# DIFFUSION, CONVECTION AND CHEMICAL REACTION IN A CHANNEL

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(Received 14 October 1974 and in revised form 18 August 1975)

Abstract—For laminar flow between a flat conduit exact solutions of the problem of steady-state diffusion and convection are presented for constant wall concentration, constant flux across the wall and a heterogeneous chemical reaction of the first order. The initial conditions were considered to be arbitrary functions of the coordinate across the channel. The same was performed for the cases of simultaneous diffusion, convection and homogeneous chemical reaction for constant wall concentration and heterogeneous chemical reaction. The eigenvalues are presented in tables and the eigenfunctions are presented in analytical form, which contains the confluent hypergeometric function.

# NOMENCLATURE

- b, width of channel;
- c, concentration,  $c_w$  wall concentration,  $c_i$ initial concentration,  $c_0$  concentration outside the duct,  $\hat{c}$  mean concentration across the channel;
- D, diffusion coefficient;

$$Da, = \frac{\pi b}{2D}$$
, Damköhler number

- $f_0$ , constant flux across the channel wall;
- $_1F_1$ , confluent hypergeometric function;
- k, heterogeneous chemical reaction coefficient;

;

- $k^*$ , homogeneous chemical reaction coefficient;
- p, pressure of liquid;
- Pe, = ReSc, Péclet number; $Re, = \frac{2u_0b}{3v}, Reynolds number;$
- Sc,  $=\frac{v}{D}$ , Schmidt number;
- $(at \ v = 0);$
- x, axial coordinate;
- y, coordinate perpendicular to channel axis;

 $y^*, \quad = y \Big/ \frac{b}{2}.$ 

- $\beta_n$ , eigenvalues;
- $\Gamma$ , gamma function;
- $\gamma$ , incomplete gamma function;
- $\eta$ , dynamic viscosity of liquid;
- $\kappa^2$ , proportionality factor;
- $\Psi$ ,  $\Psi$ -function.

#### **1. INTRODUCTION**

THE PROBLEM of steady state diffusion and convection in a straight channel has been treated previously for certain boundary conditions. Mathematically it represents nothing but the problem of forced heat convection in laminar flow assuming the Poiseuille flow velocity profile [1-3]. During the course of the analysis the partial differential equation has been transformed into an ordinary differential equation describing the concentration in the direction normal to the channel. The solution of this ordinary differential equation and the eigenvalues have been obtained numerically. Only the lower eigenvalues were given, until less than twenty years ago [4] asymptotic values were obtained for higher modes.

The purpose of this paper is to present the exact solution of the problem of steady state diffusion and convection with various boundary conditions, including the problem of a heterogeneous chemical reaction of the first order, as well as the problem of simultaneous diffusion, convection and chemical reaction. All eigenvalues may be easily and expediently obtained from the confluent hypergeometric function. In addition the orthogonality relations for the various cases are presented. With these the determination of the remaining integration constants may be performed even for arbitrarily given initial conditions exhibiting a function of the normal coordinate as their initial concentration distribution at the tube inlet.

## 2. BASIC EQUATIONS AND SOLUTION

For the determination of the local concentration of a component in a moving liquid between two parallel plates with a fully developed velocity profile, where molecular diffusion in axial direction is neglected, the second order differential equation (Fig. 1)

$$\frac{\partial^2 c}{\partial y^2} - \frac{u_0}{D} \left[ 1 - \frac{y^2}{(b/2)^2} \right] \frac{\partial c}{\partial x} - \frac{k^*}{D} c = 0$$
(1)

has to be solved. The width of the channel is b and

$$u_0 = -\frac{\partial p}{\partial x}\frac{b^2}{8\eta}$$

is the maximum velocity of the liquid. With the substitution  $y^* = y/(b/2)$  this yields

$$\frac{\partial^2 c}{\partial y^{*2}} - \frac{u_0 b^2}{4D} \left[ 1 - y^{*2} \right] \frac{\partial c}{\partial x} - \frac{k^* b^2}{4D} c = 0.$$
(1')

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F1G. 1. Geometry of the system.

This problem encounters the absorption of a substance by another through which it can diffuse convectively and molecularly and with which it can react chemically. It is assumed here, that the diffusing substance is immobilized by an irreversible first order reaction. If there is no simultaneous homogeneous chemical reaction the homogeneous chemical reaction coefficient  $k^*$  vanishes.

The problem has to be solved with the boundary condition

$$\mp A \frac{\partial c}{\partial y^*} = Bc + C \quad \text{at} \quad y^* = \pm 1$$
 (2)

which contains the cases of

- (a) constant surface concentration, i.e.  $A = 0, B = 1, C = -c_w$
- (b) heterogeneous chemical reaction of the first order, i.e. A = D, B = kb/2, C = 0
- (c) evaporation, i.e. A = D,  $B = \kappa^2 b/2$ ,  $C = -(\kappa^2 b/2) \cdot c_0$
- (d) constant flux across the wall, i.e. A = D, B = 0,  $C = f_0 b/2$ .

