

# Tema 4

## LEYES DE TRANSPORTE MOLECULAR

*4.1 Cálculo de difusividades en fase gas*

*4.2 Cálculo de difusividades en fase líquida*

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## Cálculo de difusividad en fase gas (I)

*Se pide evaluar el coeficiente de difusión del dióxido de carbono en aire a 20 °C y presión atmosférica. Comparar el valor obtenido con el valor experimental de  $1,55 \cdot 10^{-5} \text{ m}^2/\text{s}$  a la misma temperatura. Emplear la ecuación de Hirschfelder.*

# Cálculo de difusividad en fase gas (I)

## Anexo – Constantes de Lennard-Jones

**Table K.2** Lennard–Jones force constants calculated from viscosity data<sup>†</sup>

| Compound         | Formula                        | $\epsilon_A/\kappa$ , in (K) | $\sigma$ , in Å |
|------------------|--------------------------------|------------------------------|-----------------|
| Acetylene        | C <sub>2</sub> H <sub>2</sub>  | 185                          | 4.221           |
| Air              |                                | 97                           | 3.617           |
| Argon            | A                              | 124                          | 3.418           |
| Arsine           | AsH <sub>3</sub>               | 281                          | 4.06            |
| Benzene          | C <sub>6</sub> H <sub>6</sub>  | 440                          | 5.270           |
| Bromine          | Br <sub>2</sub>                | 520                          | 4.268           |
| <i>i</i> -Butane | C <sub>4</sub> H <sub>10</sub> | 313                          | 5.341           |
| <i>n</i> -Butane | C <sub>4</sub> H <sub>10</sub> | 410                          | 4.997           |
| Carbon dioxide   | CO <sub>2</sub>                | 190                          | 3.996           |

# Cálculo de difusividad en fase gas (I)

## Anexo

### Appendix K

#### Lennard–Jones Constants

Table K.1 The collision integrals,  $\Omega_\mu$  and  $\Omega_D$  based on the Lennard–Jones potential<sup>†</sup>

| $\kappa T/\epsilon$ | $\Omega_\mu = \Omega_k$<br>(for viscosity<br>and thermal<br>conductivity) | $\Omega_D$ (for mass<br>diffusivity) | $kT/\epsilon$ | $\Omega_\mu = \Omega_k$<br>(for viscosity<br>and thermal<br>conductivity) | $\Omega_D$<br>(for mass<br>diffusivity) |
|---------------------|---------------------------------------------------------------------------|--------------------------------------|---------------|---------------------------------------------------------------------------|-----------------------------------------|
| 0.30                | 2.785                                                                     | 2.662                                | 1.75          | 1.234                                                                     | 1.128                                   |
| 0.35                | 2.628                                                                     | 2.476                                | 1.80          | 1.221                                                                     | 1.116                                   |
| 0.40                | 2.492                                                                     | 2.318                                | 1.85          | 1.209                                                                     | 1.105                                   |
| 0.45                | 2.368                                                                     | 2.184                                | 1.90          | 1.197                                                                     | 1.094                                   |
| 0.50                | 2.257                                                                     | 2.066                                | 1.95          | 1.186                                                                     | 1.084                                   |
| 0.55                | 2.156                                                                     | 1.966                                | 2.00          | 1.175                                                                     | 1.075                                   |
| 0.60                | 2.065                                                                     | 1.877                                | 2.10          | 1.156                                                                     | 1.057                                   |
| 0.65                | 1.982                                                                     | 1.798                                | 2.20          | 1.138                                                                     | 1.041                                   |
| 0.70                | 1.908                                                                     | 1.729                                | 2.30          | 1.122                                                                     | 1.026                                   |
| 0.75                | 1.841                                                                     | 1.667                                | 2.40          | 1.107                                                                     | 1.012                                   |
| 0.80                | 1.780                                                                     | 1.612                                | 2.50          | 1.093                                                                     | 0.9996                                  |
| 0.85                | 1.725                                                                     | 1.562                                | 2.60          | 1.081                                                                     | 0.9878                                  |
| 0.90                | 1.675                                                                     | 1.517                                | 2.70          | 1.069                                                                     | 0.9770                                  |
| 0.95                | 1.629                                                                     | 1.476                                | 2.80          | 1.058                                                                     | 0.9672                                  |
|                     |                                                                           |                                      | 2.90          | 1.048                                                                     | 0.9576                                  |

