A Note on the Film–Penetration Model for Mass Transfer with First Order Chemical Reaction

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Systems involving mass transfer operation accompanied by chemical reaction are usually designed by using some of the models found in the technical literature on the subject. These models allow us to understand and predict the phenomena.

The two principal models for the mechanism of mass transfer between two phases are the film model (*1*) and the penetration model (*4, 5*). Toor and Marchello (*2*) proposed the film-penetration model that includes the two above mentioned as limiting cases and explains the fact that in the proportionality

$$k_L \sim D^{\nu}$$

ν varies widely.

Huang and Kuo (3) extended Toor and Marchello's work by taking into account a simultaneous first-order chemical reaction. The differential equation representing the case is

$$\frac{\partial C_A}{\partial t} = D_A \frac{\partial^2 C_A}{\partial x^2} - k\,C_A \tag{1}$$

with the boundary conditions

$$\left.\begin{array}{lll} x = 0 & t > 0 & C_A = C_{Ai} \\ x = L & t > 0 & C_A = C_{AL} \\ x > 0 & t = 0 & C_A = C_{AL} \end{array}\right\} \tag{2}$$

They gave two equivalent solutions, one of which is

$$C_A = C_{Ai} - \frac{C_{Ai} - C_A}{L}\left\{ x + \frac{2L}{\pi}\sum_{n=1}^{\infty} \frac{1 + n^2\pi^2\alpha \cdot \exp[-(1 + n^2\pi^2\alpha)kt]}{n(1 + n^2\pi^2\alpha)} \sin\left(\frac{n\pi x}{L}\right)\right\} \tag{3}$$

The other is obtained by the Laplace transform method. It has the advantage of showing a rapid convergence for short contact times; on the other hand, Equation (3) converges rapidly for long contact times.

However, solution (3) cannot be reduced for extreme values to Hatta's general solution for the film model (*6, 7*); it gives instead another expression of Hatta's that is valid only for low bulk concentration of the dissolving gas.

The present work was undertaken to find a more general solution to the differential Equation (1) with boundary conditions (2).

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THE CONCENTRATION PROFILE INSIDE THE ELEMENT

The method used to solve the differential Equation (1) with boundary conditions (2) is based on the sum of two solutions (*8*). First, the steady state differential equation

$$\frac{d^2u}{dx^2} = ku \tag{4}$$

is solved with the boundary conditions

$$\left.\begin{array}{ll} u = C_{Ai} & x = 0 \\ u = C_{AL} & x = L \end{array}\right\} \tag{5}$$

Then from a second differential equation

$$\frac{\partial w}{\partial t} = D_A \frac{\partial^2 w}{\partial t} - kw \tag{6}$$

is solved with the boundary conditions

$$\left.\begin{array}{l} w = 0 \text{ in } x = 0 \text{ and } x = L \text{ for } t > 0 \\ w = C_{AL} - u(x) \quad \text{for} \quad t = 0 \end{array}\right\} \tag{7}$$

where $u(x)$ is the solution of Equation (4). Finally the solution of our system is

$$C = \frac{1}{\sinh(1/\sqrt{\alpha})}\left\{ C_{Ai}\sinh\left[\frac{(1 - x/L)}{\sqrt{\alpha}}\right] + C_{AL}\sinh\left[\frac{x/L}{\sqrt{\alpha}}\right]\right\} + \frac{2}{\pi}\sum_{n=1}^{\infty}\left[-(C_{Ai} - C_{AL}) + \frac{C_{Ai} - C_{AL}(-1)^n}{1 + \alpha n^2\pi^2}\right]\frac{\sin(n\pi x/L)}{n} \cdot \exp\left[-t\left(\frac{D_A n^2\pi^2}{L^2} + k\right)\right] \tag{8}$$

THE MASS TRANSFER RATE

The point mass transfer rate will be

$$N_A = -D_A\left(\frac{\partial C_A}{\partial x}\right)_{x=0} \tag{9}$$

and using Equation (8) for C_A

$$N_A = \frac{D_A}{L}\left\{\frac{1}{\sqrt{\alpha}}\left[C_{Ai}\coth(1/\sqrt{\alpha}) - C_{AL}\,\mathrm{csch}(1/\sqrt{\alpha})\right] - 2\sum_{n=1}^{\infty}\left[-(C_{Ai} - C_{AL}) + \frac{C_{Ai} - C_{AL}(-1)^n}{1 + \alpha n^2\pi^2}\right]\right.$$

