Transport by convection. Coupling convection-diffusion

28 mars 2017

1 When can we neglect diffusion ?

When the Peclet number is not very small we cannot ignore the convection term in the transport equation. The first question that we might ask is : are there situations where we cannot completely ignore the diffusion term ? We have already mentioned that there are similarities between the transport equations for heat and mass and the equation of evolution of vorticity in a two dimensional flow of a newtonian fluid. We know that ignoring completely the viscosity of the fluid leads to non physical results for fluid flows : if we do not take into account the existence of viscous boundary layers, it is impossible to derive correctly the drag force on an object. There are many situations in transport of heat and mass where there are also boundary layers but for the temperature or concentration field and we will have to take into account the diffusion term (even at $Pe \gg 1$) to derive the heat and mass fluxes towards a solid boundary.

But before analyzing these boundary layer situations, let's go back to the question : when can we ignore the diffusion term ? Figure 1 illustrates the mixing of a dye within a liquid by a flow field, periodic in time, which is designed to produce alternative stretching and folding of the initial dye spot. The diffusion coefficient of the dye is so small (typical values are 10^{-9} or 10^{-10} m^2/s) that even if the dye is stretched in very thin filaments, the concentration contrast between the dyed and the undyed fluid remains very sharp. Eventually, but after a very long time, diffusion will play a role to smooth out the strong concentration gradients. At the beginning of this *mixing* process,we can ignore diffusion and analyze the problem by considering only the advection of fluid particles by the flow field. The design of flow fields which are able to stretch and fold an initially localized blob of material is crucial for the efficient mixing of liquids at low Reynolds number, either in microfluidic devices or in macroscopic mixers for very viscous fluids such as polymer melts. We will discuss these mixing strategies later, but for now we consider the interplay between convection and diffusion.

2 Coupling convection-diffusion

2.1 A simple problem : uniform velocity perpendicular to the concentration gradient

2.1.1 Simplifying the transport equation

To understand the coupling between convection and diffusion, let us start with a simple problem : a Y junction in a microfluidic device (fig. 2). The flow rates in the two inlets are equal. In one of the inlets we introduce a liquid with a soluble dye (say water with fluoresceine), in the other inlet the same liquid but without dye. Downstream of the inlets, the flow within the channel is a Poiseuille type laminar flow with a single component of velocity $u_x(y, z)$ depending on the transverse coordinates y and z. Some of you already used this kind of device in the fluid mechanics laboratory sessions to determine the diffusion coefficient of fluoresceine. In the experiment, we start with a device completely filled with water, then we introduce the dyed fluid in one of the inlets. After some time, say a few minutes, the concentration field, measured by the fluorescence
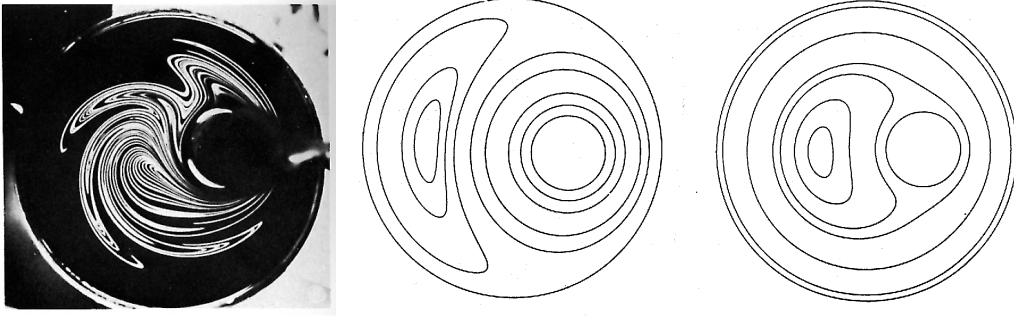
FIGURE 1 – Flow (at very low Reynolds number) of a liquid due to the rotation of two excentric cylinders. Left : stretching and folding of an initially localized spot of dye, after 12 periods of alternative rotation of the inner and outer cylinders (après 12 périodes de rotation). Center : streamlines when the inner cylinder is rotating. Right : streamlines when the outer cylinder is rotating. Figures reproduced from Chaiken, Chevray, Tabor et Tan, *Proc. Roy. Soc.* **A408** 165 (1986)