### Appendix K

#### Lennard–Jones Constants

Table K.1 The collision integrals,  $\Omega_\mu$  and  $\Omega_D$  based on the Lennard–Jones potential<sup>†</sup>

| $\kappa T/\epsilon$ | $\Omega_\mu = \Omega_k$<br>(for viscosity<br>and thermal<br>conductivity) | $\Omega_D$ (for mass<br>diffusivity) | $kT/\epsilon$ | $\Omega_\mu = \Omega_k$<br>(for viscosity<br>and thermal<br>conductivity) | $\Omega_D$<br>(for mass<br>diffusivity) |
|---------------------|---------------------------------------------------------------------------|--------------------------------------|---------------|---------------------------------------------------------------------------|-----------------------------------------|
| 1.00                | 1.587                                                                     | 1.439                                | 3.00          | 1.039                                                                     | 0.9490                                  |
| 1.05                | 1.549                                                                     | 1.406                                | 3.10          | 1.030                                                                     | 0.9406                                  |
| 1.10                | 1.514                                                                     | 1.375                                | 3.20          | 1.022                                                                     | 0.9328                                  |
| 1.15                | 1.482                                                                     | 1.346                                | 3.30          | 1.014                                                                     | 0.9256                                  |
| 1.20                | 1.452                                                                     | 1.320                                | 3.40          | 1.007                                                                     | 0.9186                                  |
| 1.25                | 1.424                                                                     | 1.296                                | 3.50          | 0.9999                                                                    | 0.9120                                  |
| 1.30                | 1.399                                                                     | 1.273                                | 3.60          | 0.9932                                                                    | 0.9058                                  |
| 1.35                | 1.375                                                                     | 1.253                                | 3.70          | 0.9870                                                                    | 0.8998                                  |
| 1.40                | 1.353                                                                     | 1.233                                | 3.80          | 0.9811                                                                    | 0.8942                                  |
| 1.45                | 1.333                                                                     | 1.215                                | 3.90          | 0.9755                                                                    | 0.8888                                  |
| 1.50                | 1.314                                                                     | 1.198                                | 4.00          | 0.9700                                                                    | 0.8836                                  |
| 1.55                | 1.296                                                                     | 1.182                                | 4.10          | 0.9649                                                                    | 0.8788                                  |
| 1.60                | 1.279                                                                     | 1.167                                | 4.20          | 0.9600                                                                    | 0.8740                                  |
| 1.65                | 1.264                                                                     | 1.153                                | 4.30          | 0.9553                                                                    | 0.8694                                  |

(continued)

# Cálculo de difusividad en fase gas (I)

Solución:

Ecuación de Hirschfelder

$$D_{AB} = 1,858 \cdot 10^{-7} T^{3/2} \frac{\sqrt{\frac{1}{M_A} + \frac{1}{M_B}}}{\left[ \left( \frac{P}{101325} \right) \left( \frac{\sigma_A + \sigma_B}{2} \right)^2 \Omega \left( T \sqrt{\left( \frac{k}{\varepsilon_A} \right) \cdot \left( \frac{k}{\varepsilon_B} \right)} \right) \right]} \quad \text{m}^2 \cdot \text{s}^{-1}$$

| Término         | Definición                                        | Unidades                         |
|-----------------|---------------------------------------------------|----------------------------------|
| $M_i$           | Peso molecular de la especie i (A soluto, B aire) | $\text{g} \cdot \text{mol}^{-1}$ |
| $\sigma_i$      | Diámetros de colisión de la especie i             | Amstrong                         |
| $\Omega(T_D)$   | Integral de colisión                              |                                  |
| $\varepsilon_i$ | Energía característica de la especie i            | J                                |
| $P$             | Presión                                           | Pa                               |
| $T$             | Temperatura                                       | K                                |
| $k$             | Constante de Boltzmann, $1,38 \cdot 10^{-23}$     | $\text{J} \cdot \text{K}^{-1}$   |

