# A mathematical model for kraft pulping expressed by a logarithmic straight-line equation

Vlado Mašura

*ABSTRACT: A mathematical model for the kraft pulping of trembling aspen is defined by a logarithmic straight-line equation for the relationship between kappa number or permanganate number and the H-factor. The model was derived using effective-alkali charges of 11%, 13%, and 15% (on $Na_2O$ basis). The correlation coefficient for the derived model was r =0.998–0.999. The relationship between the mathematical model and the studied charge of alkali is also characterized by a logarithmic straight-line equation. The power form of the logarithmic straight-line equation is the most suitable form for practical application of the pulping model. The relationships between yield and kappa number and between yield and permanganate number can also be expressed by the logarithmic straight-line equation.*

*KEYWORDS: Coefficients, computers, equations, kraft pulping, logarithms, mathematical models, pulping processes.*

Mathematical models for the pulping process derived up to now are complicated and do not predict the experimental results with sufficient precision (*1–9*). Efforts to improve the environment will require a remarkable decrease in the degree of pulping during the cooking process. Controlling and checking the pulping process with a computer depends mainly on the accuracy of the pulping model. The objective of the present work is to present a precise mathematical model of the pulping process. The new model has a correlation coefficient equal to or close to 1.

## Experimental

The experimental results reported by Hatton and Hejjas (*10*) were used to develop a mathematical model for the pulping process. The cited authors studied kraft pulping of trembling aspen (*Populus tremuloides* Michx.) under the following conditions: effective alkali (EA) charges of 11%, 13%, and 15% (on $Na_2O$ basis); maximum pulping temperature 160°C and 170°C; cooking-liquor sulfidity 24.4%; liquor-to-wood ratio 4.5:1.

## Results and discussion

### Relationship of yield to kappa number and permanganate number

**Figure 1** shows the variation of yield with kappa number and with permanganate number. It is evident that the relationship between yield and both kappa number and permanganate number is given in a log–log plot by a straight line.

The variation of the ratios "yield/kappa number" and "1/(yield x kappa number)" with kappa number is expressed in logarithmic coordinates by the straight lines in **Fig. 2**. Similarly, the variation of the ratios "yield/permanganate number" and "1/(yield x permanganate number)" is expressed in logarithmic coordinates by the straight lines in **Fig 3**. The similarity is valid also for the mathematically modified relationships expressed as the ratio "1/(yield x kappa number)" with kappa number as well as the ratio "1/(yield x permanganate number)" with permanganate number in log–log plots (given in Figs. 2 and 3), and also as the product "yield x kappa number" with kappa number or the product "yield x permanganate number" with permanganate number in log–log plots (not shown).

Mašura is consultant with the Pulp and Paper Research Institute, Lamačská Street 3, 815 20 Bratislava, Slovak Republic.

From the foregoing, it follows that the relationship between yield and either kappa number or permanganate number, as well as the modified forms of these relationships, can be mathematically expressed by the logarithmic straight line given by Eq. 1.

$$\ln\ y = (k \ln x) + \ln b \qquad (1)$$

where

$x$ =pulp kappa number or permanganate number

k =slope constant

b =intercept constant

and where $y$ represents one of the following:

$y$ =yield, %

=yield/kappa number

=yield/permanganate number

=yield x kappa number

=yield x permanganate number

=1/(yield x kappa number)

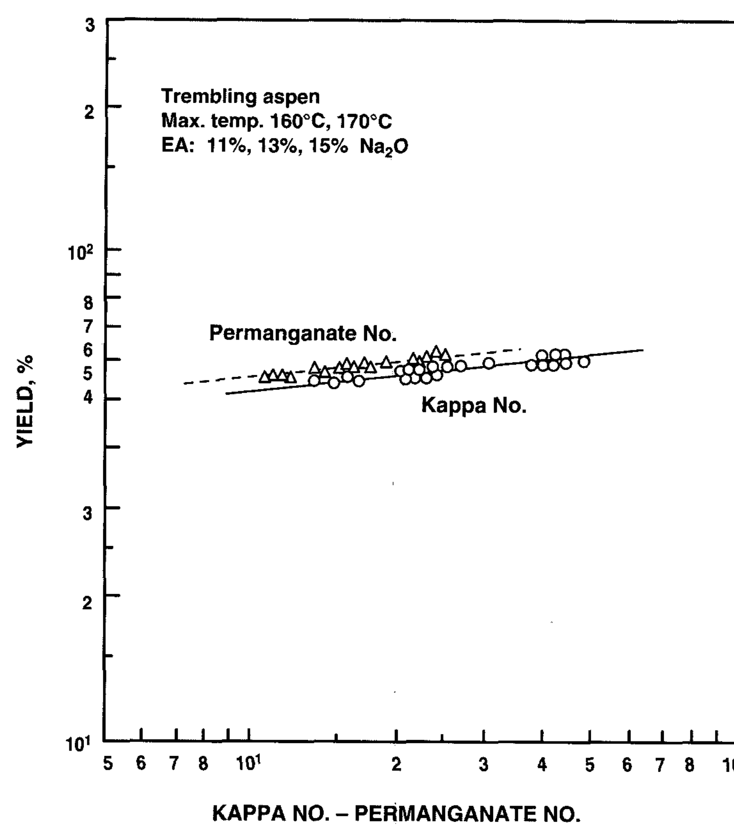
=1/(yield x permanganate number)