If a chemical reaction takes place in the surface of the channel wall, we talk then about a heterogeneous chemical reaction, in addition to the homogeneous chemical reaction. The value kb/2D = Da is called the Damköhler number. Assuming

$$c = c_1(y^*) + c_2(x, y^*)$$

the partial differential equation (1') yields

$$\frac{\mathrm{d}^2 c_1}{\mathrm{d} y^{*2}} - \frac{k^* b^2}{4D} c_1 = 0 \tag{3}$$

with

$$\overline{+} A \frac{\partial c_1}{\partial y^*} = B c_1 + C \quad \text{at} \quad y^* = \pm 1$$

and

$$\frac{\partial^2 c_2}{\partial y^{*2}} - \frac{u_0 b^2}{4D} (1 - y^{*2}) \frac{\partial c_2}{\partial x} - \frac{k^* b^2}{4D} c_2 = 0 \qquad (4)$$

with

$$\mp A \frac{\partial c_2}{\partial y^*} = Bc_2 \quad \text{at} \quad y^* = \pm 1.$$

The solution of equation (3) yields

$$c_1 =$$

$$-\frac{C\cosh\left[\frac{b}{2}\left(\frac{k^{*}}{D}\right)^{\frac{1}{2}}y^{*}\right]}{\left\{B\cosh\left[\frac{b}{2}\left(\frac{k^{*}}{D}\right)^{\frac{1}{2}}\right]+A\frac{b}{2}\left(\frac{k^{*}}{D}\right)^{\frac{1}{2}}\sinh\left[\frac{b}{2}\left(\frac{k^{*}}{D}\right)^{\frac{1}{2}}\right]\right\}}.$$
(5)

With  $c_2 = \overline{C} e^{-xx}$  equation (4) exhibits with  $\beta^2 \equiv (u_0 b^2 \alpha / 4D)$  [5] the solution

$$\bar{C} = \bar{A} e^{-\frac{\beta}{2}y^{*2}} {}_{1}F_{1}\left(\frac{1}{4}\left(1-\beta+\frac{k^{*}b^{2}}{4D\beta}\right), \frac{1}{2}; \beta y^{*2}\right)$$
(6)

where  ${}_{1}F_{1}$  represents the confluent hypergeometric series

$$_{\lambda}F_{1}(\alpha,\gamma;z) = \sum_{\lambda=0}^{\infty} \frac{\Gamma(\gamma)\Gamma(\alpha+\lambda)z^{\lambda}}{\Gamma(\alpha)\Gamma(\gamma+\lambda)\lambda!}$$

The boundary condition for  $c_2$  yields the equation for the determination of the eigenvalues  $\beta_n$ :

$$B = \frac{A}{2} \left( 1 + \beta + \frac{k^* b^2}{4D\beta} \right) - \frac{A}{2} \left( 1 - \beta + \frac{k^* b^2}{4D\beta} \right)$$
$$\times \frac{{}_{1}F_1 \left( \frac{1}{4} \left( 5 - \beta + \frac{k^* b^2}{4D\beta} \right), \frac{1}{2}; \beta \right)}{{}_{1}F_1 \left( \frac{1}{4} \left( 1 - \beta + \frac{k^* b^2}{4D\beta} \right), \frac{1}{2}; \beta \right)}.$$
 (7)

These eigenvalues  $\beta_n$  are presented for constant surface concentration, for heterogeneous chemical reaction and evaporation, and for constant flux ( $k^* = 0$ -case) in Tables 1–3. The solution of the problem is then given by the expression

$$c = -\frac{C \cosh\left[\frac{b}{2}\left(\frac{k^*}{D}\right)^{\frac{1}{2}}y^*\right]}{\left\{B \cosh\left[\frac{b}{2}\left(\frac{k^*}{D}\right)^{\frac{1}{2}}\right] + A \frac{b}{2}\left(\frac{k^*}{D}\right)^{\frac{1}{2}} \sinh\left[\frac{b}{2}\left(\frac{k^*}{D}\right)^{\frac{1}{2}}\right]\right\}} + \sum_{n=1}^{\infty} \overline{A}_n e^{-\frac{\beta_n}{2}y^{*2}} \cdot {}_1F_1\left(\frac{1}{4}\left(1 - \beta_n + \frac{k^*b^2}{4D\beta_n}\right), \frac{1}{2}; \beta_n y^{*2}\right)} \times e^{-\frac{4\beta_n^2 D}{u_0 b^2}x}$$
(8)

The constants  $\overline{A}_n$  are obtained from the initial condition at the inlet x = 0, which reads  $c(0, y^*) = c_i(y^*)$  and results for  $c_2$  in

$$c_{2}(0, y^{*}) = c_{i}(y^{*})$$

$$+ \frac{C \cosh\left[\frac{b}{2}\left(\frac{k^{*}}{D}\right)^{\frac{1}{2}}y^{*}\right]}{\left\{B \cosh\left[\frac{b}{2}\left(\frac{k^{*}}{D}\right)^{\frac{1}{2}}\right] + A\frac{b}{2}\left(\frac{k^{*}}{D}\right)^{\frac{1}{2}} \sinh\left[\frac{b}{2}\left(\frac{k^{*}}{D}\right)^{\frac{1}{2}}\right]\right\}}.$$
(9)

With the abbreviation

$$\bar{C}_{n}(y^{*}) \equiv e^{-\frac{\beta_{n}}{2}y^{*2}} \cdot {}_{1}F_{1}\left(\frac{1}{4}\left(1-\beta_{n}+\frac{k^{*}b^{2}}{4D\beta_{n}}\right), \frac{1}{2}; \beta_{n}y^{*2}\right) (10)$$

which satisfies the differential equation

$$\frac{d^2 \bar{C}}{dy^{*2}} + \left[\beta^2 (1 - y^{*2}) - \frac{k^* b^2}{4D}\right] \bar{C} = 0$$