intensity, is steady. This steady state concentration field c is described by the convection diffusion equation :

$$\mathbf{u}.\nabla c = u_x(y, z)\frac{\partial c}{\partial x} = D\Delta c \tag{1}$$

where D is the diffusion coefficient of the dye.
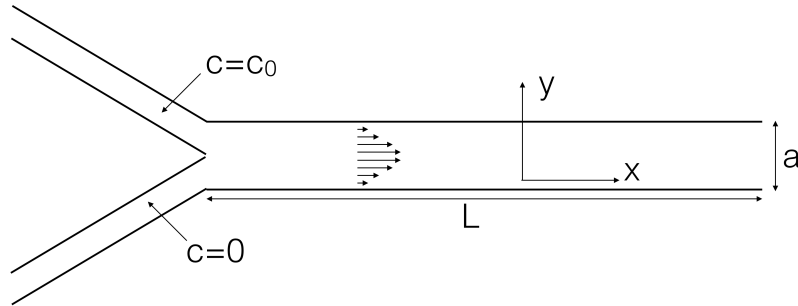

FIGURE 2 – Geometry of the microfluidics Y junction.

At the inlet, the dye concentration has a step profile : in the lower half of the channel ($y < a/2$), $c = 0$ and the upper half ($y > a/2$), $c = c_0$. The large concentration gradient in the middle of the channel will create a flux of dye from the upper half to the lower half and, as the dye is advected downstream by the flow, the width δ of the transition zone between the two sides will become wider and wider. We know, from a scaling analysis of the diffusion equation that δ should increase with $\sqrt{Dt}$ where t is the amount of time available to diffuse. We are dealing here with a steady state problem so instead of t, we have to use x/U where x is the position along the channel and U is the mean velocity of the fluid. So we get :

$$\delta \propto \sqrt{Dx/U}. \tag{2}$$

This is exactly the same type of argument that was used to define the width of a viscous boundary layer and the essential of the physics is contained in the scaling relation (2). But we will proceed to solve analytically the transport equation.

Now, let us suppose that δ remains small compared to the channel width a. Then, in the middle of the channel ($\pm\delta$) the velocity has a value which is very close U_0 and for the transport equation, we can make the approximation $u_x \equiv U_0$ and the equation becomes :

$$U_0 \frac{\partial c}{\partial x} = D\Delta c. \tag{3}$$

At the inlet, the concentration depends on the transverse coordinate y, but we can assume that it is uniform in the third dimension z and that c will remain independent of z downstream. If we assume that $\delta < a \ll L$, the components of the concentration gradient are, in order of magnitude : $\partial c/\partial x \approx c_0/L$ and $\partial c/\partial y \approx c_0/\delta$, so that $\partial c/\partial y \gg \partial c/\partial x$ and we can make the approximation $\Delta c \approx \partial^2 c/\partial y^2$. The transport equation is then :

$$U_0 \frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial y^2}. \tag{4}$$

We have to solve it with the boundary conditions $c = c_0$ at $x = 0$, $a > y > a/2$ and $c = 0$ at $x = 0$, $0 < y < a/2$. Strictly speaking, downstream of the inlet ($x > 0$) we have a condition of zero flux at the boundaries of the channel (at $y = 0, a$), but since we made the assumption that $\delta < a$ we can use a boundary condition at infinity $c \to c_0$ when $y \to \infty$ and $c \to 0$ when $y \to -\infty$.