$$\cdot \exp\left[-tk(1+\alpha n^2\pi^2\right]\Bigg\} \quad (10)$$

The average rate of mass transfer across the entire interface will be

$$\bar{N}_A = \int_0^\infty s \cdot \exp(-st) \cdot N_A \cdot dt \quad (11)$$

After integration we obtain

$$\bar{N}_A = \frac{D_A}{L}\left\{\frac{1}{\sqrt{\alpha}}\left[C_{Ai}\cdot\coth(1/\sqrt{\alpha}) - C_{AL}\cdot\operatorname{csch}(1/\sqrt{\alpha})\right] + 2\sum_{n=1}^{\infty}\frac{(C_{Ai}-C_{AL}) - \dfrac{C_{Ai}-C_{AL}(-1)^n}{1+\alpha n^2\pi^2}}{1+\beta^{-1}+\gamma n^2\pi^2}\right\} \quad (12)$$

LIMITING CASES

The general equations may be investigated in the light of limiting cases. When $C_{Ai} >> C_{AL}$ Equation (10) is reduced to

$$N_A = \frac{D_A}{L}(C_{Ai}-C_{AL})\left\{1+2\sum_{n=1}^{\infty}\frac{1+\alpha n^2\pi^2\exp\left[-kt(\alpha n^2\pi^2+1)\right]}{1+\alpha n^2\pi^2}\right\} \quad (13)$$

which is exactly the same as the equation derived by Huang and Kuo (*4*).

When the dimensionless groups α^{-1} and β^{-1} approach zero, Equation (12) is reduced to

$$\bar{N}_A{}^0 = \frac{D_A}{L}(C_{Ai}-C_{AL})\left[1+2\sum_{n=1}^{\infty}\frac{1}{1+n^2\pi^2\gamma}\right] \quad (14)$$

which is identical to the rate equation for physical mass transfer derived by Toor and Marchello (*2*).

When $t \to \infty$, Equation (10) is reduced to

$$N_A = \bar{N}_A = \frac{D_A}{L}\cdot\frac{1}{\sqrt{\alpha}}\left[C_{Ai}\cdot\coth(1/\sqrt{\alpha}) - C_{AL}\operatorname{csch}(1/\sqrt{\alpha})\right] \quad (15)$$

which is exactly the same general equation derived by Hatta (*7, 8*) for mass transfer with chemical reaction in a stagnant film. Here as $k \to 0$ we get the rate of physical mass transfer as predicted by the film model

$$N_A{}^0 = \frac{D_A}{L}(C_{Ai}-C_{AL}) \quad (16)$$

Equation (12) may be written in an alternative form as

$$\bar{N}_A = \sqrt{D_A k(1+\beta)}\left\{\left(C_{Ai} - \frac{\beta C_{AL}}{1+\beta}\right)\coth\sqrt{\frac{1+\beta}{\alpha}} - C_{AL}\left[\sqrt{\frac{\alpha}{1+\beta}}\left\{\frac{\beta}{\beta+1} - \frac{\operatorname{csch}(1/\sqrt{\alpha})}{\sqrt{\alpha}}\right.\right.\right.$$

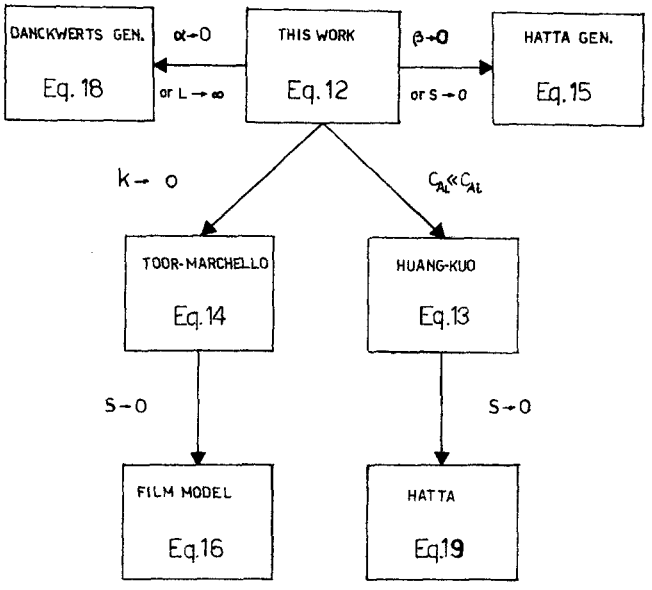

Fig. 1. Limiting cases of the derived equation.

$$\left.\left.\left. + 2\sum_{n=1}^{\infty}\frac{(-1)^n}{(1+\beta^{-1}+\gamma n^2\pi^2)(1+\alpha n^2\pi^2)}\right\}\right]\right\} \quad (17)$$

If $L \to \infty$ or $\alpha \to 0$, Equation (17) is reduced to

$$\bar{N}_A = C_{Ai}\sqrt{D_A(s+k)} - C_{AL}\sqrt{D_A s}\cdot\sqrt{\frac{s}{s+k}} \quad (18)$$

first proposed by Danckwerts for the penetration model (*6*).