# Cálculo de difusividad en fase gas (I)

Solución:

Ecuación de Hirschfelder

$$D_{AB} = 1,858 \cdot 10^{-7} T^{3/2} \frac{\sqrt{\frac{1}{M_A} + \frac{1}{M_B}}}{\left[ \left( \frac{P}{101325} \right) \left( \frac{\sigma_A + \sigma_B}{2} \right)^2 \Omega \left( T \sqrt{\left( \frac{k}{\epsilon_A} \right) \cdot \left( \frac{k}{\epsilon_B} \right)} \right) \right]} \quad \text{m}^2 \cdot \text{s}^{-1}$$

A → CO<sub>2</sub>  
 B → Aire

$$P = 101325 \text{ Pa}$$

$$M_A = 44 \frac{\text{g}}{\text{mol}}$$

$$M_B = 29 \frac{\text{g}}{\text{mol}}$$

**Table K.2** Lennard-Jones force constants calculated from viscosity data<sup>†</sup>

| Compound         | Formula                        | $\epsilon_A/k$ , in (K) | $\sigma$ , in Å |
|------------------|--------------------------------|-------------------------|-----------------|
| Acetylene        | C <sub>2</sub> H <sub>2</sub>  | 185                     | 4.221           |
| Air              |                                | 97                      | 3.617           |
| Argon            | A                              | 124                     | 3.418           |
| Arsine           | AsH <sub>3</sub>               | 281                     | 4.06            |
| Benzene          | C <sub>6</sub> H <sub>6</sub>  | 440                     | 5.270           |
| Bromine          | Br <sub>2</sub>                | 520                     | 4.268           |
| <i>i</i> -Butane | C <sub>4</sub> H <sub>10</sub> | 313                     | 5.341           |
| <i>n</i> -Butane | C <sub>4</sub> H <sub>10</sub> | 410                     | 4.997           |
| Carbon dioxide   | CO <sub>2</sub>                | 190                     | 3.996           |

$$\sigma_A = 3,996 \text{ Å} \quad \sigma_B = 3,617 \text{ Å}$$

$$\frac{\epsilon_A}{k} = 190$$

$$\frac{\epsilon_B}{k} = 97$$

# Cálculo de difusividad en fase gas (I)

Solución:

Ecuación de Hirschfelder

$$D_{AB} = 1,858 \cdot 10^{-7} T^{3/2} \frac{\sqrt{\frac{1}{M_A} + \frac{1}{M_B}}}{\left[ \left( \frac{P}{101325} \right) \left( \frac{\sigma_A + \sigma_B}{2} \right)^2 \Omega \left( T \sqrt{\left( \frac{k}{\varepsilon_A} \right) \cdot \left( \frac{k}{\varepsilon_B} \right)} \right) \right]} \quad \text{m}^2 \cdot \text{s}^{-1}$$