2.1.2 Equation in dimensionless variables and self-similar solutions

To solve the equation, it is convenient to rewrite it with dimensionless variables : $\hat{c} = c/c_0$, $\hat{x} = x/a$ and $\hat{y} = (y - a/2)/a$, where we choose the channel width as a lengthscale :

$$\frac{\partial \hat{c}}{\partial \hat{x}} = \frac{D}{U_0 a}\frac{\partial^2 \hat{c}}{\partial \hat{y}^2} = \frac{1}{Pe}\frac{\partial^2 \hat{c}}{\partial \hat{y}^2} \tag{5}$$

and we introduced the Peclet number based on the channel width, $Pe = U_0\, a/D$. The boundary conditions are then at $\hat{x} = 0$, $\hat{c} = 1$ if $\hat{y} > 0$, $\hat{c} = 0$ if $\hat{y} < 0$ and, when $\hat{x} > 0$, $\hat{c} \to 1$ if $\hat{y} \to \infty$, $\hat{c} \to 0$ if $\hat{y} \to -\infty$. The equation reduces formally to a simple diffusion equation and we can use different techniques to solve it. Here we seek self-similar solution of the form $\hat{c} = f(\zeta = \hat{y}/\hat{\delta})$ where :

$$\hat{\delta} = \frac{\delta(x)}{a} = \sqrt{\frac{Dx}{a^2 U_0}} = \sqrt{\frac{D}{aU_0}}\sqrt{\frac{x}{a}} = Pe^{-1/2}\hat{x}^{1/2}$$

and the rescaled variable in the y direction ζ is :

$$\zeta = \frac{\hat{y}}{\hat{\delta}} = \hat{y}\hat{x}^{-1/2}Pe^{1/2}.$$

We rewrite eqn. 5 with variable ζ using

$$\frac{\partial^2 \hat{c}}{\partial \hat{y}^2} = \frac{d^2 \hat{c}}{d\zeta^2}\left(\frac{\partial \zeta}{\partial \hat{y}}\right)^2 = \frac{1}{\hat{\delta}^2}\frac{d^2 \hat{c}}{d\zeta^2} = \frac{Pe}{\hat{x}}\frac{d^2 \hat{c}}{d\zeta^2}$$

and

$$\frac{\partial \hat{c}}{\partial \hat{x}} = \frac{d\hat{c}}{d\zeta}\frac{\partial \zeta}{\partial \hat{x}} = -\frac{1}{2}\hat{y}\hat{x}^{-3/2}Pe^{1/2}\frac{d\hat{c}}{d\zeta} = -\frac{1}{2}\frac{\zeta}{\hat{x}}\frac{d\hat{c}}{d\zeta} :$$

$$-\frac{1}{2}\zeta\frac{d\hat{c}}{d\zeta} = \frac{d^2 \hat{c}}{d\zeta^2}. \tag{6}$$

Using the rescaled variable ζ we have transformed the transport equation into an ordinary differential equation (instead of a P.D.E.) which we can solve more easily noting that $d_x(\exp(-x^2/4)) = -x/2\exp(-x^2/4)$. Hence we have : $d\hat{c}/d\zeta = A\exp(-\zeta^2/4)$ and :

$$\hat{c} = A\int_0^\zeta \exp(-u^2/4)\, du + B \ \ \text{or} \ \ \hat{c} = A'\frac{\sqrt{\pi}}{2}\text{erf}(\zeta/2) + B \tag{7}$$

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The appropriate boundary conditions with the rescaled variable are $\hat{c} \to 1$ if $\zeta \to \infty$ and $\hat{c} \to 0$ if $\zeta \to -\infty$. The limits of the error function are ± 1 at $\zeta \to \pm\infty$, so the dimensionless concentration is given by

$$\hat{c} = \frac{1}{2}[1 + \mathrm{erf}(\zeta/2)] \tag{8}$$

and in dimensional variables :

$$c = \frac{c_0}{2}\left[1 + \mathrm{erf}\left(\frac{y}{2}\sqrt{\frac{U_0}{Dx}}\right)\right] \tag{9}$$

