

**PQI-5776 Fenômenos de Transporte I**AULA 8 - APLICAÇÕES

Difusão em um filme líquido descendente - Absorção gasosa com reação química. Aplicação desenvolvida a partir do exemplo apresentado no §18.5 do Bird (2002). Incluir no exemplo a reação de consumo de A na fase líquida por uma reação de primeira ordem, expressa por:  $-r_A = k''\rho_A$ .

a) Obter uma expressão para a taxa de absorção do gás A no solvente B em função dos adimensionais  $Pe$  e  $Da$ .

b) Analisar o caso de reação lenta. Obter uma expressão simplificada para a taxa de absorção.

c) Analisar o caso de reação rápida. Obter uma expressão simplificada para a taxa de absorção.

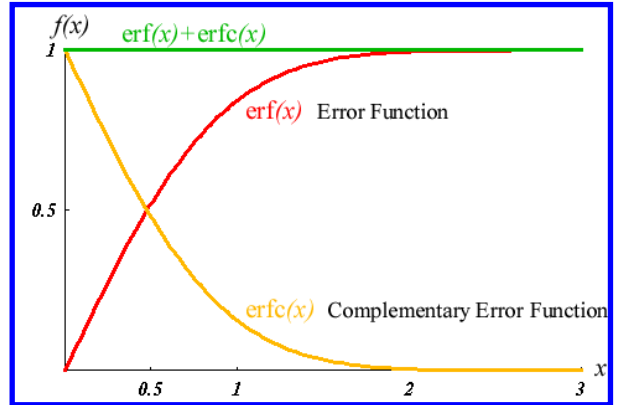
**FUNÇÃO ERRO - ERROR FUNCTION-**

$$\text{erf } x = \frac{2}{\sqrt{\pi}} \int_0^x e^{-\xi^2} d\xi,$$

$$\text{erf } \infty = 1,$$

$$\text{erf}(-x) = -\text{erf } x.$$

$$\text{erfc } x = 1 - \text{erf } x = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-\xi^2} d\xi.$$



Para  $x \ll 1$

$$\text{erf } x = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n+1}}{(2n+1)n!}.$$

Para  $x \gg 1$

$$\frac{\sqrt{\pi}}{2} \text{erfc } x = \int_x^\infty e^{-\xi^2} d\xi = \frac{1}{2} e^{-x^2} \left( \frac{1}{x} - \frac{1}{2x^3} + \frac{1 \cdot 3}{2^2 x^5} - \dots + (-1)^{n-1} \frac{1 \cdot 3 \dots (2n-3)}{2^{n-1} x^{2n-1}} \right) +$$

$$+ (-1)^n \frac{1 \cdot 3 \dots (2n-1)}{2^n} \int_x^\infty \frac{e^{-\xi^2} d\xi}{\xi^{2n}}.$$