The values of the constants and correlation coefficients in the logarithmic straight-line equation computed by the least-squares method are listed in **Table I**. These data reveal that the correlation coefficients of Eq.1 for the variation of yield with kappa number and of yield with permanganate number are low, 0.896 and 0.902, respectively. For the modified form of the relationship, expressed as the ratio or product, the correlation coefficients are close to 1, with $r$ =0.999 for yield/kappa number vs. kappa number and $r$ =0.997 for yield/permanganate number vs. permanganate number.

### Logarithmic form of the model for the pulping process

In order to develop the mathematical model for kraft pulping, the variation of the ratios "kappa number/$H$-factor" and "permanganate number/$H$-factor" with $H$-factor were evaluated (**Figs. 4** and **5**). From these figures, it is obvious that the relationship of these quantities is logarithmic for EA charges of 11%, 13%, and 15% (on $Na_2O$ basis).

**1.** Logarithmic variations of yield with kappa number and yield with permanganate number for kraft pulps at EA charges of 11%, 13%, and 15% (on $Na_2O$ basis)




Also, the relationship between yield/$H$-factor and $H$-factor is expressed by a straight line in logarithmic coordinates.

The results confirm that the variation of "kappa number/$H$-factor" and "permanganate number/$H$-factor" with $H$-factor is profoundly influenced by the alkali charge. Also, the values of the constants in the derived mathematical model are dependent on the alkali charge. The slope constants of these variations corresponding to EA charges of 13% and 15% (on $Na_2O$ basis) have the same value. [Results obtained using an EA charge of 11% (on $Na_2O$ basis) were excluded because this charge is insufficient.] However, different values of the constant b in Eq. 1 and of constant A in Eq. 2 were observed at the alkali charges given in **Tables II** and **III**.

### Power form of the model for the pulping process

By using antilogarithms and solving Eq. 1, one obtains the power form of the relationships between $H$-factor and kappa number or yield. Also, the aforementioned ratios and products can be expressed by the power form:

$$Y = A \times X^{a} \qquad (2)$$

where

$Y$ =yield, kappa number, or permanganate number

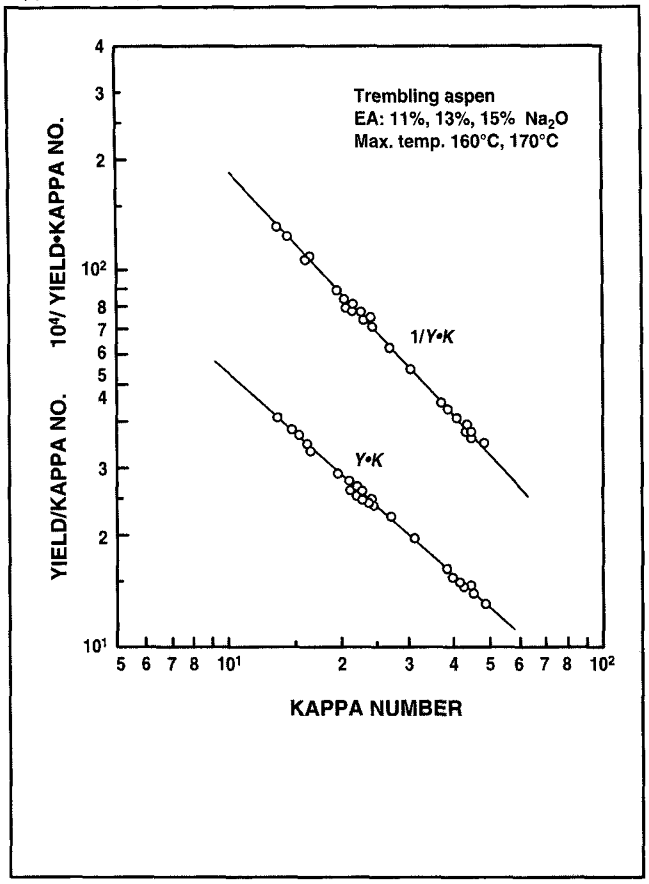
$X$ =$H$-factor, kappa number, or permanganate number