When $t \to \infty$, Equation (10) and Equation (13), when $C_{AL} >> C_{Ai}$, are both reduced to Hatta's expression for low bulk concentration.

$$N_A = \bar{N}_A = \frac{D_A}{L}(C_{Ai}-C_{AL})\frac{\coth(1/\sqrt{\alpha})}{\sqrt{\alpha}} \quad (19)$$

All these limiting cases and their connections can be seen in Figure 1.

CONCLUSIONS

A general mathematical solution based on the film-penetration concept accompanied by a first-order chemical reaction has been obtained. For extreme values of the dimensionless numbers α, β, kt or for $C_{AL} \to 0$, it is reduced to the equations developed by previous workers that appear as limiting cases.

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NOTATION

A = reactant A
C_A = concentration of component A in solution, g.-mole/liter
C_{Ai} = concentration of component A at interface, g.-mole/liter
C_{AL} = concentration of component A at the outer edge of a surface element, g.-mole/liter

D = molecular diffusivity, sq.cm./sec.
D_A = molecular diffusivity of A, sq.cm./sec.
L = thickness of a surface element, cm.
N_A = point rate of chemical mass transfer for component A, g.-mole/(sq.cm.)(sec.)
$\overline{N}_A$ = average rate of chemical mass transfer for component A, g.-mole/(sq.cm.)(sec.)
$\overline{N}_A^0$ = average rate of physical mass transfer for component A, g.-mole/(sq.cm.)(sec.)
k_L = liquid side mass transfer coefficient with chemical reaction, cm./sec.
k = reaction velocity constant, 1/sec.
n = integer
s = surface renewal rate, 1/sec.
t = time, sec.
u = dummy variable
w = dummy variable
x = distance, cm.

Greek Letters

α = dimensionless group $D_A/(k \cdot L^2)$
β = dimensionless group s/k
γ = dimensionless group, α/β or $D_A/(SL^2)$
ν = exponent

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Comments on Hybrid Computing Time of A DI Method

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A recent article (*1*) by Bishop and Green discusses what appears to be a promising method for hybrid computer solution of multidimensional partial differential equations. However, in making a time comparison between hybrid and digital implementation of the method, the authors make some assumptions which I feel are questionable. They assume that timing will be completely determined by the time it takes the digital to perform its operations. They also assume that hybrid calculations on the digital are carried out using floating point arithmetic.

Because A/D and D/A converters are of limited accuracy, the use of floating point arithmetic is not justified. If the original dimensionless temperature equations are programmed on the analog, one has to A/D convert T^*i, j and D/A convert either the quantity

$$(T^*_{i+1,j} - 2T^*_{i,j} + T^*_{i-1,j}) \qquad (1)$$

or

$$(T^*_{i,j+1} - 2T^*_{i,j} + T^*_{i,j-1}) \qquad (2)$$

at each mode. This can be accomplished by using single precision fixed points arithmetic and calculating, for example

$$(T^*_{i,j+1} - T^*_{i,j}) + (T^*_{i,j-1} - T^*_{i,j}) \qquad (3)$$

The accuracy of the above quantity would be the same as that of the A/D converter. The use of fixed point arithmetic results in the digital portion of the hybrid becoming a very fast function storage and playback device rather than a slow calculating device. For an all digital implementation of the A *DI* method single precision fixed point arithmetic is out of the question because of the accumulation of numerical errors.

Based on the above considerations I have made a time estimate for digital and hybrid implementation of the A *DI* method assuming the use of a P DP-8 digital computer. The all digital implementation would take about 6 milliseconds per node assuming .5 msec. per addition and 2 msec. per multiplication or division. For the hybrid implementation the calculation of equation 3 would take about 30 microseconds. Thus, the hybrid appears to be about 200 times faster than the digital. However, the speed of the linkage would be an important factor in the hybrid. Assuming 35 μsec. for an A/D conversion and 10 μsec. for a D/A conversion then the hybrid appears to be about 80 times faster than the digital. It is realized that this estimate is rough, but it is felt that this is a much more realistic estimate than the value of 2 given in the paper. Previous time comparisons which have appeared in the literature (*2* to *4*) have shown that a hybrid computer is anywhere from 20 to 120 times faster than a digital computer for solving partial differential equations.

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