**Derivadas**

$$\Phi_n(x) = \frac{d^n}{dx^n} \text{erf } x,$$

$$\Phi_1(x) = \frac{2}{\sqrt{\pi}} e^{-x^2},$$

$$\Phi_2(x) = -\frac{4}{\sqrt{\pi}} x e^{-x^2},$$

CONDUCTION  
OF  
HEAT IN SOLIDS

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$x$	$e^{x^2} \operatorname{erfc} x$	$4\pi^{-1/2} x e^{-x^2}$	$2\pi^{-1/2} e^{-x^2}$	$\operatorname{erf} x$	$\operatorname{erfc} x$	$2 \operatorname{ierfc} x$	$4 i^2 \operatorname{erfc} x$	$6 i^3 \operatorname{erfc} x$
0	1.0	0	1.1284	0	1.0	1.1284	1.0	0.5642
0.05	0.9460	0.1126	1.1256	0.056372	0.943628	1.0312	0.8921	0.4933
0.1	0.8965	0.2234	1.1172	0.112463	0.887537	0.9396	0.7936	0.4301
0.15	0.8509	0.3310	1.1033	0.167996	0.832004	0.8537	0.7040	0.3740
0.2	0.8090	0.4336	1.0841	0.222703	0.777297	0.7732	0.6227	0.3243
0.25	0.7703	0.5300	1.0600	0.276326	0.723674	0.6982	0.5491	0.2805
0.3	0.7346	0.6188	1.0313	0.328627	0.671373	0.6284	0.4828	0.2418
0.35	0.7015	0.6988	0.9983	0.379382	0.620618	0.5639	0.4233	0.2079
0.4	0.6708	0.7692	0.9615	0.428392	0.571608	0.5043	0.3699	0.1782
0.45	0.6423	0.8294	0.9215	0.475482	0.524518	0.4495	0.3223	0.1522
0.5	0.6157	0.8788	0.8788	0.520500	0.479500	0.3993	0.2799	0.1297
0.55	0.5909	0.9172	0.8338	0.563323	0.436677	0.3535	0.2423	0.1101
0.6	0.5678	0.9447	0.7872	0.603856	0.396144	0.3119	0.2090	0.0932
0.65	0.5462	0.9614	0.7395	0.642029	0.357971	0.2742	0.1798	0.0787
0.7	0.5259	0.9678	0.6913	0.677801	0.322199	0.2402	0.1541	0.0662
0.75	0.5069	0.9644	0.6429	0.711156	0.288844	0.2097	0.1316	0.0555
0.8	0.4891	0.9520	0.5950	0.742101	0.257899	0.1823	0.1120	0.0464
0.85	0.4723	0.9314	0.5479	0.770668	0.229332	0.1580	0.0950	0.0386
0.9	0.4565	0.9035	0.5020	0.796908	0.203092	0.1364	0.0803	0.0321
0.95	0.4416	0.8695	0.4576	0.820891	0.179109	0.1173	0.0677	0.0265
1.0	0.4276	0.8302	0.4151	0.842701	0.157299	0.1005	0.0568	0.0218
1.1	0.4017	0.7403	0.3365	0.880205	0.119795	0.0729	0.0396	0.0147
1.2	0.3785	0.6416	0.2673	0.910314	0.089686	0.0521	0.0272	0.0097
1.3	0.3576	0.5413	0.2082	0.934008	0.065992	0.0366	0.0184	0.0063
1.4	0.3387	0.4450	0.1589	0.952285	0.047715	0.0253	0.0122	0.0041
1.5	0.3216	0.3568	0.1189	0.966105	0.033895	0.0172	0.0080	0.0026
1.6	0.3060	0.2791	0.0872	0.976348	0.023652	0.0115	0.0052	0.0016
1.7	0.2917	0.2132	0.0627	0.983790	0.016210	0.0076	0.0033	0.0010
1.8	0.2786	0.1591	0.0442	0.989091	0.010909	0.0049	0.0021	0.0006
1.9	0.2665	0.1160	0.0305	0.992790	0.007210	0.0031	0.0013	0.0003
2.0	0.2554	0.0827	0.0207	0.995322	0.004678	0.0020	0.0008	0.0002
2.1	0.2451	0.0576	0.0137	0.997021	0.002979	0.0012	0.0005	0.0001
2.2	0.2356	0.0393	0.0089	0.998137	0.001863	0.0007	0.0003	
2.3	0.2267	0.0262	0.0057	0.998857	0.001143	0.0004	0.0002	
2.4	0.2185	0.0171	0.0036	0.999311	0.000689	0.0002	0.0001	
2.5	0.2108	0.0109	0.0022	0.999593	0.000407	0.0001		
2.6	0.2036	0.0068	0.0013	0.999764	0.000236	0.0001		
2.7	0.1969	0.0042	0.0008	0.999866	0.000134			
2.8	0.1905	0.0025	0.0004	0.999925	0.000075			
2.9	0.1846	0.0015	0.0003	0.999959	0.000041			
3.0	0.1790	0.0008	0.0001	0.999978	0.000022			