A → CO<sub>2</sub>  
B → Aire

$$P = 101325 \text{ Pa}$$

$$M_A = 44 \frac{\text{g}}{\text{mol}}$$

$$M_B = 29 \frac{\text{g}}{\text{mol}}$$

$$\sigma_A = 3,996 \text{ Å} \quad \sigma_B = 3,617 \text{ Å}$$

$$\Omega \left( T \sqrt{\left( \frac{k}{\varepsilon_A} \right) \cdot \left( \frac{k}{\varepsilon_B} \right)} \right) = \Omega(293,15 \text{ K} \sqrt{\left( \frac{1}{190} \right) \cdot \left( \frac{1}{97} \right)}) = 2,159$$

$$\frac{\varepsilon_A}{k} = 190$$

$$\frac{\varepsilon_B}{k} = 97$$

# Cálculo de difusividad en fase gas (I)

Solución:

$$\Omega \left( T \sqrt{\left( \frac{k}{\epsilon_A} \right) \cdot \left( \frac{k}{\epsilon_B} \right)} \right) = \Omega \left( 293,15 \text{ K} \sqrt{\left( \frac{1}{190} \right) \cdot \left( \frac{1}{97} \right)} \right) = 2,159$$

$$\frac{kT}{\epsilon} = 2,10 \longrightarrow \Omega_D = 1,057$$

$$\frac{kT}{\epsilon} = 2,20 \longrightarrow \Omega_D = 1,041$$

Interpolación

$$\Omega_D = 1,048$$

## Appendix K

### Lennard-Jones Constants

Table K.1 The collision integrals,  $\Omega_\mu$  and  $\Omega_D$  based on the Lennard-Jones potential<sup>1</sup>

| $kT/\epsilon$ | $\Omega_\mu = \Omega_k$<br>(for viscosity<br>and thermal<br>conductivity) | $\Omega_D$ (for mass<br>diffusivity) | $kT/\epsilon$ | $\Omega_\mu = \Omega_k$<br>(for viscosity<br>and thermal<br>conductivity) | $\Omega_D$<br>(for mass<br>diffusivity) |
|---------------|---------------------------------------------------------------------------|--------------------------------------|---------------|---------------------------------------------------------------------------|-----------------------------------------|
| 0.30          | 2.785                                                                     | 2.662                                | 1.75          | 1.234                                                                     | 1.128                                   |
| 0.35          | 2.628                                                                     | 2.476                                | 1.80          | 1.221                                                                     | 1.116                                   |
| 0.40          | 2.492                                                                     | 2.318                                | 1.85          | 1.209                                                                     | 1.105                                   |
| 0.45          | 2.368                                                                     | 2.184                                | 1.90          | 1.197                                                                     | 1.094                                   |
| 0.50          | 2.257                                                                     | 2.066                                | 1.95          | 1.186                                                                     | 1.084                                   |
| 0.55          | 2.156                                                                     | 1.966                                | 2.00          | 1.175                                                                     | 1.075                                   |
| 0.60          | 2.065                                                                     | 1.877                                | 2.10          | 1.156                                                                     | 1.057                                   |
| 0.65          | 1.982                                                                     | 1.798                                | 2.20          | 1.138                                                                     | 1.041                                   |
| 0.70          | 1.908                                                                     | 1.729                                | 2.30          | 1.122                                                                     | 1.026                                   |
| 0.75          | 1.841                                                                     | 1.667                                | 2.40          | 1.107                                                                     | 1.012                                   |
| 0.80          | 1.780                                                                     | 1.612                                | 2.50          | 1.093                                                                     | 0.9996                                  |
| 0.85          | 1.725                                                                     | 1.562                                | 2.60          | 1.081                                                                     | 0.9878                                  |
| 0.90          | 1.675                                                                     | 1.517                                | 2.70          | 1.069                                                                     | 0.9770                                  |
| 0.95          | 1.629                                                                     | 1.476                                | 2.80          | 1.058                                                                     | 0.9672                                  |
|               |                                                                           |                                      | 2.90          | 1.048                                                                     | 0.9576                                  |