This self-similar concentration field is shown on fig. 3 together with profiles in the y direction at different locations in x.
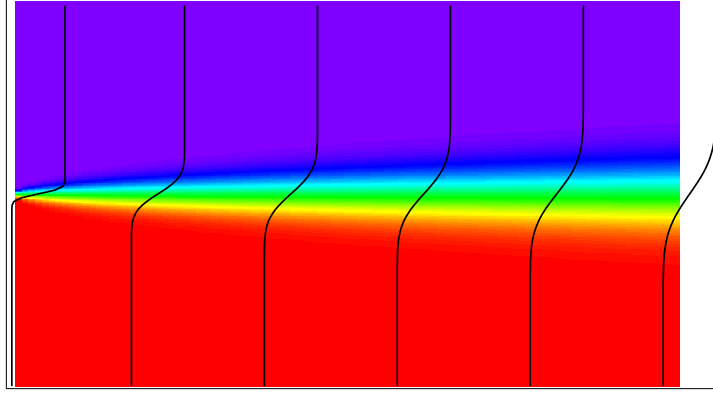

FIGURE 3 – Self-similar concentration profiles which are solutions of eqn. 6

The solutions derived above are valid only on the condition that δ, the thickness of the diffusion layer, remains small compared to the width of the channel a. Since $\delta(x) = \sqrt{U_0 x/D}$, its maximum value is $\delta(L) = \sqrt{U_0 L/D}$. So the condition is :

$$\sqrt{\frac{U_0 L}{D}} = a\sqrt{\frac{U_0}{Da}}\sqrt{\frac{L}{a}} \ll a \ \ \text{or} \ \ Pe \gg \frac{L}{a}. \tag{10}$$

We could anticipate a condition of the type $Pe \gg 1$ since the scaling relation (2) implies that δ increases with $\sqrt{Pe}$, but we have a more precise condition involving the aspect ratio L/a of the channel. We can test this criterion by solving numerically the transport equation for various values of the Peclet number. Some numerical solutions are shown on fig. 4 for an aspect ratio L/a of 10. When $Pe = 8 < L/a$, lateral diffusion is rather fast compared to convection and the transverse gradient of concentration disappears almost completely at $x = 4a$. On the other hand, when $Pe = 833 \gg L/a$, the thickness of the diffusion layer remains much smaller than a and the transverse concentration profiles are accurately described by the self similar solutions (9).

2.1.3 Transverse fluxes

From the solution for the concentration field, it is possible to compute the transverse flux of mass. To understand the physics, an order of magnitude calculation is sufficient : the local vertical concentration gradient $\partial c/\partial y$ can be approximated as $C_0/\delta(x)$ and the local mass flux is $-DC_0/\delta(x)$, the total mass exchange per unit time along the channel (per unit width in the z direction) is then :

$$J_{total} = \int_0^L -D\frac{C_0}{\delta(x)}dx = -DC_0\int_0^L \sqrt{\frac{U}{D}}x^{-1/2}dx = -2DC_0\sqrt{\frac{U}{D}}\sqrt{L} \tag{11}$$
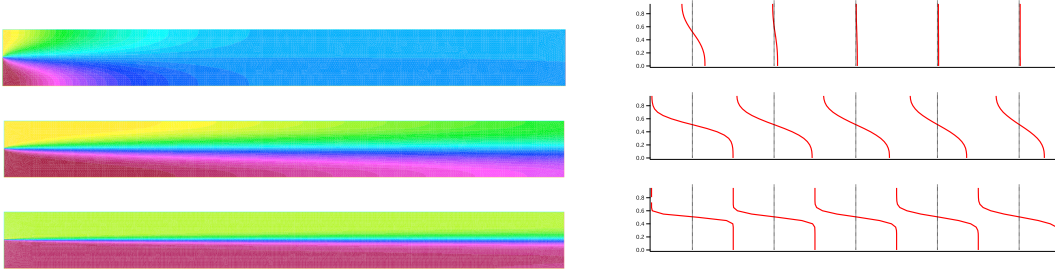
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FIGURE 4 – Diffusion within a two dimensional channel of aspect ration $L/a = 10$. The flow has a parabolic velocity profile. At the inlet, the concentration is 1 in the top half, 0 in the bottom half. Left, concentration fields. Right vertical concentration profiles at $x = 2a$, $4a$, $6a$, $8a$ and $10a$. Top, $Pe = 8$, middle, $Pe = 83$, bottom, $Pe = 833$.