**PQI-5776 - Fenômenos de Transporte I**  
**Lista de Exercícios 6 e 7**

- 1) Bird - 2002 - § 18.3 e exemplo 18.3-1 - anexo.
  - a) A equação (18.3-1) é válida mesmo para reação lenta?
  - b)  $x_{A0}$  (condição 18.3-6) varia ao longo do leito?
  - c) Obtenha a expressão 18.3-9 a partir da 18.3-14, admitindo-se  $Da^{II} \rightarrow \infty$ .
  - d) Qual a expressão de  $N_{Az}$ , no caso do processo controlado pela reação, que corresponde à condição  $Da^{II} \rightarrow 0$  (reação extremamente lenta).
  
- 2) (Incropera F. P., de Witt D.P., Fundamentals of Heat Transfer, 2<sup>nd</sup> edition - Exemplo 6.2 - Anexo.
  - a) Obtenha a expressão para a velocidade  $U_1$  (comentário 1) e as expressões para  $q''_0$  e  $q''_L$  para esta velocidade.
  - b) Calcule a força aplicada à placa superior (considere placa com 1m x 1m) e a potência (W) para manter a placa com velocidade  $U = 10$  m/s. Obtenha o valor da função de dissipação de Rayleigh ( $W/m^3$ ) multiplicada pelo volume de fluido. Compare este último resultado com a potência.
  
- 3) Considerando-se o caso de absorção com reação rápida (discutido em aula) expresse o coeficiente de transferência de massa em termos de números adimensionais.

- 4) Nos parágrafos 18.5 e 18.6 (lista de exercícios -aula 4) a velocidade do centro de massa é igual à do centro molar? Comente.
- 5) No parágrafo 18.5 (lista de exercícios -aula 4) equacione a conservação de A, na forma lagrangeana, para um elemento de volume do filme líquido próximo à interface. Qual a interpretação para o tempo de contato?
- 6) No caso da absorção de um sistema gasoso A/inerte(ar) pode-se considerar  $C_{A0}$  constante na interface gás-líquido(parágrafo 18.5 - lista de exercícios -aula 4)?
- 7) Equacione um modelo para estimativa do tempo necessário para a evaporação de uma gota de tolueno em ar estagnado à temperatura de 25 °C. Adote a hipótese de regime pseudo-permanente.

§18.3 DIFFUSION WITH A HETEROGENEOUS CHEMICAL REACTION

Let us now consider a simple model for a catalytic reactor, such as that shown in Fig. 18.3-1a, in which a reaction  $2A \rightarrow B$  is being carried out. An example of a reaction of this type would be the solid-catalyzed dimerization of  $\text{CH}_3\text{CH}=\text{CH}_2$ .

We imagine that each catalyst particle is surrounded by a stagnant gas film through which  $A$  has to diffuse to reach the catalyst surface, as shown in Fig. 18.3-1b. At the catalyst surface we assume that the reaction  $2A \rightarrow B$  occurs instantaneously, and that the product  $B$  then diffuses back out through the gas film to the main turbulent stream composed of  $A$  and  $B$ . We want to get an expression for the local rate of conversion from  $A$  to  $B$  when the effective gas-film thickness and the main stream concentrations  $x_{A0}$  and  $x_{B0}$  are known. We assume that the gas film is isothermal, although in many catalytic reactions the heat generated by the reaction cannot be neglected.

