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Forced Convection in Three-Dimensional Flows: I. Asymptotic Solutions for Fixed Interfaces

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In geometrically complicated flows it is seldom feasible to solve the energy or diffusion equation exactly. However, in laminar flows with a sufficiently high Prandtl or Schmidt number, the thermal or diffusional effects become localized in thin boundary layers and can be predicted analytically in some detail. Lighthill (*1*), Levich (*2*), and Acrivos (*3, 4*) have given solutions of this type for systems of arbitrary two-dimensional or axially symmetric form. Here the same basic technique is extended to three-dimensional systems with any number of interfaces. The results may be used either for prediction of transfer behavior a priori, or as guides in correlation of experimental data.

The present treatment is for fixed interfaces, but can also be applied to moving ones under certain conditions. Thus, rigid-body translation and rotation of any interface can be handled without modification of the formulae if the boundary layer is at steady state when viewed from the moving interface. More general types of surface motion will be considered in a subsequent paper.

Only steady, laminar flows are considered here. No attempt is made to treat the flow in a laminar sublayer of a turbulent stream; sublayers exhibit a fluctuating motion to which the present analysis does not apply.

The main assumptions in the present treatment are as follows:

1. The heat-conduction and diffusion fluxes in the fluid are assumed to be directed along the normal to the neighboring interface; the flux components parallel to the interface are neglected.

2. The tangential fluid velocity in the thermal or diffusional boundary layer is assumed to be proportional to the distance from the interface.

3. The thermal or diffusional boundary-layer thickness is assumed to be small with respect to the local radii of curvature of the interface, and small enough that neighboring thermal or diffusional boundary layers do not significantly overlap. The energy or diffusion equation can then be solved near each interface as if no other interfaces were present.

The above assumptions hold asymptotically with increasing Prandtl or Schmidt number under given laminar-flow conditions except near points of flow separation or of discontinuity in the solutions. The results are frequently accurate down to Prandtl or Schmidt numbers less than unity. Detailed criteria of accuracy will be given later.

This paper is mainly concerned with general results rather than specific applications. Some general solutions are first derived for heat transfer in a pure fluid, and the corresponding results for diffusion are then indicated by analogy. Criteria of accuracy are then discussed, and some illustrative applications are given.

BASIC EQUATIONS FOR ENERGY TRANSPORT

Consider a pure fluid of constant density ρ, viscosity μ, heat capacity C_p, and thermal conductivity k in steady flow along a fixed surface. The steady state energy equation with radiation and dissipation neglected

$$(\mathbf{v} \bullet \nabla T) = \alpha \nabla^2 T \qquad (1)$$

is to be simplified according to assumptions 1 to 3.

The choice of coordinates is crucial. The present analysis is based on curvilinear coordinates x, y, z, where y is the distance from the surface along its local normal, x is measured along the surface following the adjacent streamlines, and z is measured along the surface perpendicular to the adjacent streamlines. In the boundary-layer region where assumption 3 holds, these coordinates are essentially orthogonal, so that

$$(ds)^2 = (h_x dx)^2 + (h_y dy)^2 + (h_z dz)^2 \qquad (2)$$

where ds is the distance between the points (x, y, z) and $(x + dx, y + dy, z + dz)$. Here h_y is unity, whereas h_x and h_z may depend on x and z. An elementary discussion of orthogonal curvilinear coordinates is given by Hildebrand (5).

Now in the region near the surface, the velocity components may be expressed as truncated Taylor series valid for Newtonian or non-Newtonian flow:

$$v_x = y\,\beta(x, z) \qquad + O(y^2) \qquad (3)$$

$$v_y = v_0(x, z) + y^2\,\gamma(x, z) \qquad + O(y^3) \qquad (4)$$

$$v_z = 0 \qquad + O(y^2) \qquad (5)$$

with

$$\gamma = -\frac{1}{2h_x h_z}\frac{\partial}{\partial x}(h_z\beta) \qquad (6)$$

These velocity components satisfy the continuity equation for constant density

$$(\nabla \bullet \mathbf{v}) = \frac{1}{h_x h_y h_z}\left[\frac{\partial}{\partial x}(h_y h_z v_x) + \frac{\partial}{\partial y}(h_x h_z v_y) + \frac{\partial}{\partial z}(h_x h_y v_z)\right] = 0 \qquad (7)$$

to the first degree in y when h_x, h_y, and h_z are evaluated as described above. The flow near the surface is thus described by the functions $\beta(x, z)$ and $v_0(x, z)$ together with the shape of the coordinate grid. The function $\beta(x, z)$ is proportional to the surface shear stress; it vanishes at points of stagnation or separation and is positive elsewhere. The function $v_0(x, z)$ is the fluid velocity through the interface; it is needed to describe vaporization, melting, transpiration, and other mass transfer processes which may accompany heat transfer in pure fluids.

Equation (1) can now be simplified. On physical grounds one knows that as $\alpha \to 0$, the nonseparated thermal boundary layer becomes thin and Equations (3), (4), and (5) accurately describe the flow conditions therein. Also, within the thermal boundary layer, the derivatives of T with respect to y become infinite as $\alpha \to 0$; thus, if the derivatives with respect to distance in the x and z directions remain locally finite, assumption 1 holds and $\nabla^2 T / (\partial^2 T/\partial y^2) \to 1$. The energy equation then reduces to

$$\frac{y\beta}{h_x}\frac{\partial T}{\partial x} + (v_0 + \gamma y^2)\frac{\partial T}{\partial y} = \alpha\frac{\partial^2 T}{\partial y^2} \qquad (8)$$

for a thin thermal boundary layer on a fixed surface.

The simplification of $\nabla^2 T$ employed here greatly facilitates the analysis, but causes discontinuities of the resulting T-function or its derivatives to appear in certain parts of the boundary layer whenever such discontinuities are present on the wall. The boundary-layer discontinuities are easily located by inspection of the solutions, which retain their asymptotic validity (for $\alpha \to 0$) except at the discontinuities.

The energy equation is now in two-dimensional form, since no derivatives with respect to z appear in Equation (8). The equation can therefore be integrated at constant z, and the complete solution for the given surface can be obtained by varying z. This integration is done in the next four sections for various boundary conditions and any sufficiently differentiable positive function $\beta(x, z)$.