We can rearrange this expression as follows :

$$J_{total} = -\frac{2DC_0}{a}L\sqrt{\frac{Ua}{D}}\sqrt{\frac{a}{L}} = 2J_{dif}\sqrt{Pe\frac{a}{L}} \tag{12}$$

where we have used the Peclet number already defined and where $J_{dif} = DC_0/a \times L$ would be the purely diffusive flux resulting from a transverse concentration gradient on the length scale a, integrated over the channel length L.

The ratio between J_{total} and J_{dif} is called the *Sherwood number Sh*; it shows the enhancement of transport due to the interplay between convection and diffusion. The self similar solutions are valid if $Pe \gg L/a$, so $Pe(a/L) \gg 1$ and eqn. 12 shows that $Sh \gg 1$. The enhancement of the transverse mass flux is due to the small value of δ at large Peclet numbers, because of the macroscopic flow, thus maintaining large transverse gradients of concentration.

2.1.4   An analogy between mass flux and viscous drag ?

Just a side remark : yes, there is an analogy between mass flux and viscous drag. Consider the viscous boundary layer on a flat plate : the thickness of the boundary layer scales as $\delta_\nu = \sqrt{\nu x/U}$ wher U is the velocity outside the boundary layer. The shear stress on the plate is $\sigma_{xy} = \eta\partial u_x/\partial y \sim \eta U/\delta_\nu(x)$ where η is the dynamic viscosity. The drag force on the plate of length L (per unit length in the third dimension z) is $F_d = \int_0^L \sigma_{xy}dx = \eta U \int_0^L \delta_\nu(x)^{-1}dx$. Using the expression for δ_ν, we get :

$$F_d \sim \eta U\sqrt{\frac{UL}{\nu}} = \eta U Re_L^{1/2} \tag{13}$$

Equation 13 is similar to eqn. (12) if we identify ηU as a drag force (per unit length) resulting from a purely diffusive transport of momentum and if the Reynolds number plays a role similar to the Peclet number. Note that the ratio L/a does not appear here because we have not considered a characteristic length scale in the y direction.

2.2   Transport boundary layers

We can now use the ideas developed above to solve slightly more complicated problems, provided that we can make the approximation that there exits a thin boundary layer in which the concentration or temperature changes rapidly in the direction transverse (say y) to the main flow. If the thickness of this boundary layer increases slowly in the streamwise direction (say x), we can ignore the diffusive flux in the x direction $-D\partial c/\partial x$ compared to the diffusive flux in the y direction $-D\partial c/\partial y$ and this simplifies greatly the mathematical solution of the problem.

2.2.1 Concentration boundary layer on a flat plate. Velocity field invariant in the streamwise direction

We consider first the case described in the "micro biochemical sensor" problem (fig. 5). Liquid containing a tracer molecule at concentration C_0 flows within a channel of height a. On the bottom of the channel there is a reactive region which adsorbs quickly the tracer molecules. We make the assumption that the adsorption process is very fast, so that we can consider that the concentration is 0 on the reactive plate. We want to compute the flux of molecules towards the reacting plate. This flux is fixed by the concentration gradient on the bottom wall of the channel, located at $y = 0 : J = -D(\partial c/\partial y)$ at $y = 0$.
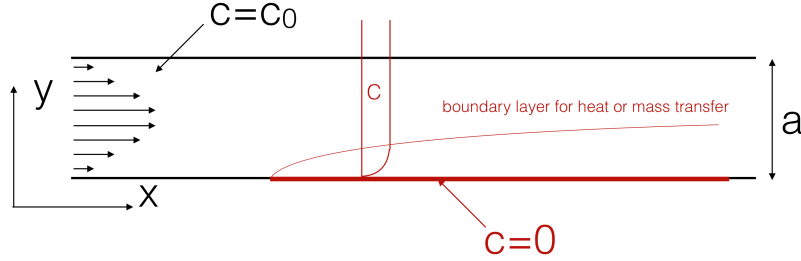

FIGURE 5 – Concentration boundary layer within a channel. Reactive plate in red.