For the situation depicted in Fig. 18.3-1b, there is one mole of  $B$  moving in the minus  $z$  direction for every two moles of  $A$  moving in the plus  $z$  direction. We know this from the stoichiometry of the reaction. Therefore we know that at steady state

$$N_{Bz} = -\frac{1}{2}N_{Az} \tag{18.3-1}$$

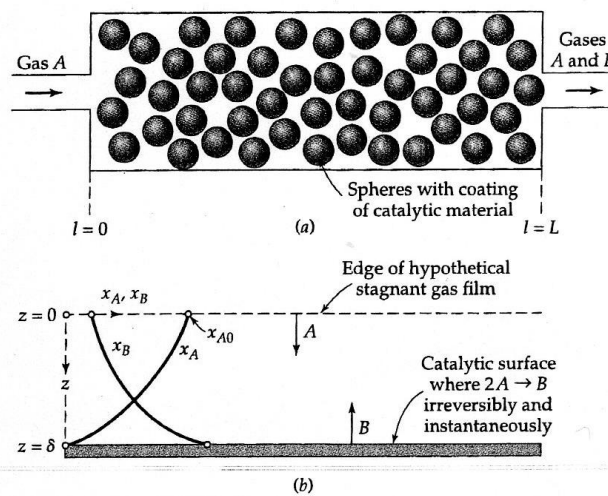


Fig. 18.3-1. (a) Schematic diagram of a catalytic reactor in which  $A$  is being converted to  $B$ . (b) Idealized picture (or "model") of the diffusion problem near the surface of a catalyst particle.

at any value of  $z$ . This relation may be substituted into Eq. 18.0-1, which may then be solved for  $N_{Az}$  to give

$$N_{Az} = -\frac{c\mathcal{D}_{AB}}{1 - \frac{1}{2}x_A} \frac{dx_A}{dz} \tag{18.3-2}$$

Hence, Eq. 18.0-1 plus the stoichiometry of the reaction have led to an expression for  $N_{Az}$  in terms of the concentration gradient.

We now make a mass balance on species  $A$  over a thin slab of thickness  $\Delta z$  in the gas film. This procedure is exactly the same as that used in connection with Eqs. 18.2-2 and 3 and leads once again to the equation

$$\frac{dN_{Az}}{dz} = 0 \tag{18.3-3}$$

Insertion of the expression for  $N_{Az}$  developed above, into this equation gives (for constant  $\mathcal{D}_{AB}$ )

$$\frac{d}{dz} \left( \frac{1}{1 - \frac{1}{2}x_A} \frac{dx_A}{dz} \right) = 0 \tag{18.3-4}$$

Integration twice with respect to  $z$  gives

$$-2 \ln(1 - \frac{1}{2}x_A) = C_1z + C_2 = -(2 \ln K_1)z - (2 \ln K_2) \tag{18.3-5}$$

It is somewhat easier to find the integration constants  $K_1$  and  $K_2$  than  $C_1$  and  $C_2$ . The boundary conditions are

B.C. 1:  $z = 0, \quad x_A = x_{A0} \tag{18.3-6}$

B.C. 2:  $z = \delta, \quad x_A = 0 \tag{18.3-7}$

$$\left(1 - \frac{1}{2}x_A\right) = \left(1 - \frac{1}{2}x_{A0}\right)^{1-(z/\delta)} \quad (18.3-8)$$

for the concentration profile in the gas film. Equation 18.3-2 may now be used to get the molar flux of reactant through the film:

$$N_{Az} = \frac{2c\mathcal{D}_{AB}}{\delta} \ln\left(\frac{1}{1 - \frac{1}{2}x_{A0}}\right) \quad (18.3-9)$$

The quantity  $N_{Az}$  may also be interpreted as the local rate of reaction per unit area of catalytic surface. This information can be combined with other information about the catalytic reactor sketched in Fig. 18.3-1(a) to get the overall conversion rate in the entire reactor.

One point deserves to be emphasized. Although the chemical reaction occurs instantaneously at the catalytic surface, the conversion of  $A$  to  $B$  proceeds at a finite rate because of the diffusion process, which is "in series" with the reaction process. Hence we speak of the conversion of  $A$  to  $B$  as being *diffusion controlled*.

In the example above we have assumed that the reaction occurs instantaneously at the catalytic surface. In the next example we show how to account for finite reaction kinetics at the catalytic surface.