SOLUTION FOR STEP CHANGE IN SURFACE TEMPERATURE

Consider a surface for which the following thermal conditions apply:

$$\text{At } y >> \delta_T(x, z),\ T = T_\infty \qquad (9)$$

$$\text{At } y = 0 \text{ and } x > x_1(z),\ T = T_0 = \text{constant} \qquad (10)$$

Here δ_T is a thermal boundary-layer thickness, and $x_1(z)$ is a single-valued function of z so that no streamline enters the heat transfer region more than once.

From Equation (8) it is clear that the function $v_0(x, z)$ will appear in the solution. This function is left free for the moment and a solution is sought in the form

$$(T - T_0)/(T_\infty - T_0) = \Pi_T\,(\eta_T) \qquad (11)$$

where

$$\eta_T = y/\delta_T(x, z) \qquad (12)$$

Equation (8) then becomes

$$\left[\frac{v_0\,\delta_T}{\alpha} + \eta_T^2\left(-\frac{\delta_T^2\beta}{\alpha h_x}\frac{\partial\delta_T}{\partial x} + \frac{\delta_T^3\gamma}{\alpha}\right)\right]\frac{d\Pi_T}{d\eta_T} = \frac{d^2\Pi_T}{d\eta_T^2} \qquad (13)$$

and the boundary conditions on T give

$$\Pi_T(\infty) = 1 \qquad \Pi_T(0) = 0 \qquad (14), (15)$$

Now from Equation (13) one sees that the transformation assumed in Equation (11) holds only if the following quantities are independent of x in the region $x > x_1(z)$:

$$v_0\delta_T/\alpha = C_T \qquad (16)$$

TABLE 1. DIMENSIONLESS FUNCTIONS FOR DIFFUSION AND HEAT TRANSFER DERIVED FROM EQUATION (21)

$\phi \frac{\delta}{\delta^0}$	$\Pi'(0)$	R	$\theta \frac{\delta}{\delta^0}$	$\phi \frac{\delta}{\delta^0}$	$\Pi'(0)$	R	$\theta \frac{\delta}{\delta^0}$
+0.00	1.1198	0.0	1.0000	—0.00	1.1198	0.0	1.0000
0.10	1.0574	0.1059	0.9443	—0.10	1.1842	—0.0946	1.0575
0.20	0.9970	0.2246	0.8903	—0.20	1.2504	—0.1791	1.1166
0.30	0.9385	0.3580	0.8381	—0.30	1.3185	—0.2548	1.1774
0.40	0.8821	0.5078	0.7877	—0.40	1.3884	—0.3226	1.2398
0.50	0.8278	0.6764	0.7392	—0.50	1.4601	—0.3835	1.3038
0.60	0.7755	0.8665	0.6925	—0.60	1.5335	—0.4382	1.3694
0.70	0.7253	1.0808	0.6476	—0.70	1.6085	—0.4873	1.4364
0.80	0.6771	1.3230	0.6047	—0.80	1.6852	—0.5316	1.5048
0.90	0.6311	1.5970	0.5636	—0.90	1.7633	—0.5716	1.5746
1.00	0.5872	1.9072	0.5243	—1.00	1.8430	—0.6076	1.6458
1.10	0.5453	2.2590	0.4870	—1.10	1.9242	—0.6402	1.7183
1.20	0.5055	2.6584	0.4514	—1.20	2.0067	—0.6696	1.7920
1.30	0.4678	3.1124	0.4177	—1.30	2.0906	—0.6964	1.8669
1.40	0.4320	3.6291	0.3858	—1.40	2.1758	—0.7206	1.9429
1.50	0.3982	4.2181	0.3556	—1.50	2.2622	—0.7425	2.0201
1.60	0.3664	4.8901	0.3272	—1.60	2.3498	—0.7625	2.0983
1.70	0.3365	5.6579	0.3005	—1.70	2.4385	—0.7807	2.1776
1.80	0.3084	6.5363	0.2754	—1.80	2.5284	—0.7972	2.2578
1.90	0.2821	7.5424	0.2519	—1.90	2.6192	—0.8123	2.3389
2.00	0.2576	8.6963	0.2300	—2.00	2.7111	—0.8261	2.4209
2.50	0.1586	17.654	0.1416	—2.50	3.1837	—0.8794	2.8430
3.00	0.0929	36.144	0.0830	—3.00	3.6750	—0.9142	3.2817
4.00	0.0276	162.03	0.0247	—4.00	4.6979	—0.9535	4.1951
∞	0.0	∞	0.0	—∞	∞	—1.0	∞

and

$$\frac{\delta_T^2\beta}{\alpha h_x}\frac{\partial \delta_T}{\partial x} + \frac{\delta_T^3}{2\alpha h_x h_z}\frac{\partial}{\partial x}(h_z\beta) = C_0 \qquad (17)$$

A constant value of C_T in Equation (16) requires that the interfacial mass flux vary inversely with the boundary-layer thickness; it also leads to a constant ratio of the interfacial heat and mass fluxes in a given system as will be seen later. Thus the boundary condition C_T = constant leads to simple and physically interesting results. The value of C_T indicates the direction and intensity of mass transfer.

The constant C_0 can be assigned any positive value. Setting $C_0 = 3$ and integrating Equation (17) with $\delta_T^2 h_z\beta = 0$ at $x = x_1(z)$ gives

$$\delta_T = \frac{1}{\sqrt{h_z\beta}}\left\{9\alpha\int_{x_1(z)}^{x}\sqrt{h_z\beta}\,h_x h_z dx\right\}^{1/3} \qquad (18)$$

Equation (13) then becomes

$$(C_T - 3\eta_T^2)\frac{d\Pi_T}{d\eta_T} = \frac{d^2\Pi_T}{d\eta_T^2} \qquad (19)$$

Integration of this equation under the above boundary conditions gives the dimensionless temperature profile

$$\Pi_T = \frac{\int_0^{\eta_T}\exp(C_T\eta_T - \eta_T^3)\,d\eta_T}{\int_0^{\infty}\exp(C_T\eta_T - \eta_T^3)\,d\eta_T} \qquad (20)$$

and the dimensionless temperature gradient at the interface:

$$\Pi'_T(0) = \left[\int_0^{\infty}\exp\ (C_T\eta_T - \eta_T^3)\,d\eta_T\right]^{-1} \qquad (21)$$

Some profiles of Π_T are plotted in Figure 1 and some values of $\Pi'_T(0)$ are given in Table 1 for various values of the parameter $\phi_T\delta_T/\delta_T^0 = C_T\Gamma(4/3)$. Analogous results hold for diffusion as will be shown later. Table 1 is an extension of results derived originally by Stewart (6, 7, 8) and independently by Merk (9) for the flat-plate geometry at high Prandtl or Schmidt number.