|    | 4 <i>D</i> |           |           |           |           |  |  |
|----|------------|-----------|-----------|-----------|-----------|--|--|
| n  | 0          | 0.1       | 1.0       | 10        | 100       |  |  |
| 1  | 1.680706   | 1.705408  | 1.973668  | 3.753472  | 10.517979 |  |  |
| 2  | 5.668724   | 5.677812  | 5.777087  | 6.804868  | 12.807847 |  |  |
| 3  | 9.667103   | 9.667270  | 9.731214  | 10.417786 | 15.480656 |  |  |
| 4  | 13.666522  | 13.667353 | 13.711603 | 14.217085 | 18.474449 |  |  |
| 5  | 17.666236  | 17.667500 | 17.700241 | 18.100188 | 21.716535 |  |  |
| 6  | 21.666069  | 21.668438 | 21.692764 | 22.026755 | 25,147685 |  |  |
| 7  | 25.665961  | 25.669741 | 25.687459 | 25.974962 | 28,701792 |  |  |
| 8  | 29.665886  | 29.669244 | 29.683496 | 29,936296 | 32.364750 |  |  |
| 9  | 33.665832  | 33.668869 | 33.680420 | 33.906250 | 36.085944 |  |  |
| 10 | 37.665791  | 37.668575 | 37.677963 | 37.882206 | 39.851775 |  |  |

| Table 1. $\beta_n$ -values for constant wall concentratio | Table 1. | $\beta_n$ -values | for | constant | wall | concentration |
|---|----------|-------------------|-----|----------|------|---------------|
|---|----------|-------------------|-----|----------|------|---------------|

Table 2(a).  $\beta_n$ -values for various Damköhler-numbers and  $\frac{k^*b^2}{4D}$ -values

|    |           |           | Da        |           |                    |
|----|-----------|-----------|-----------|-----------|--------------------|
| n  | 0.1       | 1.0       | 10        | 100       |                    |
| 1  | 0.374941  | 1.000000  | 1.550312  | 1.666035  |                    |
| 2  | 4.332076  | 4.654545  | 5.397629  | 5.636888  |                    |
| 3  | 8.327079  | 8.542446  | 9.293999  | 9.613329  |                    |
| 4  | 12.328510 | 12.498990 | 13.217682 | 13.603544 |                    |
| 5  | 16.328308 | 16.472657 | 17,157799 | 17.592962 |                    |
| 6  | 20.328448 | 20.454484 | 21.108539 | 21.583684 |                    |
| 7  | 24.328478 | 24.440997 | 25.066797 | 25.574979 |                    |
| 8  | 28.328517 | 28.430519 | 29.030707 | 29.566814 |                    |
| 9  | 32.328542 | 32.422099 | 32.999038 | 33.559075 | $k^*b^2$           |
| 10 | 36.328563 | 36.415158 | 36.970926 | 37.551700 | $\frac{1}{4D} = 0$ |
| 11 | 40.328580 | 40.409318 | 40.945737 | 41.544639 | 15                 |
| 12 | 44.328594 | 44,404324 | 44.922990 | 45.537853 |                    |
| 13 | 48.328605 | 48.399996 | 48.902310 | 49.531312 |                    |
| 14 | 52.328615 | 52.396200 | 52.883399 | 53.524989 |                    |
| 15 | 56.328624 | 56.392840 | 56.866021 | 57.518866 |                    |
| 16 | 60.328631 | 60.389841 | 60.849977 | 61.512923 |                    |
| 17 | 64.328637 | 64.387143 | 64.835107 | 65.507147 |                    |
| 18 | 68.328643 | 68.384702 | 68.821127 | 69.501523 |                    |

|    |           | 1000000000000000000000000000000000000 |           |           |                      |
|----|-----------|---------------------------------------|-----------|-----------|----------------------|
|    |           |                                       | Da        |           |                      |
| n  | 0.1       | 1.0                                   | 10        | 100       |                      |
| 1  | 0.535742  | 1.062995                              | 1.588564  | 1.701239  |                      |
| 2  | 4.354768  | 4.675074                              | 5.411420  | 5.649568  |                      |
| 3  | 8.327215  | 8.556917                              | 9.308817  | 9.627288  |                      |
| 4  | 12.320443 | 12.516351                             | 13.234488 | 13.615060 |                      |
| 5  | 16.318533 | 16.488570                             | 17.172599 | 17.603504 | $k^{*}b^{2}$         |
| 6  | 20.317606 | 20.469858                             | 21.121587 | 21.593502 | $\frac{1}{4D} = 0.1$ |
| 7  | 24.317032 | 24.455803                             | 25.078521 | 25.584289 | -10                  |
| 8  | 28.316629 | 28.444917                             | 29.041443 | 29.575743 |                      |
| 9  | 32.316329 | 32.436162                             | 33.009016 | 33.567708 |                      |
| 10 | 36.316096 | 36.428949                             | 36.980305 | 37.560097 |                      |
| 1  | 1.260792  | 1.524110                              | 1.891290  | 1.979940  |                      |
| 2  | 4.555467  | 4.851578                              | 5.536855  | 5.763207  |                      |
| 3  | 8.437837  | 8.661265                              | 9.375170  | 9.687909  |                      |
| 4  | 12.408832 | 12.576553                             | 13.277000 | 13.650642 |                      |
| 5  | 16.391302 | 16.533770                             | 17.206441 | 17.627249 | $k^*b^2$             |
| 6  | 20.380700 | 20.504780                             | 21.150324 | 21.609643 | $\frac{1}{4D} = 1.0$ |
| 7  | 24.373283 | 24.483994                             | 25.103766 | 25.595218 |                      |
| 8  | 28.367904 | 28.468167                             | 29.064093 | 29.582809 |                      |
| 9  | 32.363802 | 32.455677                             | 33.029653 | 33.571799 |                      |
| 10 | 36.360577 | 36.445530                             | 36.999332 | 37.561820 |                      |