A =constant

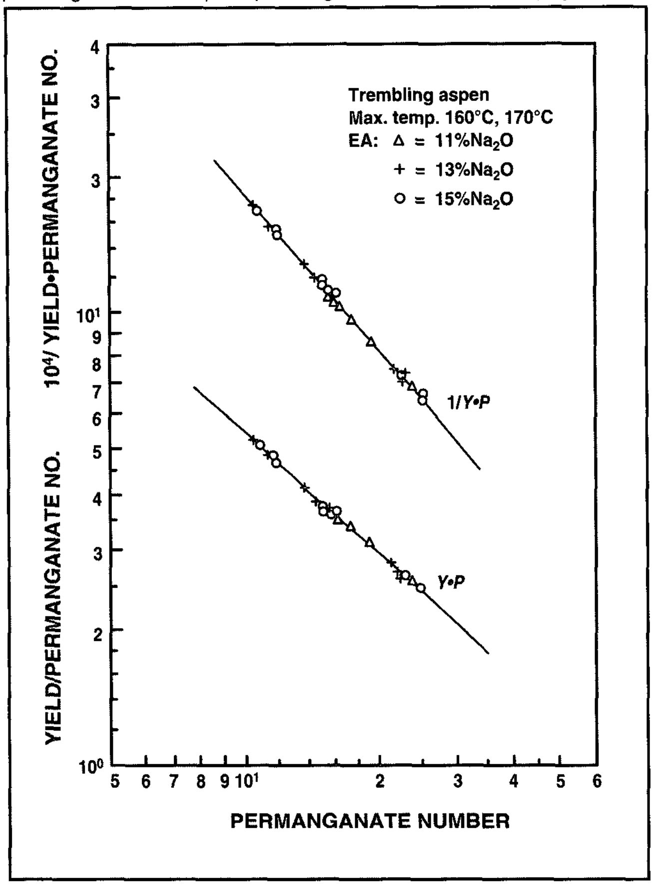
$a$ =exponent, whose value is dependent on the relation being expressed and can correspond to $a$ =k+1, $a$ =k–1, and $a$ =1–k.

Values for constant A and $a$ in Eq. 2 for the individual variations given in

**2.** Logarithmic variations of "yield/kappa number" and "1/(yield x kappa number)" vs. kappa number for kraft pulps




**3.** Logarithmic variations of "yield/permanganate number" and "1/(yield x permanganate number)" vs. permanganate number for kraft pulps

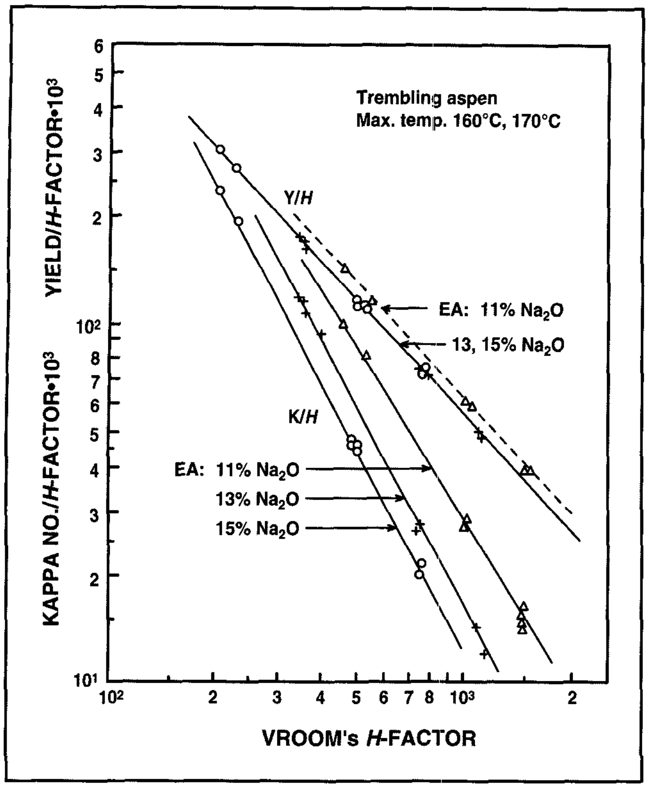



**I.** Values of constants and correlation coefficients of Eqs. 1 and 2 of the variation of yield with kappa number, yield with permanganate number, and yield with *H*-factor