Table 1 provides a convenient basis for three-dimensional heat transfer calculations at finite mass transfer rates. The conductive heat flux into the fluid at any point on the interface is given by

$$q_0 = -k\left.\frac{\partial T}{\partial y}\right|_{y=0} = \frac{k}{\delta_T}(T_0 - T_\infty)\,\Pi'_T(0) \qquad (22)$$

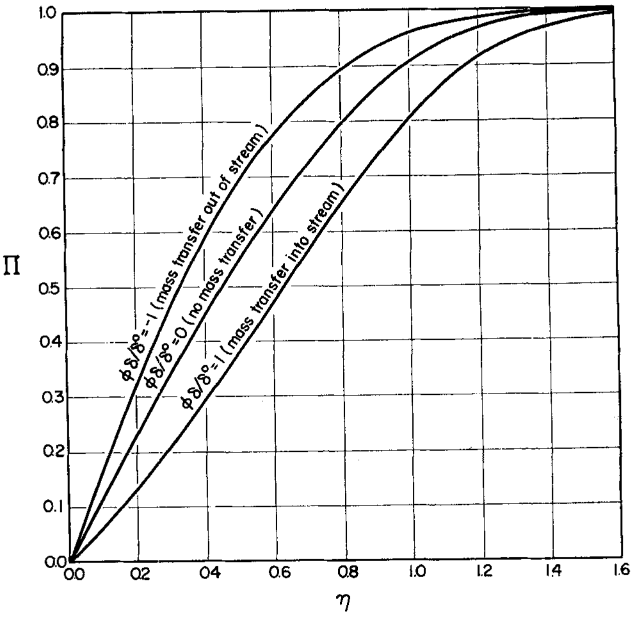

Fig. 1. Boundary-layer temperature or concentration profiles according to Equation (20).

and $\Pi'_T(0)$ is obtainable from the table if either the quantity $\phi_T\delta_T/\delta_T^0$, or the flux ratio (*8*)

$$R_T = \frac{v_0\rho\hat{C}_p(T_0 - T_\infty)}{q_0} = \frac{w_0\hat{C}_p(T_0 - T_\infty)}{Q} \qquad (23)$$

is known. The quantity ϕ_T is used to simplify calculations when the heat transfer coefficient h^0 at zero mass transfer rate is known; the quantity δ_T can then be expressed as (δ_T/δ_T^0) 1.1198 k/h^0 to avoid dealing with Equation (18). The ratio δ_T/δ_T^0 is close to unity for high Prandtl numbers and finite ϕ_T or for lower Prandtl numbers when $/\phi_T/ << 1$; for closer estimation the ratio may be taken as $(\beta^0/\beta)^{1/3} = \theta_v^{-1/3}$ from the flat-plate solutions in reference *8*.

The rate of heat loss from a given surface region may be found by integration of $q_0h_xh_z\,dxdz$ over the region or by a boundary-layer energy balance. The result for a region of the form $x_1(z) < x < x_2(z)$, $z_I < z < z_{II}$, is

$$Q = \frac{3^{1/3}k}{2\alpha^{1/3}}(T_0 - T_\infty)\,\Pi'_T(0)\int_{z_I}^{z_{II}} \left\{\int_{x_1(z)}^{x_2(z)} \sqrt{h_z\beta}h_xh_zdx\right\}^{2/3} dz \qquad (24)$$

This equation, together with Table 1, gives the heat transfer rate as a function of the fluid properties, the mass transfer rate, the velocity profiles, and the geometry of the heat transfer surface. This equation provides useful predictions, as will be shown later, even if one does not carry out the integration explicitly.

The results in this section confirm several known solutions for heat transfer or diffusion in special geometries. Thus, for two-dimensional systems one sets $h_x = h_z = 1$, and with appropriate substitutions for β in Equations (18) and (24) one obtains the results of Stewart (*6, 7, 8*), Merk (*9*), Spalding and Evans (*10*), and Acrivos (*4*) for boundary-layer flows at high Prandtl or Schmidt numbers in the presence of mass transfer. The results of Lévêque (*11*) for heat transfer in the Poiseuille flow, and of Levich (*2, 13*), Natanson (*12, 13*), and Acrivos and Taylor (*14*) for creeping flows with high Prandtl or Schmidt numbers are also obtainable by suitably restricting h_x, h_z, and β. Some new predictions will be given at the end of this paper.

SOLUTION WITH GIVEN SURFACE TEMPERATURE DISTRIBUTION

The results obtained above can be superimposed to get the solution when the surface has the temperature T_∞ for $x \leqq 0$ and a given temperature distribution $T_0(x, z)$ for $x > 0$. The resulting temperature profile for positive x and $v_0 = 0$ is

$$T(x, y, z) - T_\infty = \int_{0_-}^{x} (1 - \Pi_T)\Big|_{x,z,x_1=\xi} dT_0(\xi, z) \qquad (25)$$

where the integrand is found from Equations (12), (18), and (20) with $x_1 = \xi$ and $C_T = 0$. The corresponding expression for the conductive heat flux at the wall is

$$q_0 = \frac{k}{\Gamma(4(/3)}\int_{0-}^{x}\frac{1}{\delta_T}\Big|_{x,z,x_1=\xi} dT_0(\xi, z) = \frac{k\sqrt{h_z\beta}}{(9\alpha)^{1/3}\Gamma(4/3)} \int_{0_-}^{x}\left\{\int_{\xi}^{x}\sqrt{h_z\beta}\,h_xh_zdx\right\}^{-1/3} dT_0(\xi, z) \qquad (26)$$

in which $1/\Gamma(4/3) = 1.1198\ldots$ is the value of $\Pi'_T(0)$ at $\phi_T = 0$. For two-dimensional flows Equation (25) reduces to a solution previously given by Acrivos (*3*). The lower limit of x is taken on the negative side of $x = 0$ to insure that any step change in wall temperature will be properly included.