#### EXAMPLE 18.3-1

##### Diffusion with a Slow Heterogeneous Reaction

Rework the problem just considered when the reaction  $2A \rightarrow B$  is not instantaneous at the catalytic surface at  $z = \delta$ . Instead, assume that the rate at which  $A$  disappears at the catalyst-coated surface is proportional to the concentration of  $A$  in the fluid at the interface,

$$N_{Az} = k_1''c_A = k_1''cx_A \quad (18.3-10)$$

in which  $k_1''$  is a rate constant for the pseudo-first-order surface reaction.

#### SOLUTION

We proceed exactly as before, except that B.C. 2 in Eq. 18.3-7 must be replaced by

$$\text{B.C. 2':} \quad \text{at } z = \delta, \quad x_A = \frac{N_{Az}}{k_1''c} \quad (18.3-11)$$

$N_{Az}$  being, of course, a constant at steady state. The determination of the integration constants from B.C. 1 and B.C. 2' leads to

$$\left(1 - \frac{1}{2}x_A\right) = \left(1 - \frac{1}{2}\frac{N_{Az}}{k_1''c}\right)^{z/\delta} \left(1 - \frac{1}{2}x_{A0}\right)^{1-(z/\delta)} \quad (18.3-12)$$

From this we evaluate  $(dx_A/dz)|_{z=0}$  and substitute it into Eq. 18.3-2, to get

$$N_{Az} = \frac{2c\mathcal{D}_{AB}}{\delta} \ln\left(\frac{1 - \frac{1}{2}(N_{Az}/k_1''c)}{1 - \frac{1}{2}x_{A0}}\right) \quad (18.3-13)$$

This is a transcendental equation for  $N_{Az}$  as a function of  $x_{A0}$ ,  $k_1''$ ,  $c\mathcal{D}_{AB}$ , and  $\delta$ . When  $k_1''$  is large, the logarithm of  $1 - \frac{1}{2}(N_{Az}/k_1''c)$  may be expanded in a Taylor series and all terms discarded but the first. We then get

$$N_{Az} = \frac{2c\mathcal{D}_{AB}/\delta}{1 + \mathcal{D}_{AB}/k_1''\delta} \ln\left(\frac{1}{1 - \frac{1}{2}x_{A0}}\right) \quad (k_1 \text{ large}) \quad (18.3-14)$$

Note once again that we have obtained the rate of the *combined* reaction and diffusion process. Note also that the dimensionless group  $\mathcal{D}_{AB}/k_1''\delta$  describes the effect of the surface reaction kinetics on the overall diffusion-reaction process. The reciprocal of this group is known as the *second Damköhler number*<sup>1</sup>  $Da^{\text{II}} = k_1''\delta/\mathcal{D}_{AB}$ . Evidently we get the result in Eq. 18.3-9 in the limit as  $Da^{\text{II}} \rightarrow 0$ .

<sup>1</sup>G. Damhöhler, Z. Elektrochem., 42, 846-862 (1936).

EXAMPLE 6.2

328 One of the few situations for which exact solutions to the convection transfer equations may be obtained involves what is termed *parallel flow*. In this case fluid motion is only in one direction. Consider a special case of parallel flow involving stationary and moving plates of infinite extent separated by a distance  $L$ , with the intervening space filled by an incompressible fluid. This situation is referred to as Couette flow and occurs, for example, in a journal bearing.

1. What is the appropriate form of the continuity equation (6.13)?
2. Beginning with the momentum equation (6.22), determine the velocity distribution between the plates.
3. Beginning with the energy equation (6.34), determine the temperature distribution between the plates.
4. Consider conditions for which the fluid is engine oil with  $L = 3$  mm. The speed of the moving plate is  $U = 10$  m/s, and the temperatures of the stationary and moving plates are  $T_0 = 10^\circ\text{C}$  and  $T_L = 30^\circ\text{C}$ , respectively. Calculate the heat flux to each of the plates and determine the maximum temperature in the oil.