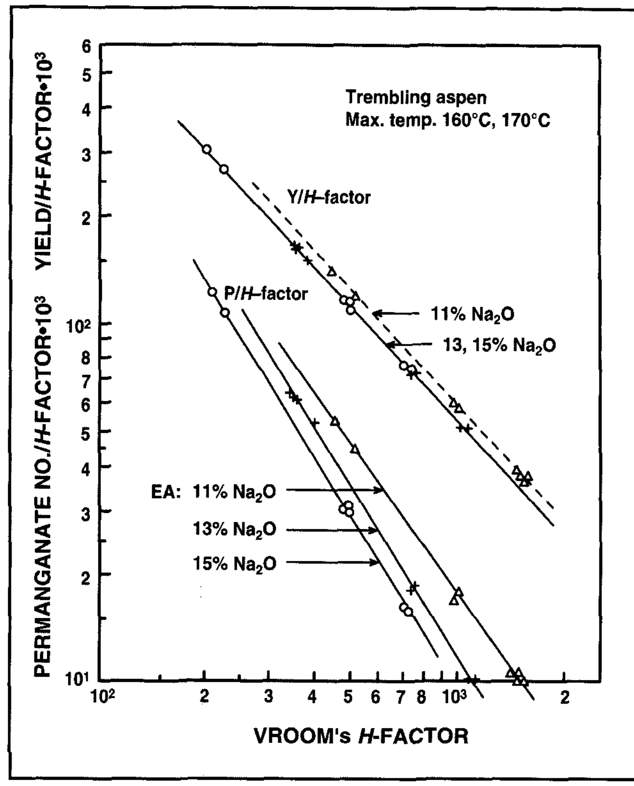
| *Variation* | *Slope constant k in Eq. 1* | *Intercept constant ln b in Eq. 1* | *Correlation coefficient r in Eq. 1* | *Constant A in Eq. 2* | *Exponent a in Eq. 2* | *Degree of freedom* |
|---|---|---|---|---|---|---|
| | | | Variation of yield with kappa number | | | |
| Yield with kappa No. | 0.09463 | 3.759 | 0.896 | 42.9055 | 0.09463 | 24 |
| Yield/kappa with kappa No. | -0.90538 | 3.759 | 0.999 | 42.9055 | 0.09462 | 24 |
| | | | Variation of yield with permanganate number | | | |
| Yield with permanganate No. | 0.13859 | 3.678 | 0.902 | 39.56718 | 0.13859 | 24 |
| Yield/perm. No. with permanganate No. | -0.86141 | 3.678 | 0.997 | 39.5672 | 0.13859 | 24 |
| | | | Variation of yield with *H*-factor[a] | | | |
| Yield/*H*-factor with *H*-factor | -1.0637 | 4.4522 | 0.999 | 85.81936 | -0.0637 | 16 |

[a] Alkali charge EA = 13% and 15% $Na_2O$

4. Logarithmic variations of "kappa number/*H*-factor" and "yield/*H*-factor" with the *H*-factor used during kraft pulping




5. Logarithmic variations of "permanganate number/*H*-factor" and "yield/*H*-factor" with the *H*-factor used during kraft pulping




II. Values of constants and correlation coefficients of Eqs. 1 and 2 of the variation of kappa number with *H*-factor and variation of permanganate number with the *H*-factor

| *Variation* | *EA, %* | *Slope constant k in Eq. 1* | *Intercept constant ln b in Eq. 1* | *Correlation coefficient r in Eq. 1* | *Constant A in Eq. 2* | *Exponent a in Eq. 2* | *Degree of freedom* |
|---|---|---|---|---|---|---|---|
| | | Variation of kappa number with *H*-factor | | | | | |
| Kappa No./*H*-factor with *H*-factor | 13 | -1.8823 | 8.8842 | 0.998 | 7217.361 | -0.8823 | 8 |
| Kappa No./*H*-factor with *H*-factor | 15 | -1.8690 | 8.4932 | 0.999 | 4881.680 | -0.8690 | 8 |
| | | Variation of permanganate number with *H*-factor | | | | | |
| Perm. No/*H*-factor with *H*-factor | 13 | -1.6210 | 6.7552 | 0.999 | 858.5498 | -0.6210 | 8 |
| Perm. No/*H*-factor with *H*-factor | 15 | -1.5894 | 6.3622 | 0.999 | 579.5458 | -0.5894 | 8 |

Tables I–III were computed by the least-squares method.