The total rate of heat conduction from the surface region $0 < x < x_2(z)$, $z_I < z < z_{II}$ may be found by integration of Equation (26) over the surface, or by a boundary-layer energy balance using Equation (25). The result in either case is

$$Q = \frac{3^{1/3}k}{2\Gamma(4/3)\alpha^{1/3}}\int_{z_I}^{z_{II}}\int_{\xi=0_-}^{x_2(z)} \left\{\int_{x=\xi}^{x_2(z)}\sqrt{h_z\beta}h_xh_zdx\right\}^{2/3} dT_0(\xi, z)dz \qquad (27)$$

which shows the dependence of Q on the fluid properties, the velocity profiles, the surface geometry and the surface temperature distribution. For two-dimensional systems Equation (27) reduces to the well-known Lighthill formula (*1*).

For flows with significant mass transfer rates the results of the previous section cannot be superimposed, because the distributions of v_0 required by Equation (16) differ markedly for different values of x_1. However, Equation (25) may be used with little error if $|v_0\delta_T(x, z, x_1 = 0)/\alpha| << 1$ in the region of integration. Then if one computes the surface heat flow by Fourier's law, Equations (26) and (27) are obtained as approximations for small v_0. On the other hand, if one computes the surface heat flow by a boundary-layer energy balance, the following alternate equations are obtained for small v_0:

$$q_0 + v_0\rho\hat{C}_p(T_0 - T_\infty) \doteq \frac{k\sqrt{h_z\beta}}{(9\alpha)^{1/3}\Gamma(4/3)}\int_{0_-}^{x} \left\{\int_{\xi}^{x}\sqrt{h_z\beta}h_xh_zdx\right\}^{-1/3} dT_0(\xi, z) \qquad (26a)$$

and

$$Q + w_0\hat{C}_p(\bar{T}_0 - T_\infty) \doteq \frac{3^{1/3}k}{2\Gamma(4/3)\alpha^{1/3}}\int_{z_I}^{z_{II}}\int_{\xi=0_-}^{x_2(z)} \left\{\int_{\xi}^{x_2(z)}\sqrt{h_z\beta}h_xh_zdx\right\}^{2/3} dT_0(\xi, z)dz \qquad (27a)$$

Evidently Equations (26*a*) and (27*a*) differ from (26) and (27) by the bulk flow terms $v_0\rho\hat{C}_p(T_0 - T_\infty)$ and $w_0\hat{C}_p(\bar{T}_0 - T_\infty)$, respectively, which correspond approximately to the uncertainties of these equations. A closer approximation to the heat flow is expected if one uses Equation (26*a*) or (27*a*) with the bulk flow term multiplied by 0.566; this gives q_0 or Q within 0.7% for $|\phi_T| < 0.25$ under the conditions of the previous section if β is corrected for the effect of v_0.

SOLUTION FOR A LINE HEAT SOURCE

The results of the previous section are convenient to apply only if the surface temperature distribution $T_0(x, z)$ is given. The inverse problem with given heat flux distribution $q_0(x, z)$ and unknown $T_0(x, z)$ is easily solved, however, if one has the solution for a line heat source on the surface. The boundary conditions for the line-source problem are conveniently written as follows:

At $y >> \delta_T(x, z)$, $\quad T = T_\infty \quad$ (28)
At $y = 0$, $\quad q_0h_xh_z = \delta(x - x_1(z)) \quad$ (29)
At $y = 0$, $\quad v_0 = 0 \quad$ (30)

That is, a line heat source is distributed as a Dirac δ-function across the line $x = x_1(z)$, the surface is insulated everywhere else, and there is no mass transfer. The function $x = x_1(z)$ is single-valued as in Equation (10).

Equation (8) can be solved under these boundary conditions by a modification of the combination of variables previously given:

$$T - T_\infty = (T_0 - T_\infty) g(\eta_T) \tag{31}$$

Here the coordinate η_T is the same as before, but $(T_0 - T_\infty)$ is now a function of x and z. The latter function can be eliminated by writing an energy balance across the line source for the fluid flowing between z and $z + dz$:

$$\int_{0_-}^{x} q_0 h_x h_z dx = \int_0^\infty \rho\hat{C}_p (T - T_\infty) v_x h_z \Big|_{x,z} dy \tag{32}$$

Here the boundary condition in Equation (28) has been used to obtain the right-hand integral. Integration with the aid of Equations (3), (29), and (31) gives, for the region downstream of the source,

$$1 = \rho\hat{C}_p \delta^2 \beta h_z (T_0 - T_\infty) \Big|_{x,z} \int_0^\infty g \eta_T d\eta_T \tag{33}$$

in which the integral is, by definition, independent of x and z. Insertion of Equations (31) and (33) in Equation (8) then gives the differential equation for $g(\eta_T)$:

$$-6\, g \eta_T - 3\eta_T^2 \frac{dg}{d\eta_T} = \frac{d^2 g}{d\eta_T^2} \tag{34}$$

The boundary conditions that correspond to Equations (29) and (31) are

$$\text{At } \eta_T = 0, \quad \frac{dg}{d\eta_T} = 0 \text{ and } g = 1 \quad (35),\ (36)$$

and the solution of Equation (34) with these boundary conditions is

$$g = \exp(-\eta_T^3) \tag{37}$$

Insertion of this result in Equations (31) and (33) gives the complete temperature distribution downstream of the source:

$$T - T_\infty = \frac{\exp(-\eta_T^3)}{\frac{1}{3}\Gamma\left(\frac{2}{3}\right) \rho\hat{C}_p \beta h_z \delta_T^2} \tag{38}$$

Here δ_T and η_T are given by Equations (12) and (18) as before.