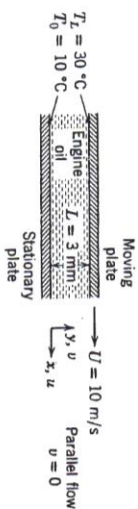
SOLUTION

**Known:** Couette flow with heat transfer.

**Find:**

1. Form of the continuity equation.
2. Velocity distribution.
3. Temperature distribution.
4. Surface heat fluxes and maximum temperature for prescribed conditions.

**Schematic:**



**Assumptions:**

1. Steady-state conditions.
2. Two-dimensional flow (no variations in  $z$ ).

3. Incompressible fluid with constant properties.
4. No body forces.
5. No internal energy generation.

**Properties:** Table A.5, engine oil ( $20^\circ\text{C}$ ):  $\rho = 888.2$  kg/m<sup>3</sup>,  $k = 0.145$  W/m · K,  $\nu = 900 \times 10^{-6}$  m<sup>2</sup>/s,  $\mu = \nu\rho = 0.799$  N · s/m<sup>2</sup>.

**Analysis:**

1. For an incompressible fluid (constant  $\rho$ ) and parallel flow ( $v = 0$ ), Equation 6.13 reduces to

$$\frac{\partial u}{\partial x} = 0$$

The important implication of this result is that, while depending on  $y$ , the  $x$ -velocity component  $u$  is independent of  $x$ . It may then be said that the velocity field is *fully developed*.

2. For two-dimensional, steady-state conditions with  $v = 0$ ,  $(\partial u/\partial x) = 0$  and  $X = 0$ , Equation 6.22 reduces to

$$0 = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial y} \left( \mu \frac{\partial u}{\partial y} \right)$$

However, in Couette flow, motion of the fluid is sustained not by the pressure gradient,  $\partial p/\partial x$ , but by an external force that provides for motion of the top plate relative to the bottom plate. Hence  $(\partial p/\partial x) = 0$ . Accordingly, with constant viscosity, the  $x$ -momentum equation reduces to

$$\frac{\partial^2 u}{\partial y^2} = 0$$

The desired velocity distribution may be obtained by solving this equation. Integrating twice, we obtain

$$u(y) = C_1 y + C_2$$

where  $C_1$  and  $C_2$  are the constants of integration. Applying the boundary conditions

$$u(0) = 0 \quad \text{and} \quad u(L) = U$$

it follows that  $C_2 = 0$  and  $C_1 = U/L$ . The velocity distribution is then

$$u(y) = \frac{y}{L} U$$



3. The energy equation, (6.34), may be simplified for the prescribed conditions. In particular for two-dimensional, steady-state conditions with  $v = 0$ ,  $(\partial u/\partial x) = 0$ , and  $\dot{q} = 0$ , it follows that

$$\rho c_p \mu \frac{\partial T}{\partial x} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) + \mu \left( \frac{\partial u}{\partial y} \right)^2$$

However, because the top and bottom plates are at uniform temperatures, the temperature field must also be fully developed, in which case  $(\partial T/\partial x) = 0$ . For constant thermal conductivity, the appropriate form of the energy equation is then

$$0 = k \frac{\partial^2 T}{\partial y^2} + \mu \left( \frac{\partial u}{\partial y} \right)^2$$

The desired temperature distribution may be obtained by solving this equation. Rearranging and substituting for the velocity distribution,

$$k \frac{\partial^2 T}{\partial y^2} = -\mu \left( \frac{du}{dy} \right)^2 = -\mu \left( \frac{U}{L} \right)^2$$

