-ka) = \frac{(s+a)^{s-2}}{s!} \{a(s-1) + (1-ka)(s+a)\}.$$

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Finally

$$\frac{C_n(a)}{C_0} = 1 - (1-k)e^{-ka} \left[n - \sum_{t=1}^{n-1} \sum_{s=1}^t k^{s-1} e^{-sk} \frac{(s+a)^{s-2}}{s!} \{a(s-1) + (1-ka)(s+a)\} \right]$$

may be used if $C_n(a)$ is required for a series of values of n , and

$$\frac{C_n(a)}{C_0} = 1 - (1-k)e^{-ka} \left[n - \sum_{s=1}^{n-1} (n-s) k^{s-1} e^{-sk} \frac{(s+a)^{s-2}}{s!} \{a(s-1) + (1-ka)(s+a)\} \right]$$

is better if computing for only a single value of n .

For $k < 1$, it can be shown that this last equation is equivalent to

$$\frac{C_n(a)}{C_0} = \frac{1-k}{k} e^{-ka} \sum_{s=n+1}^{\infty} (s-n) \frac{(s+a)^{s-2}}{s!} (ke^{-k})^s \{a(s-1) + (1-ka)(s+a)\}.$$

The infinite series is useful only when k is small enough to force rapid convergence. In such cases, the absence of subtraction from unity has the definite advantage of preserving accuracy.

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¹ N. W. Lord: *Trans. AIME* (1953) **197**, p. 1531; JOURNAL OF METALS (November 1953).