This development is easily extended to include mass transfer downstream of the heat source, provided that $v_0\delta_T/\alpha$ is independent of x for $x > x_1(z)$. The surface heat flux q_0 in Equations (29) and (32) is then replaced by the surface energy flux $q_0 + v_0\rho\hat{C}_p(T_0 - T_\infty)$, and the final solution for the temperature is

$$T - T_\infty = \frac{\exp(C_T\eta_T - \eta_T^3)}{\rho\hat{C}_p \beta h_z \delta_T^2 \int_0^\infty \exp(C_T\eta_T - \eta_T^3)\eta_T d\eta_T} \tag{38a}$$

in which C_T is again constant for $x > x_1(z)$.

SOLUTION WITH GIVEN SURFACE HEAT FLUX DISTRIBUTION

Now if the temperature is constant at T_∞ for $x \leqq 0$, and if the surface heat flux $q_0(x, z)$ is a given function for $x > 0$, the temperature distribution for $v_0 = 0$ may be found by the superposition formula

$$T(x, y, z) - T_\infty = \int_{0_-}^{x} (T - T_\infty)\Big|_{x_1 = \xi} (q_0 h_x h_z)\Big|_{\xi} d\xi \tag{39}$$

where the temperature function inside the integral is that given in Equation (38). In particular, the wall temperature distribution is given by

$$T_0(x, z) - T_\infty = \frac{1}{\frac{1}{3}\Gamma\left(\frac{2}{3}\right)\rho\hat{C}_p(9\alpha)^{2/3}} \int_{0_-}^{x} \left[\int_{\xi}^{x} \sqrt{h_z\beta} h_z h_x dx\right]^{-2/3} (q_0 h_x h_z)\Big|_{\xi} d\xi \tag{40}$$

which is the inverse of Equation (26).

For flows with slow mass transfer, Equations (39) and (40) can be used as approximations. The limitation, as in Equations (25) to (27*a*), is that $|v_0\delta_T(x, z, x_1 = 0)/\alpha|$ should be small compared with unity in the region of integration. The modification corresponding to Equation (26*a*) is Equation (40) with q_0 replaced by $q_0 + v_0\rho C_p(T_0 - T_\infty)$; the latter quantity is more readily specified than q_0 in many problems.

SOLUTIONS FOR ISOTHERMAL BINARY DIFFUSION

In diffusional systems the density usually varies with the composition so that the usual concept of incompressibility does not apply. However, if there are no volume changes owing to mixing, a simple treatment can still be given.

Consider an isothermal stream composed of chemical species A and B. A convenient equation of state is provided by the identity

$$c_A\overline{V}_A + c_B\overline{V}_B = 1 \tag{41}$$

in which the partial molar volumes $\overline{V}_A$ and $\overline{V}_B$ will be assumed constant. Such a linear relation between c_A and c_B holds in any isothermal binary system at constant pressure, at least for moderate changes in composition. For ideal gases it holds over the whole composition range.

The equation of continuity of either species in the mixture, in the absence of homogeneous chemical reactions, is

$$\frac{\partial c_i}{\partial t} + (\nabla \bullet \mathbf{N}_i) = 0 \tag{42}$$

Multiplying Equation (42) by $\overline{V}_i$ and summing on i gives

$$\frac{\partial}{\partial t}(c_A\overline{V}_A + c_B\overline{V}_B) + (\nabla \bullet (\mathbf{N}_A\overline{V}_A + \mathbf{N}_B\overline{V}_B)) = 0 \tag{43}$$

Now if one defines

$$\mathbf{v}^{\blacksquare} = \mathbf{N}_A\overline{V}_A + \mathbf{N}_B\overline{V}_B \tag{44}$$

then Equations (41) and (43) give

$$(\nabla \bullet \mathbf{v}^{\blacksquare}) = 0 \tag{45}$$

which is similar to the incompressibility condition given in Equation (7) for a pure fluid. The quantity $\mathbf{v}^{\blacksquare}$ is known as the *volume average velocity* (8).

When the diffusion is referred to the velocity $\mathbf{v}^{\blacksquare}$, Fick's law becomes (8)

$$\mathbf{N}_A = c_A\mathbf{v}^{\blacksquare} - \mathcal{D}_{AB}\nabla c_A \tag{46}$$

Insertion of this expression in Equation (42) gives, for constant $\mathcal{D}_{AB}$,

$$\partial c_A/\partial t + (\mathbf{v}^{\blacksquare} \bullet \nabla c_A) = \mathcal{D}_{AB}\nabla^2 c_A \tag{47}$$

and for steady state this becomes similar to Equation (1).

The analysis in section 2 can now be restated in diffusional terms. The components of the velocity $\mathbf{v}^{\blacksquare}$ near the surface $y = 0$ are

$$v_x^{\blacksquare} = y\beta(x, z) \qquad + O(y^2) \tag{48}$$

$$v_y^{\blacksquare} = v_0^{\blacksquare} + y^2\gamma(x, z) \quad + \quad O(y^3) \tag{49}$$

$$v_z^{\blacksquare} = 0 \quad + O(y^2) \tag{50}$$

in which $v_0^{\blacksquare} = N_{A0}\overline{V}_A + N_{B0}\overline{V}_B$. It should be noted that under assumption 1 the diffusion velocities in the x and z directions are neglected, so that $v_x^{\blacksquare}$ and $v_z^{\blacksquare}$ may be equated with the corresponding mass-average velocity components. Application of Equation (45) gives the same result for γ as before, namely, Equation (6).

The boundary-layer diffusion equation can now be obtained by arguments analogous to those given for Equation (8). The result is

$$\frac{y\beta}{h_x}\frac{\partial c_A}{\partial x} + [v_0^{\blacksquare} + \gamma y^2]\frac{\partial c_A}{\partial y} = \mathcal{D}_{AB}\frac{\partial^2 c_A}{\partial y^2} \tag{51}$$

for steady state diffusion and sufficiently small $\mathcal{D}_{AB}$.