Integrating twice, we obtain

$$T(y) = -\frac{\mu}{2k} \left( \frac{U}{L} \right)^2 y^2 + C_3 y + C_4$$

The constants of integration may be obtained from the boundary conditions

$$T(0) = T_0 \quad \text{and} \quad T(L) = T_L$$

in which case

$$C_4 = T_0 \quad \text{and} \quad C_3 = \frac{T_L - T_0}{L} + \frac{\mu}{2k} \frac{U^2}{L}$$

and

$$T(y) = T_0 + \frac{\mu}{2k} U^2 \left[ \frac{y}{L} - \left( \frac{y}{L} \right)^2 \right] + (T_L - T_0) \frac{y}{L}$$

4. Knowing the temperature distribution, the surface heat fluxes may be obtained by applying Fourier's law. Hence

$$q''_y = -k \frac{dT}{dy} = -k \left[ \frac{\mu}{2k} U^2 \left( \frac{1}{L} - \frac{2y}{L^2} \right) + \frac{T_L - T_0}{L} \right]$$

At the bottom and top surfaces, respectively, it follows that

$$q''_0 = -\frac{\mu U^2}{2L} - \frac{k}{L} (T_L - T_0) \quad \text{and} \quad q''_L = +\frac{\mu U^2}{2L} - \frac{k}{L} (T_L - T_0)$$

Hence, for the prescribed numerical values,

$$q''_0 = -\frac{0.799 \text{ N} \cdot \text{s}/\text{m}^2 \times 100 \text{ m}^2/\text{s}^2}{2 \times 3 \times 10^{-3} \text{ m}} - \frac{0.145 \text{ W}/\text{m} \cdot \text{K}}{3 \times 10^{-3} \text{ m}} (30 - 10)^\circ\text{C}$$

$$q''_0 = -13,315 \text{ W}/\text{m}^2 - 967 \text{ W}/\text{m}^2 = -14,3 \text{ kW}/\text{m}^2 \quad \blacktriangleleft$$

$$q''_L = +13,315 \text{ W}/\text{m}^2 - 967 \text{ W}/\text{m}^2 = 12.3 \text{ kW}/\text{m}^2 \quad \blacktriangleleft$$

The location of the maximum temperature in the oil may be found from the requirement that

$$\frac{dT}{dy} = \frac{\mu}{2k} U^2 \left( \frac{1}{L} - \frac{2y}{L^2} \right) + \frac{T_L - T_0}{L} = 0$$

Solving for  $y$  it follows that

$$y_{\text{max}} = \left[ \frac{k}{\mu U^2} (T_L - T_0) + \frac{1}{2} \right] L$$

or for the prescribed conditions

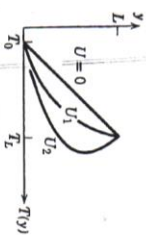
$$y_{\text{max}} = \left[ \frac{0.145 \text{ W}/\text{m} \cdot \text{K}}{0.799 \text{ N} \cdot \text{s}/\text{m}^2 \times 100 \text{ m}^2/\text{s}^2} (30 - 10)^\circ\text{C} + \frac{1}{2} \right] L = 0.536L$$

Substituting the value of  $y_{\text{max}}$  into the expression for  $T(y)$ , it follows that

$$T_{\text{max}} = 89.3^\circ\text{C} \quad \blacktriangleleft$$

**Comments:**

1. Due to the strong effect of viscous dissipation for the prescribed conditions, the maximum temperature occurs in the oil and there is heat transfer to the hot, as well as to the cold, plate. The temperature distribution is a function of the velocity of the moving plate, and the effect is shown schematically below.



For velocities less than  $U_1$  the maximum temperature corresponds to that of the hot plate. For  $U = 0$  there is no viscous dissipation, and the temperature distribution is linear.

2. The properties were evaluated at  $\bar{T} = (T_L + T_0)/2 = 20^\circ\text{C}$ , which is *not* a good measure of the average oil temperature. For more precise calculations, the properties should be evaluated at a more appropriate value of the average temperature (e.g.,  $\bar{T} \approx 55^\circ\text{C}$ ), and the calculations should be repeated.