Table 2(b).  $\beta_n$ -values for various Damköhler-numbers and  $\frac{k^*b^2}{4D}$ -value

|                      |           | Da        |           |           |    |
|----------------------|-----------|-----------|-----------|-----------|----|
|                      | 100       | 10        | 1.0       | 0.1       | n  |
|                      | 3.751998  | 3.728017  | 3.662817  | 3.634360  | 1  |
|                      | 6.786674  | 6.650157  | 6.302725  | 6.164637  | 2  |
|                      | 10.382907 | 10.144622 | 9.623018  | 9.458632  | 3  |
|                      | 14.169056 | 13.853489 | 13.268780 | 13.123793 | 4  |
| $k^*b^2$ 10          | 18.041197 | 17.670843 | 17.071151 | 16.920771 | 5  |
| $\frac{1}{4D} = 10$  | 21.957940 | 21.544618 | 20.947287 | 20.808017 | 6  |
|                      | 25.897039 | 25.447850 | 24.850416 | 24.733057 | 7  |
|                      | 29.849860 | 29.364876 | 28.779554 | 28.678850 | 8  |
|                      | 33.811783 | 33.295308 | 32.726025 | 32.637726 | 9  |
|                      | 37.780114 | 37.236902 | 36.684193 | 36.605433 | 10 |
|                      | 10.513046 | 10.512967 | 10.512884 | 10.512867 | 1  |
|                      | 12.810292 | 12.807572 | 12.804609 | 12.803990 | 2  |
|                      | 15.478601 | 15.462683 | 15.444667 | 15.440815 | 3  |
|                      | 18.463462 | 18.416132 | 18.361220 | 18.349319 | 4  |
| $k^*b^2$ 100         | 21.698263 | 21.607042 | 21.499196 | 21.475687 | 5  |
| $\frac{1}{4D} = 100$ | 25.124777 | 24.976323 | 24.796645 | 24.758169 | 6  |
|                      | 28.662403 | 28.467537 | 28.239946 | 28.191912 | 7  |
|                      | 32.308009 | 32.056028 | 31.776408 | 31.719559 | 8  |
|                      | 36.029106 | 35.726379 | 35.407249 | 35.345068 | 9  |
|                      | 39.790099 | 39.455769 | 39.109924 | 39.045408 | 10 |

Table 3.  $\beta_n$ -values for constant flux across the walls ( $k^* = 0$ )

n

1

2 3

4

5 6 7

8 9

10

11 12

13

14

15

16 17

18 19

20

 $\beta_n$ 

4.286418

8.303518

12.291126

16.297552 20.299898

24.301932 28.303424 32.304607

36.305567

40.306364 44.307038

48.307617

52.308121

56.308564

60.308957

64.309308

68.309624 72.309911

76.310172

80.310410

Table 2(c).  $\beta_n$ -values for various Damköhler-numbers and  $\frac{k^*b^2}{4D}$ -values

| $\int_0^1 (1 - y^{*2}) \overline{C}_m(y^*) \overline{C}_n(y^*)  \mathrm{d}y^*$  |  |
|---|--|
| $= \begin{cases} 0 \text{ for } m \neq n \\ \frac{1}{2\beta_n} \left[ \frac{\partial \bar{C}_n}{\partial \beta_n} \cdot \frac{\partial \bar{C}_n}{\partial y^*} \right]_{y^*=1} & \text{for constant} \\ 1 \left[ \partial \bar{C}_n \partial \bar{C}_n - \bar{c} \right]_{z^*=1} & \text{wall concentration} \end{cases}$  |  |
| $\begin{bmatrix} \overline{2\beta_n} \begin{bmatrix} \overline{\partial y^*} & \overline{\partial \beta_n} & -C_n & \overline{\partial y^* \partial \beta_n} \end{bmatrix}_{y^*=1} \text{ all other cases} \\ = -\frac{\overline{C}_n(1)}{2\beta_n} \begin{bmatrix} \overline{\partial^2 \overline{C}_n} \\ \overline{\partial y^* \partial \beta_n} + \frac{B}{A} & \overline{\partial y^*} \end{bmatrix}_{y^*=1} \text{ for } m = n.$ |  |

The value for m = n was obtained from an indeterminate expression by applying the rule of l'Hospital. The values

we obtain the orthogonality relation

$$\left[\frac{\partial \bar{C}_n}{\partial \beta_n}\right]_{y^*=1} \quad \text{and} \quad \left[\frac{\partial \bar{C}_n}{\partial y^*}\right]_{y^*=1}$$

may be obtained from (10) and the confluent hypergeometric function. They are given by [6]:

$$\begin{bmatrix} \frac{\partial \bar{C}_n}{\partial y^*} \end{bmatrix}_{y^*=1} = \frac{1}{2} e^{-\frac{\beta_n}{2}} \begin{bmatrix} 1 - \beta_n + \frac{k^*b^2}{4D\beta_n} \end{bmatrix}_1 F_1 \left( \frac{1}{4} \left( 5 - \beta_n + \frac{k^*b^2}{4D\beta_n} \right), \frac{1}{2}; \beta_n \right) \\ - \frac{1}{2} e^{-\frac{\beta_n}{2}} \begin{bmatrix} 1 + \beta_n + \frac{k^*b^2}{4D\beta_n} \end{bmatrix}_1 F_1 \left( \frac{1}{4} \left( 1 - \beta_n + \frac{k^*b^2}{4D\beta_n} \right), \frac{1}{2}; \beta_n \right).$$

and

$$\left[\frac{\partial \bar{C}_n}{\partial \beta_n}\right]_{y^{*}=1} = \frac{e^{-\frac{\beta_n}{2}}}{4\beta_n} {}_1F_1\left(\frac{1}{4}\left(5-\beta_n+\frac{k^*b^2}{4D\beta_n}\right),\frac{1}{2};\beta_n\right)\left[1-\beta_n+\frac{k^*b^2}{4D\beta_n}\right]$$