Solutions of Equation (51) can be obtained by analogy from the corresponding solutions of Equation (8). The following notational changes are required.

$$\begin{gathered}
T \rightarrow c_A \\
\alpha \rightarrow \mathcal{D}_{AB} \\
\mathrm{k} \rightarrow \mathcal{D}_{AB} \\
\rho\hat{C}_p \rightarrow 1 \\
v_0 \rightarrow N_{A0}\overline{V}_A + N_{B0}\overline{V}_B \\
q_0 \rightarrow N_{A0} - c_{A0}(N_{A0}\overline{V}_A + N_{B0}\overline{V}_B) \\
Q \rightarrow \mathcal{W}_{A0} - \overline{c_{A0}}(\mathcal{W}_{A0}\overline{V}_A + \mathcal{W}_{B0}\overline{V}_B) \\
q_0 + v_0\rho\hat{C}_p(T_0 - T_\infty) \rightarrow N_{A0} - c_{A\infty}(N_{A0}\overline{V}_A + N_{B0}\overline{V}_B) \\
Q + w_0\hat{C}_p(\overline{T_0} - T_\infty) \rightarrow \mathcal{W}_{A0} - c_{A\infty}(\mathcal{W}_{A0}\overline{V}_A + \mathcal{W}_{B0}\overline{V}_B) \\
\text{Subscript } T \rightarrow \text{Subscript } AB
\end{gathered} \tag{52}$$

The presence of two chemical species in the diffusional problems makes it necessary to specify an additional boundary condition at the wall. Thus, in transcribing Equations (9) to (24) to diffusion, one must set

$$N_{A0}/N_{B0} = \text{constant} \tag{53}$$

so that the diffusional flux ratio

$$R_{AB} = \frac{(N_{A0}\overline{V}_A + N_{B0}\overline{V}_B)(c_{A0} - c_{A\infty})}{N_{A0} - c_{A0}(N_{A0}\overline{V}_A + N_{B0}\overline{V}_B)} \tag{54}$$

will be independent of x as the analogous quantity R_T was for pure-fluid heat transfer. Equation (53) must also be applied in transcribing Equation (38a), in order that $N_{A0} - c_{A\infty}(N_{A0}\overline{V}_A + N_{B0}\overline{V}_B)$ vanish downstream of the line source. In transcribing results for $v_0 = 0$, Equation (53) again applies with the constant equal to $-\overline{V}_B/\overline{V}_A$. The only exceptions to Equation (53) arise in using the superposition formulae as approximations for small values of $v_0^{\blacksquare}$; in those equations N_{A0}/N_{B0} need not be constant, but knowledge of N_{A0}/N_{B0} or $\mathcal{W}_{A0}/\mathcal{W}_{B0}$ is still needed to obtain a solution.

Other diffusional notations which lead to exact analogies with heat transfer are obtainable from Equations (41) to (54) by placing restrictions on $\overline{V}_A$ and $\overline{V}_B$. Thus, if $\overline{V}_A = \overline{V}_B$, then c is constant, and the notations can be simplified slightly by introducing the mole fraction $x_A = c_A/c$; whereas if $\overline{V}_A/M_A = \overline{V}_B/M_B$, then ρ is constant, and the use of the mass fraction $\omega_A = c_AM_A/\rho$ is appropriate. The former condition holds accurately for gases at moderate, constant pressure; neither condition is commonly met in liquids.

CRITERIA OF ACCURACY

The validity of assumptions 1 to 3 will be analyzed here for the solution shown in Figure 1. The criteria thus found can be adapted to other boundary conditions by the superposition method.

It is convenient to define a local boundary-layer thickness, $\delta_{0.99}$, as the value of y for which $\Pi = 0.99$ in Figure 1. For moderate values of ϕ this thickness is about 1.5δ, where δ is given by Equation (18) or its diffusional analog. Then assumptions 1 to 3 may be considered valid if $\delta_{0.99}$ is a sufficiently small and slowly varying function of position. It is estimated that Equations (22) and (24) (or their diffusional counterparts) will match the corresponding solutions of Equation (1) or (47) within about 5% in regions over which the following inequalities hold

$$\left|\frac{\delta}{h_xh_z}\frac{\partial}{\partial x}\left(\frac{h_z}{h_x}\frac{\partial\delta}{\partial x}\right)\right| < 0.01 \tag{55}$$

$$\left|\frac{\delta}{h_xh_z}\frac{\partial}{\partial z}\left(\frac{h_x}{h_z}\frac{\partial\delta}{\partial z}\right)\right| < 0.01 \tag{56}$$

$$\left|\frac{v_x}{\beta y} - 1\right| < 0.2 \text{ for } 0 < y < \delta_{0.99} \tag{57}$$

$$\delta_{0.99}\left|\frac{1}{r_1} + \frac{1}{r_2}\right| < 0.1 \tag{58}$$

and where there are no neighboring boundary layers, wakes, or discontinuities in the solution within a distance $\delta_{0.99}$ of the given region. In measuring distance from a discontinuity, $\delta_{0.99}$ is taken as the larger of the adjoining boundary-layer thicknesses. Here Equations (55) and (56) are obtained by integrating ∇^2T in the y-direction and applying assumption 1; Equations (57) and (58) come from assumptions 2 and 3. The quantities r_1 and r_2 are the y-coordinates of the principal centers of curvature of the surface evaluated locally.

The solutions in Equations (20) and (38) are continuous with respect to y, but predict step changes in T, ∇T or ∇^2T with respect to x or z under certain conditions. Such step changes may occur at $x = x_1(z)$, and will occur at any value of z for which x_1, ∇x_1, or ∇^2x_1 is discontinuous. There are no other discontinuities as long as the surface curvature remains finite and a physically reasonable (smooth) β function is used. Thus, for example, if one specified $x_1 = 0$ for $z < 0$ and $x_1 = 1$ for $z > 0$, the solution for T would be continuous except across $x = x_1(z)$ and across the surface $z = 0$. The superposition solutions, on the other hand, are completely continuous as long as the surface curvature is finite and the surface temperature distribution is smooth. The behavior of the diffusional solutions is analogous.