For the calculation of kappa number or permanganate number from the *H*-factor—or for the calculation of the *H*-factor necessary for the production of pulp with a required kappa number or permanganate number—one first needs to calculate the value of A in Eq. 2 that corresponds to the charge of alkali used. The constant A can be calculated using Eq. 2 with the constants given in Table III, as follows:

For the variation of kappa number with *H*-factor:

$$\text{kappa number} = 7984398.4\ \text{EA}^{-2.7323}\ H\text{-factor}^{-0.8690} \quad (3)$$

$(r = 0.999)$

**III.** Values of constants and correlation coefficients of Eqs. 1 and 2 of the variation of constant A in Eq. 2 with charge of alkali EA

| *Variation* | *Slope constant k in Eq. 1* | *Intercept constant ln b in Eq. 1* | *Correlation coefficient r in Eq. 1* | *Constant A in Eq. 2* | *Exponent a in Eq. 2* | *Degree of freedom* |
|---|---|---|---|---|---|---|
| | | For the calculation of kappa number from *H*-factor | | | | |
| Constant A with EA | -2.7323 | 15.893 | 1.000 | 7984398.4 | -2.7323 | 3 |
| | | For the calculation of permanganate number from *H*-factor | | | | |
| Constant A with EA | -2.7463 | 13.799 | 1.000 | 983625.0 | -2.7463 | 3 |
| | | For the calculation of *H*-factor from kappa number | | | | |
| Constant A with EA | -1.9147 | 14.914 | 1.000 | 2999631.5 | -1.8147 | 3 |
| | | For the calculation of *H*-factor from permanganate number | | | | |
| Constant A with EA | -0.8386 | 12.988 | 1.000 | 437136.2 | -0.8386 | 3 |

For the variation of permanganate number with *H*-factor:

$$\text{permanganate number} = 983625.0\ \text{EA}^{-2.7463}\ H\text{-factor}^{-0.5894} \quad (4)$$

$$(r = 0.999)$$

The derived mathematical model for kraft pulping of trembling aspen can also be used to calculate the *H*-factor needed to produce a pulp with a specific kappa or permanganate number from the following equations:

$$H\text{-factor} = 2999631.5\ \text{EA}^{-1.9147}\ \text{kappa number}^{-1.1368} \quad (5)$$

$$(r = 0.999)$$

$$H\text{-factor} = 437136.16\ \text{EA}^{-0.8386}\ \text{permanganate number}^{-1.5955} \quad (6)$$

$$(r = 0.999)$$

The yield can be calculated from the values of the kappa number and permanganate number using the following equations:

$$\text{yield} = 42.905\ \text{kappa number}^{0.0946} \quad (7)$$

$$(r = 0.999)$$

$$\text{yield} = 41.264\ \text{permanganate number}^{0.1205} \quad (8)$$

$$(r = 0.999)$$ TJ

## Literature cited


1. Vroom, K. E., *Pulp Paper Mag. Can.* 58(C): 228(1957).
2. Hatton, J. V., *Tappi* 56(7): 97(1973).
3. Chari, N. C. S., *Tappi* 56(7): 65(1973).
4. Hatton, J. V., *Tappi* 59(8): 48(1976).
5. Kerr, A. J. and Uprichard, J. M., Appita 30(1): 48(1976).
6. Tasman, J. E., *Pulp Paper Can*, 81(3): TR19(1980).
7. Tasman, J. E., *Tappi* 64(3): 175(1981).
8. Gustafson, R. R., Sleicher, C. A., McKean, W. T. and Finlayson, B. A., *I&EC Process Design Devt.* 22(1): 87(1983).
9. Wells, C. H., Bailey, B., and Fridley, M. L., *1988 Pulping Conference Proceedings*, TAPPI PRESS, Atlanta, p. 545.
10. Hatton, J. V. and Hejjas, J., *Pulp Paper Mag. Can.* 73(9): T218(1972).



Received for review Aug. 3, 1992.

Accepted Jan. 2, 1993.