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$$-\frac{e^{-\frac{\beta_{n}}{2}}}{4}\left[1+\frac{1}{\beta_{n}}+\frac{k^{*}b^{2}}{4D\beta_{n}}\right]_{1}F_{1}\times\left(\frac{1}{4}\left(1-\beta_{n}+\frac{k^{*}b^{2}}{4D\beta_{n}},\frac{1}{2};\beta_{n}\right)\right)-\frac{1}{4}\left(1+\frac{k^{*}b^{2}}{4D\beta_{n}^{2}}\right)\sum_{\lambda=0}^{\infty}\frac{2^{2\lambda}\beta_{n}^{\lambda}}{(2\lambda)!}\frac{\Gamma\left(\lambda+\frac{1}{4}\left(1-\beta_{n}+\frac{k^{*}b^{2}}{4D\beta_{n}}\right)\right)}{\Gamma\left(\frac{1}{4}\left(1-\beta_{n}+\frac{k^{*}b^{2}}{4D\beta_{n}}\right)\right)}\times\left[\Psi\left(\lambda+\frac{1}{4}\left(1-\beta_{n}+\frac{k^{*}b^{2}}{4D\beta_{n}}\right)\right)-\Psi\left(\frac{1}{4}\left(1-\beta_{n}+\frac{k^{*}b^{2}}{4D\beta_{n}}\right)\right)\right]e^{-\beta_{n}/2}.$$
 (11)

From the initial condition (9) the constants  $\overline{A}_n$  may be determined by the expression

$$\bar{A}_{n} = \frac{2\beta_{n} \int_{0}^{1} (1-y^{*2}) \left[ c_{i}(y^{*}) + \frac{C \cosh\left[\frac{b}{2} \left(\frac{k^{*}}{D}\right)^{\frac{1}{2}}\right] + A \frac{b}{2} \left(\frac{k^{*}}{D}\right)^{\frac{1}{2}} ] + A \frac{b}{2} \left(\frac{k^{*}}{D}\right)^{\frac{1}{2}} ] \right]}{\left[ \frac{\partial \bar{C}_{n}}{\partial y^{*}} \frac{\partial \bar{C}_{n}}{\partial \beta_{n}} - \delta \bar{C}_{n} \frac{\partial^{2} \bar{C}_{n}}{\partial y^{*} \partial \beta_{n}} \right]_{y^{*}=1}}$$
(12)

 $\delta = \begin{cases} 0 & \text{for constant wall concentration} \\ 1 & \text{for all other cases.} \end{cases}$ 

If  $c_i$  is constant the first part of the integral may be evaluated and yields

$$\int_{0}^{1} (1 - y^{*2}) \overline{C}_{n}(y^{*}) dy^{*} = \frac{k^{*}b^{2}}{4D\beta_{n}^{2}} \int_{0}^{1} \overline{C}_{n}(y^{*}) dy^{*} - \frac{\overline{C}_{n}'(1)}{\beta_{n}^{2}}.$$
(13)

For the determination of the remaining integral and that of equation (12) we refer to the appendix.

If at the inlet x = 0 the initial condition  $c_i$  is a constant value, the integration constants are with (11) given by

$$\bar{A}_{n} = -\frac{2[c_{i} - c_{w}]}{\beta_{n} \left[\frac{\partial \bar{C}_{n}}{\partial \beta_{n}}\right]_{y^{*}=1}}$$

for constant wall concentration and  $k^* = 0$ 

$$\bar{A}_{n} = -\frac{2c_{i}}{\beta_{n} \left[\frac{\partial \bar{C}_{n}}{\partial \beta_{n}} + \frac{1}{Da} \frac{\partial^{2} \bar{C}_{n}}{\partial y^{*} \partial \beta_{n}}\right]_{y^{*}=1}}$$

for heterogeneous chemical reaction and  $k^* = 0$ .

# 3. CONSTANT FLUX ACROSS THE WALL

The case of just diffusion and convection with a constant rate of diffusing material across the boundary

$$\left(\frac{\partial c}{\partial y^*} = \mp \frac{f_0 b}{2D} \quad \text{at} \quad y^* = \pm 1\right)$$

needs special treatment. For the solution of the differential equation (1') with  $k^* = 0$ , we assume  $c = c_1 + c_2$ , where  $c_1$  and  $c_2$  have to satisfy (1') with the boundary condition

$$\frac{\partial c_1}{\partial y^*} = \mp \frac{f_0 b}{2D}$$
 and  $\frac{\partial c_2}{\partial y^*} = 0$  for  $y^* = \pm 1$  (14)

respectively. With

$$c_1 = Bx + f^*(y^*)$$

and  $c_i = \text{constant}$  we obtain

$$c_1 = c_i - \frac{3f_0}{bu_0} x - \frac{3f_0 b}{8D} \left[ y^{*2} - \frac{1}{6} y^{*4} - \frac{13}{70} \right]$$
(15)

The concentration  $c_2$  is given by the series expression with  $k^* = 0$ :

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$$c_{2}(x, y^{*}) = \sum_{n=1}^{\infty} \overline{A}_{n} e^{-\frac{\beta_{n}}{2}y^{*2}} \cdot {}_{1}F_{1}(\frac{1}{4}(1-\beta_{n}), \frac{1}{2}; \beta_{n}y^{*2}) \times e^{-\frac{4\beta_{n}^{2}D}{u_{0}b^{2}} \cdot x}.$$
 (16)