So we need to determine the concentration field, given the velocity field $u_x(y)$ and the diffusion coefficient D. Again, we are looking for solutions at steady state and the transport equation is again :

$$u_x(y)\frac{\partial c}{\partial x} = D\Delta c \tag{14}$$

From the previous analysis, we know that, if the Peclet number is large enough, there will be a thin concentration boundary layer of thickness $\delta(x)$ on the bottom of the channel this time and we make the assumption $\Delta c \approx \partial^2 c/\partial y^2$ and the transport equation is :

$$u_x(y)\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial y^2}. \tag{15}$$

We cannot proceed exactly like in the previous problem because u_x does depend on y, but we can at least make a general dimensional analysis if we assume that u_x varies as a power law $u_x = U(y/a)^\alpha$ giving :

$$\left(\frac{y}{a}\right)^\alpha \frac{\partial c}{\partial x} = \frac{D}{U}\frac{\partial^2 c}{\partial y^2}. \tag{16}$$

We can then make a very crude dimensional analysis by setting $y \sim \delta$ and $\partial c/\partial x \sim c_0/x$. Then :

$$\left(\frac{\delta}{a}\right)^\alpha \frac{C_0}{x} \sim \frac{D}{U}\frac{C_0}{\delta^2} \tag{17}$$

and we derive a scaling law for $\delta(x)$:

$$\delta^{2+\alpha} \sim \frac{Dx}{U}a^{-\alpha} = \frac{D}{Ua}\frac{x}{a}a^{2-\alpha} \tag{18}$$

or :

$$\delta \sim \left(\frac{x}{a}\right)^{\frac{1}{2+\alpha}} Pe^{-\frac{1}{2+\alpha}} a^{\frac{2-\alpha}{2+\alpha}}. \tag{19}$$

Once we know $\delta(x)$ from the scaling relation (19), we estimate the local mass flux on the wall as $-DC_0/\delta(x)$ and we integrate over the total length L of the reacting plate to get the total mass exchange per unit time : $J_{total} = -DC_0 \int_0^L \delta(x)^{-1} \, dx$. Again we see that δ decreases when the Peclet number increases, but with a power law depending on the velocity profile.

There is a more rigorous way of doing this by seeking self-similar solutions of the transport equation of the form $c = C_0 f(y/\delta(x))$. It turns out that the scaling relation (19) provides the appropriate dependence for δ and the transport equation written with the rescaled variable $\zeta = y/\delta(x)$ as we did above, becomes an O.D.E. which is easier to solve. We will derive in class the exact solution in the case where the velocity profile is linear ($u_x = Uy/a$).

2.2.2 Concentration or temperature boundary layer on a curved solid. The velocity field is a viscous boundary layer.

We can generalize further by looking at situations where the surface on which the transport layer occurs is no longer flat and where the velocity field evolves (slowly) with streamwise coordinate. This type of situation is shown on fig. 6 : a heated cylinder is placed in a stream of gaz flowing at right angle to the axis of the cylinder. If the Peclet number is large enough (here $Pe \sim 100$), a thin transport boundary layer develops from the stagnation point, on the upstream side of the cylinder. If the radius of curvature of the surface is large compared to δ, we can essentially use the same arguments as above, replacing x by the curvilinear coordinate s along the object surface (fig. 7).