# Cálculo de difusividad en fase gas (I)

Solución:

$$D_{AB} = 1,858 \cdot 10^{-7} T^{3/2} \frac{\sqrt{\frac{1}{M_A} + \frac{1}{M_B}}}{\left[ \left( \frac{P}{101325} \right) \left( \frac{\sigma_A + \sigma_B}{2} \right)^2 \Omega \left( T \sqrt{\left( \frac{k}{\varepsilon_A} \right) \cdot \left( \frac{k}{\varepsilon_B} \right)} \right) \right]}$$

$$D_{AB} = 1,858 \cdot 10^{-7} \cdot 293,15^{3/2} \frac{\sqrt{\frac{1}{44} + \frac{1}{29}}}{\left[ \left( \frac{101325}{101325} \right) \left( \frac{3,996 + 3,617}{2} \right)^2 \cdot 1,048 \right]} = 1,47 \cdot 10^{-5} \frac{\text{m}^2}{\text{s}}$$

$$D_{AB}(\text{experimental}) = 1,55 \cdot 10^{-5} \frac{\text{m}^2}{\text{s}}$$

$$\text{Error} = \frac{1,55 \cdot 10^{-5} \frac{\text{m}^2}{\text{s}} - 1,47 \cdot 10^{-5} \frac{\text{m}^2}{\text{s}}}{1,55 \cdot 10^{-5} \frac{\text{m}^2}{\text{s}}} \cdot 100 = 5,18 \%$$

# Tema 4

## LEYES DE TRANSPORTE MOLECULAR

*4.1 Cálculo de difusividades en fase gas*

*4.2 Cálculo de difusividades en fase líquida*

## Cálculo de difusividad en fase líquida (I)

*El tratamiento de aguas residuales implica en ocasiones el tratamiento con cloro gas. Se pide determinar el coeficiente de difusión líquida de cloro elemental en una solución a dilución infinita a 289 K utilizando la ecuación de Wilke-Chang. Comparar los resultados con el valor experimental  $1,26 \cdot 10^{-9} \text{ m}^2/\text{s}$  a la misma temperatura.*

# Cálculo de difusividad en fase líquida (I)

## Anexo

686 Appendix I

| $T$<br>(K) | $\rho$<br>(kg/m <sup>3</sup> ) | $c_p$<br>(J/kg × K) | $\mu \times 10^6$<br>(Pa × s) | $\nu \times 10^6$<br>(m <sup>2</sup> /s) | $k$<br>(W/m × K) | $\alpha \times 10^6$<br>(m <sup>2</sup> /s) | Pr   | $g\beta\rho^2/\mu^2 \times 10^{-9}$<br>(1/K · m <sup>3</sup> ) |
|------------|--------------------------------|---------------------|-------------------------------|------------------------------------------|------------------|---------------------------------------------|------|----------------------------------------------------------------|
| Water      |                                |                     |                               |                                          |                  |                                             |      |                                                                |
| 273        | 999.3                          | 4226                | 1794                          | 1.795                                    | 0.558            | 0.132                                       | 13.6 |                                                                |
| 293        | 998.2                          | 4182                | 993                           | 0.995                                    | 0.597            | 0.143                                       | 6.96 | 2.035                                                          |
| 313        | 992.2                          | 4175                | 658                           | 0.663                                    | 0.633            | 0.153                                       | 4.33 | 8.833                                                          |
| 333        | 983.2                          | 4181                | 472                           | 0.480                                    | 0.658            | 0.160                                       | 3.00 | 22.75                                                          |
| 353        | 971.8                          | 4194                | 352                           | 0.362                                    | 0.673            | 0.165                                       | 2.57 | 46.68                                                          |
| 373        | 958.4                          | 4211                | 278                           | 0.290                                    | 0.682            | 0.169                                       | 1.72 | 85.09                                                          |
| 473        | 862.8                          | 4501                | 139                           | 0.161                                    | 0.665            | 0.171                                       | 0.94 | 517.2                                                          |
| 573        | 712.5                          | 5694                | 92.2                          | 0.129                                    | 0.564            | 0.139                                       | 0.93 | 1766.0                                                         |