The integration constants  $\overline{A}_n$  are obtained from the initial condition, with the orthogonality relation  $(\bar{C}_n'(1)=0)$ 

$$\int_{0}^{1} (1-y^{*2}) \widetilde{C}_{m}(y^{*}) \overline{C}_{n}(y^{*}) dy^{*} = \begin{cases} 0 & \text{for } m \neq n \\ -\frac{\widetilde{C}_{n}(1)}{2\beta_{n}} \cdot \frac{\partial^{2} \widetilde{C}_{n}}{\partial y^{*} \partial \beta_{n}} (1) \\ & \text{for } m = n. \end{cases}$$
(17)

Thus  $\overline{A}_n$  is with the initial condition for the concentration  $c_2$  at the inlet x = 0

$$c_2(0, y^*) = \frac{3f_0 b}{8D} \left[ y^{*2} - \frac{1}{5} y^{*4} - \frac{13}{70} \right]$$
(18)

obtained from

$$\bar{A}_{n} = -\frac{3f_{0}\beta_{n}b\int_{0}^{1}(1-y^{*2})[y^{*2}-\frac{1}{6}y^{*4}-\frac{13}{70}]\bar{C}_{n}(y^{*})dy^{*}}{4D\bar{C}_{n}(1)\cdot\frac{\partial^{2}\bar{C}_{n}}{\partial y^{*}\partial\beta_{n}}(1)}$$
(19)

which yields

$$\bar{A}_{n} = -\frac{f_{0}b}{D\beta_{n}\frac{\partial^{2}\bar{C}_{n}}{\partial y^{*}\partial\beta_{n}}(1)}$$

#### 4. REMARKS

In the previous treatment we have neglected the molecular diffusion in axial direction. This, however,

is not always permitted. Without this neglection the process would be described by the differential equation

$$\frac{\partial^2 c}{\partial y^{*2}} + \frac{b^2}{4} \frac{\partial^2 c}{\partial x^2} - \frac{u_0 b^2}{4D} (1 - y^{*2}) \frac{\partial c}{\partial x} - \frac{k^* b^2}{4D} c = 0.$$

In the usual way the substitution  $c = \overline{C} e^{-\alpha x}$  shall reduce the above equation to the ordinary differential equation

$$\frac{\mathrm{d}^2\bar{C}}{\mathrm{d}y^{*\,2}} + \left[\beta^2(1-y^{*\,2}) + \frac{4D^2\beta^4}{b^2u_0^2} - \frac{k^*b^2}{4D}\right]\bar{C} = 0.$$

The solution of this equation is

$$\overline{C} = e^{-\frac{\beta}{2}y^{*2}} {}_{1}F_{1}\left(\frac{1}{4}\left(1-\beta-\frac{4D^{2}\beta^{3}}{b^{2}u_{0}^{2}}+\frac{k^{*}b^{2}}{4D\beta}\right), \frac{1}{2}; \beta y^{*2}\right).$$

which yields

$$\frac{\partial^2 c}{\partial \eta^{*2}} - \frac{u_0 b^2}{2D} \eta^* \frac{\partial c}{\partial x} = 0$$

in the case of diffusion and convection, and

$$\frac{\partial^2 c}{\partial \eta^{*2}} - \frac{u_0 b^2}{2D} \eta^* \frac{\partial c}{\partial x} - \frac{k^* b^2}{4D} c = 0$$

in the case of simultaneous diffusion, convection and chemical reaction. By proper transformation these differential equations may be solved, as indicated by Levich [7] for the first equation. For the solution of the second differential equation a Laplace-Transformtechnique may be applied.

Table 4.  $\beta_n$ -values for various Péclet-numbers (for constant wall concentration)

|    | Pe       |           |           |           |           |  |  |
|----|----------|-----------|-----------|-----------|-----------|--|--|
| n  | 1        | 10        | 100       | 1000      | $\infty$  |  |  |
| 1  | 0.977152 | 1.636176  | 1.680206  | 1.680702  | 1.680706  |  |  |
| 2  | 1.828636 | 4.574453  | 5.645687  | 5.668488  | 5.668724  |  |  |
| 3  | 2.387047 | 6.563249  | 9.549618  | 9.665858  | 9.667103  |  |  |
| 4  | 2.838052 | 8.120181  | 13.337954 | 13.662894 | 13.666523 |  |  |
| 5  | 3.227349 | 9.436836  | 16.979712 | 17.658252 | 17.666236 |  |  |
| 6  | 3.571120 | 10.599105 | 20.458014 | 21.651175 | 21.666607 |  |  |
| 7  | 3.887497 | 11.647333 | 23.770739 | 25.641056 | 25.665961 |  |  |
| 8  | 4.178400 | 12.612735 | 26.922088 | 29.627370 | 29.665886 |  |  |
| 9  | 4.452324 | 13.509006 | 29.921406 | 33.609669 | 33.665832 |  |  |
| 10 | 4.713051 | 14.351016 | 32.780426 | 37.586289 | 37.665791 |  |  |

From this one may conclude immediately, that the above solutions tend into those of the previous section, if

$$\frac{4D^2\beta^2}{b^2u_0^2} \ll 1$$

is satisfied. This means that the Péclet number  $Pe = ReSc \gg 1$ . Only for such cases the molecular diffusion in axial direction may be neglected. It may, however, be mentioned that the functions are not orthogonal.

To show just the difference of the eigenvalues  $\beta_n$  for the classical Graetz-problem, the equation for the determination of the eigenvalues  $\beta_n$  with  $Re = (2u_0 b/3v)$ 

$${}_{1}F_{1}\left(\frac{1}{4}\left(1-\beta-\frac{16\beta^{3}}{9(Pe)^{2}}\right),\frac{1}{2};\beta\right)=0$$

has been evaluated for various Péclet numbers (Table 4).