The solutions given here can often be combined with a dimensional analysis and experimental measurements, as in the concluding example, to avoid the need for velocity-profile information. However, more detailed calculations are possible if the velocity profiles are determined. This can be done either by measurement or by solving the equations of continuity and motion (8) under the given boundary conditions. Many methods for obtaining such solutions are now available. References *16 to 19* deal with creeping or developed rectilinear flows, *20 to 23* give boundary-layer methods for two-dimensional flow, and *23* gives a boundary-layer method for three-dimensional flow. It should be noted that most of the available methods are approximate, but high accuracy is not ordinarily needed because Equation (24) is not very sensitive to errors in β. Thus, if β were overestimated everywhere by 10%, the resulting error in Q would be only 3%. The effects of inaccuracy in the calculation of the x, z coordinate net are best studied by numerical calculations in each particular problem; in two-dimensional or axisymmetric flows no such inaccuracy need arise because the contours of constant z are then known and planar.

The range of applicability of the results varies with the geometry and boundary conditions. Thus, Equation (24) with $\phi_T = 0$ agrees within 5% with more complete heat transfer solutions for the Graetz-Nusselt problem (*8*) at $N_{Re}\, N_{Pr}\, D/L \geqq 20$, for laminar flow along an isothermal plate (*15*) at $N_{Pr} \geqq 0.3$, for two-dimensional stagnation flow (*15*) at $N_{Pr} \geqq 10$, and for creeping flow around an isothermal sphere at $N_{Re}\, N_{Pr} > 100$ or thereabouts (*13*). When the heat transfer or diffusion region is preceded by an insulated region on the same interface, the accuracy of the present theory is usually enhanced because Equation (3) then holds for larger values of y.

The dependence of the Nusselt number on the Prandtl number, if known for the given system, provides a simple test of the analysis. The present theory predicts a 1/3-power dependence of N_{Nu} on N_{Pr} for any fixed distribution of q_0 or T_0, and this holds accurately down to N_{Pr} of unity or less for many flow systems. Such a test is easier to apply than the criteria given earlier, though less complete.

EXAMPLES

Consider the developed laminar flow of a Newtonian fluid in a straight circular tube with a step change in wall temperature from T_∞ for $x < 0$ to T_0 for $x > 0$. Here the x-coordinate is measured parallel to the tube axis and the z-coordinate is measured around the inner circumference of the tube. With $h_x = h_z = 1$, and $\beta = 8 <v>/D$ for Poiseuille flow, Equation (18) gives

$$\delta_T = \left(\frac{9 \alpha D x}{8<v>} \right)^{1/3} \tag{59}$$

The local Nusselt number in the absence of mass transfer is thus found to be

$$\frac{q_0 D}{k(T_0 - T_\infty)} = \frac{D}{\delta_T}\, \Pi'(0) = 1.0767 \left(\frac{D^2 <v>}{\alpha x} \right)^{1/3} \tag{60}$$

which agrees with the result found by Lévêque (*11*). The mean Nusselt number over any section of the pipe can be found from Equation (24). The heat transfer rate in the presence of mass transfer can be predicted with the aid of Table 1.

Now suppose that the pipe wall temperature is T_∞ for $x < 0$, and position-dependent for $x \geqq 0$. Equation (26) then gives

$$q_0 = 1.1198\, k \left(\frac{8<v>}{9 \alpha D} \right)^{1/3} \int_{0_-}^{x} \frac{d\, T_0(\xi, z)}{(x - \xi)^{1/3}} \tag{61}$$

which can be integrated numerically or analytically when $T_0(x, z)$ is given. Thus, if the wall temperature increases linearly with x for $x > 0$ and is axially symmetric, then $dT_0(\xi, z) = (T_0(x) - T_\infty)(d\xi)/x$, and

$$q_0 = 1.1198 k \left(\frac{8<v>}{9 \alpha D} \right)^{1/3} \frac{T_0(x) - T_\infty}{x} \int_{0_-}^{x} \frac{d\xi}{(x - \xi)^{1/3}}$$

$$= \frac{1.615 k}{D} \left(\frac{D^2 <v>}{\alpha x} \right)^{1/3} (T_0(x) - T_\infty) \tag{62}$$

This gives a Nusselt-number expression of the same form as Equation (60) but with a 50% higher coefficient.

Next suppose that the surface heat flux is zero for $x < 0$ and constant at q_0 for $x \geqq 0$. Equation (40) then gives

$$(T_0(x) - T_\infty) = \frac{1}{0.45137\, \rho \hat{C}_p\, (9 \alpha)^{2/3}} \int_{0_-}^{x} \{ \sqrt{8<v>/D}\, (x - \xi) \}^{-2/3} q_0 d\xi \tag{63}$$

which leads to the Nusselt-number expression:

$$\frac{q_0 D}{k(T_0(x) - T_\infty)} = 1.302 \left(\frac{D^2 <v>}{\alpha x} \right)^{1/3} \tag{64}$$

This is consistent with the corresponding non-Newtonian solution given by Bird (*24*).

Equations (59) to (64) can also be applied to developed Newtonian or non-Newtonian flow in straight ducts of arbitrary uniform cross section, by changing $8<v>/D$ to $\beta(z)$ and redefining the characteristic length D.

As a final example, consider the creeping flow of a Newtonian fluid through a fixed bed of solid particles. One solid particle of characteristic dimension D_p is at temperature T_0 and all others are at T_∞. For creeping flow in a given geometry it is known that

$$\frac{\mathrm{v}}{V} = f \left(\frac{x}{D_p}, \frac{y}{D_p}, \frac{z}{D_p} \right) \tag{65}$$

in the absence of mass transfer, and that the shapes of the streamlines are independent of D_p, V, ρ and μ. Thus

$$\beta = \frac{V}{D_p} f_1 \left(\frac{x}{D_p}, \frac{z}{D_p} \right) \tag{66}$$

$$h_x = f_2 \left(\frac{x}{D_p}, \frac{z}{D_p} \right) \tag{67}$$

$$h_z = f_3 \left(\frac{x}{D_p}, \frac{z}{D_p} \right) \tag{68}$$

Equation (24) then gives the heat transfer solution

$$\frac{Q\, D_p}{A_p k (T_0 - T_\infty)} = c_1 \left(\frac{D_p V}{\alpha} \right)^{1/3} \tag{69}$$

where Q is the total rate of heat transfer from the particle to the fluid. The coefficient c_1 is given by

$$c_1 = \frac{3^{1/3}(1.1198)}{2} \frac{D_p^2}{A_p} \int_{z/D_p} \left\{ \int_{x/D_p} \sqrt{f_3 f_1}\, f_2 f_3\, d\frac{x}{D_p} \right\}^{2/3} d\frac{z}{D_p} \tag{70}$$

and is constant for creeping flow in a given packed-bed geometry. The region of integration here is the wetted surface of the particle.