There is an additional complexity though : the flow field is a viscous boundary layer with a thickness δ_ν also developing from the stagnation point, so u depends both on the coordinate normal to the surface and also on the streamwise position s. Nevertheless, as long as the boundary layers remain thin (implying $Pe \gg 1$ for δ and $Re \gg 1$ for δ_ν) we can neglect the diffusive fluxes in the s direction and this allows the derivation of self-similar solutions as we have done before. δ and δ_ν will be different in general because the kinematic viscosity ν and the heat diffusivity $\kappa = \lambda/\rho CP$ or the mass diffusivity D are not equal. In particular in liquids, D is typically much smaller than ν. But the ratio ν/κ (called the Prandtl number) may be larger or smaller than 1 depending on the fluids (for example $Pr = 0.7$ for air $Pr \sim 10$ for water).

This is a basis to understand the heat transfer from a body in fluid flow and to propose an expression for the "wind chill factor".
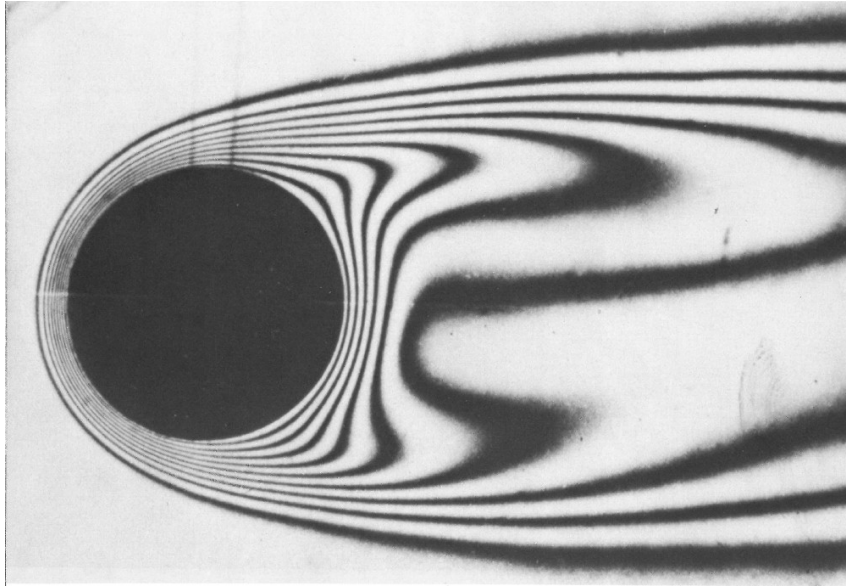
FIGURE 6 – Thermal boundary layer on a heated circular cylinder visualized by Mach-Zender interferometry. Each black line corresponds to a given value of the optical path through the interferometer and since the optical index of the fluid is directly related to the temperature, each black line is an isotherm. Reynolds number for the flow = 120. $Pe = Re(\nu/\kappa) = RePr = 84$ for air. Picture reproduced from An Album of Fluid Motion by Milton Van Dyke.
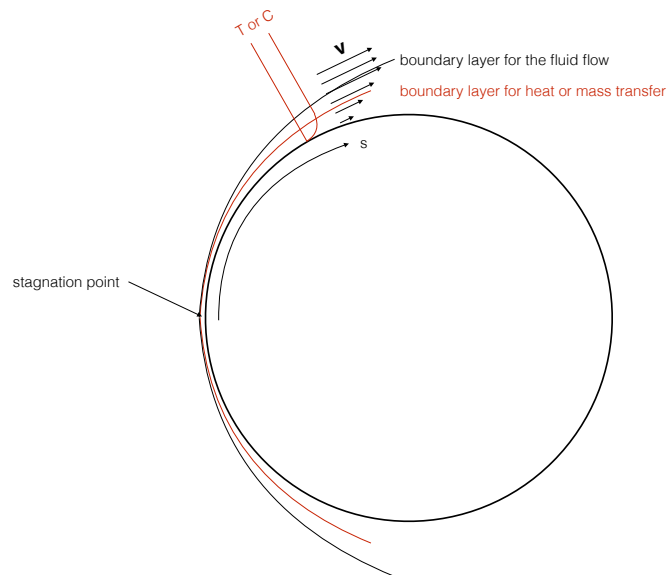

FIGURE 7 – Concentration or thermal boundary layer on a cylinder.