It may also be noted that the representation of the results in the immediate vicinity of the inlet x = 0 requires a large number of eigenvalues and eigenfunctions. This could be achieved with some increased numerical effort with the above solution. Another method could as well be adopted by noting that near x = 0 the concentration change takes place very closely to the wall in the extremely thin diffusion layer. This suggests immediately the transformation of the governing differential equation to the wall by

$$\eta = \frac{b}{2} - y \quad \text{or} \quad \eta^* = 1 - y^*$$

# 5. MEAN CONCENTRATION AND CONCENTRATION AT THE WALL

The concentration at the walls may be easily obtained from the previous results by merely introducing in the solutions presented in Sections 2 and 3 the value  $y^* = \pm 1(y = \pm b/2)$ . For constant flux across the walls the wall-concentration yields

$$c_{w} = c_{i} - \frac{3f_{0}}{bu_{0}} x - \frac{17f_{0}b}{70D} + \sum_{n=1}^{\infty} \bar{A}_{n} e^{-\frac{\beta_{n}}{2}} F_{1}(\frac{1}{4}(1-\beta_{n}), \frac{1}{2}; \beta_{n}) \cdot e^{-\frac{4\beta_{n}^{2}D}{u_{0}b^{2}}x}$$
(20)

For simultaneous diffusion, convection and chemical reaction one finds at the walls

$$c_{w} = -\frac{C}{\left\{B + A\frac{b}{2}\left(\frac{k^{*}}{D}\right)^{\frac{1}{2}} \tanh\left[\frac{b}{2}\left(\frac{k^{*}}{D}\right)^{\frac{1}{2}}\right]\right\}} + \sum_{n=1}^{\infty} \overline{A}_{n} e^{-\frac{\beta_{n}}{2}}$$
$$\times {}_{1}F_{1}\left(\frac{1}{4}\left(1 - \beta_{n} + \frac{k^{*}b^{2}}{4D\beta_{n}}\right), \frac{1}{2}; \beta_{n}\right) \cdot e^{-\frac{4\beta^{2}D}{u_{0}b^{2}}x} \quad (21)$$

where the values A, B, C have to be introduced appropriately for the various cases.

The mean concentration over the cross section of the channel is given by  $(\bar{u} = \frac{2}{3}u_0)$ 

$$\bar{c} = \frac{2}{b\bar{u}} \int_0^{b/2} u(y) c(x, y) dy = \frac{3}{2} \int_0^1 (1 - y^{*2}) c(x, y^*) dy^*$$
(22)

which is only a function of the axial coordinate x. Introducing the previous results and applying the appropriate boundary conditions and orthogonality relations yields:

$$\bar{c} = c_i - \frac{3f_0}{bu_0}x$$
 for constant flux across the walls  
and  $k^* = 0$  (23)

and

$$\bar{c} = \frac{12CD\left[1 - \frac{2}{b}\left(\frac{D}{k^*}\right)^{\frac{1}{2}} \tanh\left[\frac{b}{2}\left(\frac{k^*}{D}\right)^{\frac{1}{2}}\right]\right]}{k^*b^2\left\{B + A\frac{b}{2}\left(\frac{k^*}{D}\right)^{\frac{1}{2}} \tanh\left[\frac{b}{2}\left(\frac{k^*}{D}\right)^{\frac{1}{2}}\right]\right\}}$$
$$+ \frac{3}{2}\sum_{n=1}^{\infty}\frac{\bar{A}_n}{\beta_n^2}e^{-\frac{4D\beta^2}{n_0b^2}x} \cdot \left\{\frac{k^*b^2}{4D}\int_0^1 \bar{C}_n(y^*)dy^* + \frac{B}{A}\bar{C}_n(1)\right\} (24)$$

for all other cases.

The integral  $\int_0^1 \overline{C}_n(y^*) dy^*$  is presented in the Appendix.

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#### APPENDIX

For the determination of the integration constants of the previous sections various integrals appear, which have to be evaluated. They are of the form

$$J = \int_0^1 f(y^*) C_n(y^*) \, \mathrm{d}y^*$$

where  $f(y^*) = 1$ ;  $y^{*2m}$ ;  $y^{*2m+1}$  or combinations of those. It is therefore [6]

$$J_{1} = \int_{0}^{1} \overline{C}_{n}(y^{*}) dy^{*}$$
$$\int_{0}^{1} e^{-\frac{\beta_{n}}{2}y^{*2}} \sum_{\lambda=1}^{\infty} \frac{\Gamma(\alpha_{n}+\lambda)2^{2\lambda}\beta_{n}^{\lambda}}{\Gamma(\alpha_{n})(2\lambda)!} y^{*2\lambda} dy^{*}$$

 $\beta_* v^{*2} = z$ 

which may be reduced with the transformation

to 
$$J_1 = \sum_{\lambda=0}^{\infty} \frac{\Gamma(\alpha_n + \lambda) 2^{2\lambda-1}}{\Gamma(\alpha_n)(2\lambda)! \sqrt{\beta_n}} \int_0^{\beta_n} e^{-z/2} z^{\lambda-1/2} dz.$$

The integral is presented by

$$\int_{0}^{\beta_{n}} e^{-z/2} z^{\lambda-1/2} dz = 2^{\lambda+1/2} \gamma(\lambda + \frac{1}{2}, \frac{1}{2}\beta_{n})$$

where  $\gamma$  represents the incomplete gamma-function, which may be represented in series form as [6]

$$\gamma(\lambda+\frac{1}{2},\frac{1}{2}\beta_n) = \sum_{\nu=0}^{\infty} \frac{(-1)^{\nu} \beta_n^{\nu+\lambda+1/2}}{\nu! 2^{\nu+\lambda+1/2} (\nu+\lambda+\frac{1}{2})}.$$