Equation (69) and its diffusional analog should prove useful in correlation of transfer coefficients for packed beds. The constant c_1 is, of course, more easily obtained experimentally than from Equation (70). These results should apply also to simultaneous heat transfer from all particles in a shallow packed bed, if δ_T/D_p is sufficiently small. Further work on these points is in progress.

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NOTATION

A_p = characteristic area of solid particle
$\hat{C}_p$ = heat capacity at constant pressure ($E\, M^{-1}\, T^{-1}$)
C_T = dimensionless mass transfer rate, Equation (16)
c = $c_A + c_B$, total molar concentration (moles L^{-3})
c_A = molar concentration of species A (moles L^{-3})
c_{A0} = local concentration of A on the stream side of the interface

$\overline{c_{A0}}$ = average of c_{A0} for a given region on the interface
D = pipe diameter
D_p = characteristic particle size (L)
$\mathcal{D}_{AB}$ = mass diffusivity $(L^2 t^{-1})$
g = dimensionless function defined in Equation (31)
h = $q_0/(T_0 - T_\infty)$, local heat transfer coefficient $(Et^{-1}L^{-2}T^{-1})$
h^0 = value of h at $v_0 = 0$
h_x, h_y, h_z = scale factors defined in Equation (2); dimensions, see x, y, z
k = thermal conductivity $(Et^{-1}L^{-1}T^{-1})$
k_c = $\dfrac{N_{A0} - c_{A0}(N_{A0}\overline{V}_A + N_{B0}\overline{V}_B)}{(c_{A0} - c_{A\infty})}$, diffusional transfer coefficient (Lt^{-1})
$k_c{}^0$ = value of k_c at $N_{A0} \rightarrow 0$ and $N_{B0} \rightarrow 0$
L = length of heat transfer region in pipe
M_A = molecular weight of A
$\mathbf{N}_A$ = vector flux of species A relative to the x-y-z coordinates (moles $L^{-2}t^{-1}$)
N_{A0} = local mass transfer rate into the stream
= y-component of $\mathbf{N}_A$ at $y = 0$
N_{Nu} = Nusselt number
N_{Re} = Reynolds number
N_{Pr} = Prandtl number
$O(y^2)$ = function of second or higher degree in y
Q = rate of heat conduction into the stream from a given interfacial region $(E\,t^{-1})$
q_0 = conductive heat flux into the stream at the interface $(E\,L^{-2}t^{-1})$
R_T = dimensionless flux ratio for heat transfer; see Equation (23)
R_{AB} = dimensionless flux ratio for binary diffusion; see Equation (54)
T = temperature
T_0 = local temperature at the interface
$\overline{T_0}$ = average of T_0 for a given region on the interface
t = time
V = superficial velocity in packed bed $(L\,t^{-1})$
$\overline{V}_A$ = partial molar volume of species $A (L^3\ \text{mole}^{-1})$
$\langle v \rangle$ = mean velocity over cross section of pipe $(L\,t^{-1})$
$\mathbf{v}$ = velocity vector in pure fluid, or mass-average velocity vector in a mixture $(L\,t^{-1})$
v_x, v_y, v_z = physical components of $\mathbf{v}$ $(L\,t^{-1})$
v_0 = interfacial value of v_y
$\mathbf{v}^{\blacksquare}$ = volume-average velocity vector defined in Equation (44) $(L\,t^{-1})$
$v_x{}^{\blacksquare}, v_y{}^{\blacksquare}, v_z{}^{\blacksquare}$ = physical components of $\mathbf{v}^{\blacksquare}$ $(L\,t^{-1})$
$v_0{}^{\blacksquare}$ = interfacial value of $v_y{}^{\blacksquare}$
$\mathcal{W}_{A0}$ = molar rate of transfer of species A into the stream from a given interfacial region (moles t^{-1})
w_0 = mass rate of transfer of pure fluid into the stream from a given interfacial region $(M\,t^{-1})$
x, y, z = coordinates defined above Equation (2) $(L/h_x, L, L/h_z)$

Greek Letters

α = $k/\rho\hat{C}_p$, thermal diffusivity $(L^2\,t^{-1})$
β = function defined in Equation (3) (t^{-1})
$\Gamma(n)$ = gamma function of n
γ = function defined in Equation (4) $(L^{-1}t^{-1})$
δ = boundary-layer thickness for heat transfer or diffusion (L)
δ^0 = local value of δ at $v_0 \rightarrow 0$ for heat transfer, or $v_0{}^{\blacksquare} \rightarrow 0$ for diffusion (L)
δ_T = δ for heat transfer, given in Equation (18); for conversion to diffusion, see Equation (52)
$\delta_{0.99}$ = value of y when $\Pi = 0.99$
η = dimensionless coordinate defined in Equation (12)
θ = correction factor for effect of interfacial velocity on transfer coefficients (see below)
θ_T = h/h^0 (dimensionless)
θ_{AB} = $k_c/k_c{}^0$ (dimensionless)
μ = viscosity $(ML^{-1}t^{-1})$
ξ = dummy x-variable
Π = dimensionless temperature or composition. See Equations (11) and (52)
$\Pi'(0)$ = $d\Pi/d\eta|_{\eta=0}$
ρ = density (ML^{-3})
ϕ = dimensionless mass transfer rate (see below)
ϕ_T = $v_0\rho C_p/h^0$ for pure fluid heat transfer
ϕ_{AB} = $\dfrac{N_{A0}\overline{V}_A + N_{B0}\overline{V}_B}{k_c{}^0}$ for isothermal binary diffusion

Superscripts

0 = the condition $v_0 = 0$ for heat transfer, or $N_{A0} \rightarrow 0$ and $N_{B0} \rightarrow 0$ for binary diffusional transfer

Subscripts

0 = conditions in the stream at $y = 0$
∞ = conditions at $y >> \delta$
A = species A
B = species B
AB = diffusional variables not specific to either species
i = either species
T = thermal
v = velocity

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