The integral is therefore given by

$$U_1 = \sum_{\lambda=0}^{\infty} \frac{\Gamma(\alpha_n + \lambda) 2^{2\lambda-1}}{\Gamma(\alpha_n)(2\lambda)!} \sum_{\nu=0}^{\infty} \frac{(-1)^{\nu} \beta_n^{\nu+\lambda}}{2^{\nu} \nu! (\nu + \lambda + \frac{1}{2})}.$$

The following integrals may be obtained in a similar way. They are given by the expressions:

$$J_{2} = \int_{0}^{\infty} y^{*2m} C_{n}(y^{*}) dy^{*}$$

$$\sum_{\lambda=0}^{\infty} \frac{\Gamma(\alpha_{n}+\lambda)2^{2\lambda-1}}{\Gamma(\alpha_{n})(2\lambda)!} \sum_{\nu=0}^{\infty} \frac{(-1)^{\nu} \beta_{n}^{\nu+\lambda}}{\nu! 2^{\nu} (\lambda+\nu+m+\frac{1}{2})}$$

$$J_{3} = \int_{0}^{1} y^{*2m+1} C_{n}(y^{*}) dy^{*}$$

$$= \sum_{\lambda=0}^{\infty} \frac{\Gamma(\alpha_{n}+\lambda)2^{2\lambda-1}}{\Gamma(\alpha_{n})(2\lambda)!} \sum_{\nu=0}^{\infty} \frac{(-1)^{\nu} \beta_{n}^{\nu+\lambda}}{2^{\nu} \nu! (\nu+\lambda+m+1)}$$

$$= \sum_{\lambda=0}^{\infty} \frac{\Gamma(\alpha_{n}+\lambda)2^{3\lambda+m} (m+\lambda)!}{\Gamma(\alpha_{n})(2\lambda)! \beta_{n}^{m+1}} \cdot \left\{ 1 - e^{-\beta_{n}/2} \sum_{\nu=0}^{m+\lambda} \frac{\beta_{n}^{\nu}}{\nu! 2^{\nu}} \right\}$$

All appearing integrals in the text may be determined with these results. It is furthermore

$$\int_{0}^{1} (1 - y^{*2}) \cosh\left[\frac{b}{2} \left(\frac{k^{*}}{D}\right)^{*} y^{*}\right] C_{n}(y^{*}) dy^{*}$$

$$= \sum_{m=0}^{\infty} \frac{\left(\frac{k^{*}b^{2}}{4D}\right)^{m}}{(2m)!} \cdot \left\{\sum_{\lambda=0}^{\infty} \frac{\Gamma(\alpha_{n} + \lambda)2^{2\lambda - 1}}{\Gamma(\alpha_{n})(2\lambda)!} \times \sum_{\nu=0}^{\infty} \frac{(-1)^{\nu} \beta_{n}^{\nu + \lambda}}{2^{\nu} \nu! (\nu + \lambda + m + \frac{1}{2})(\nu + m + \lambda + \frac{3}{2})}\right\}.$$

# DIFFUSION, CONVECTION ET REACTION CHIMIQUE DANS UN CANAL

Résumé—On présente des solutions exactes du problème de diffusion et de convection stationnaires en écoulement laminaire dans un canal plat, pour une concentration constante à la paroi, un flux pariétal constant et une réaction chimique hétérogène du premier ordre. Les conditions initiales sont supposées fonctions arbitraires de la coordonnée transversale dans le canal. On a traité de même les cas d'une diffusion et convection avec réaction chimique homogène pour une concentration de paroi constante et une réaction chimique hétérogène. Les valeurs propres sont présentées dans des tables et les fonctions propres sont données sous forme analytique, à l'aide de la fonction hypergéométrique confluente.

# DIFFUSION, KONVEKTION UND CHEMISCHE REAKTION IN EINEM KANAL

Zusammenfassung—Für laminare Strömung in einem flachen Kanal wurden exakte Lösungen des Problems der stationären Diffusion und Konvektion angegeben bei konstanter Wandkonzentration, konstantem Wärmestrom an der Wand und heterogener chemischer Reaktion von erster Ordnung. Die Anfangsbedingungen wurden als beliebige Funktionen der Kanalkoordinaten angesehen.

# HELMUT F. BAUER

Dasselbe Vorgehen erfolgte für den Fall gleichzeitiger Diffusion, Konvektion und homogener chemischer Reaktion bei konstanter Wandkonzentration und heterogener chemischer Reaktion. Eigenwerte wurden in Tabellen angegeben und Eigenfunktionen in analytischer Form, die die konfluente hypergeometrische Funktion enthielten.

# ДИФФУЗИЯ, КОНВЕКЦИЯ И ХИМИЧЕСКАЯ РЕАКЦИЯ В КАНАЛЕ

Аннотация — Получены точные решения задачи установившейся диффузии и конвекции для граничных условий постоянной концентрации на стенке, постоянного потока и гетерогенной химической реакции первого порядка при ламинарном течении в плоском канале. Предполагается, что начальные условия являются произвольными функциями поперечной координаты. Эти же условия принимаются для случаев совместной диффузии, конвекции и гомогенной химической реакции при постоянной концентрации на стенке и гетерогенной химической реакции при постоянной концентрации на стенке и гетерогенной химической реакции. Собственные значения затабулированы, а собственные функции представлены аналитически в виде сходящейся гипергеометрической функции.