Table 24.4 Molecular volumes at normal boiling point for some commonly encountered compounds

| Compound                        | Molecular volume,<br>in cm <sup>3</sup> /g mol | Compound                           | Molecular volume,<br>in cm <sup>3</sup> /g mol |
|---------------------------------|------------------------------------------------|------------------------------------|------------------------------------------------|
| Hydrogen, H <sub>2</sub>        | 14.3                                           | Nitric oxide, NO                   | 23.6                                           |
| Oxygen, O <sub>2</sub>          | 25.6                                           | Nitrous oxide, N <sub>2</sub> O    | 36.4                                           |
| Nitrogen, N <sub>2</sub>        | 31.2                                           | Ammonia, NH <sub>3</sub>           | 25.8                                           |
| Air                             | 29.9                                           | Water, H <sub>2</sub> O            | 18.9                                           |
| Carbon monoxide, CO             | 30.7                                           | Hydrogen sulfide, H <sub>2</sub> S | 32.9                                           |
| Carbon dioxide, CO <sub>2</sub> | 34.0                                           | Bromine, Br <sub>2</sub>           | 53.2                                           |
| Carbonyl sulfide, COS           | 51.5                                           | Chlorine, Cl <sub>2</sub>          | 48.4                                           |
| Sulfur dioxide, SO <sub>2</sub> | 44.8                                           | Iodine, I <sub>2</sub>             | 71.5                                           |

# Cálculo de difusividad en fase líquida (I)

Solución:

Ecuación de Wilke-Chang

$$D_{BW} = 7,4 \cdot 10^{-8} T \frac{\sqrt{\Phi_W M_W}}{\mu_W [V_B^{0,6}]} \text{ cm}^2\text{s}^{-1}$$

| Término  | Definición                                              | Unidades                          |
|----------|---------------------------------------------------------|-----------------------------------|
| $M_W$    | Peso molecular del agua                                 | $\text{g}\cdot\text{mol}^{-1}$    |
| $\Phi_W$ | Factor de asociación del disolvente -agua- (2,6)        | -                                 |
| $\mu_W$  | Viscosidad del agua                                     | cP                                |
| $V_B$    | Volumen molar del soluto a su temperatura de ebullición | $\text{cm}^3\cdot\text{mol}^{-1}$ |
| T        | Temperatura                                             | K                                 |

\*  $\Phi_W = 2,6$ ;  $\Phi_{disol\ org} = 1$ ;  $\Phi_{Alcoholes} = 1,5$ ; \*\*  $\Phi_W = 2,26$ ;

# Cálculo de difusividad en fase líquida (I)

Solución:

Ecuación de Wilke-Chang

B → Cl<sub>2</sub>  
W → Agua

$$D_{BW} = 7,4 \cdot 10^{-8} T \frac{\sqrt{\Phi_W M_W}}{\mu_W [V_B^{0,6}]}$$

cm<sup>2</sup>·s<sup>-1</sup>

$$M_W = 18 \frac{\text{g}}{\text{mol}} \quad \Phi_W = 2,6$$

| Término  | Definición                                              | Unidades                           |
|----------|---------------------------------------------------------|------------------------------------|
| $M_W$    | Peso molecular del agua                                 | g·mol <sup>-1</sup>                |
| $\Phi_W$ | Factor de asociación del disolvente -agua- (2,6)        | -                                  |
| $\mu_W$  | Viscosidad del agua                                     | cP                                 |
| $V_B$    | Volumen molar del soluto a su temperatura de ebullición | cm <sup>3</sup> ·mol <sup>-1</sup> |
| $T$      | Temperatura                                             | K                                  |

686 Appendix I

| $T$<br>(K) | $\rho$<br>(kg/m <sup>3</sup> ) | $c_p$<br>(J/kg × K) | $\mu \times 10^6$<br>(Pa × s) | $\nu \times 10^6$<br>(m <sup>2</sup> /s) | $k$<br>(W/m × K) | $\alpha \times 10^6$<br>(m <sup>2</sup> /s) | Pr   | $g\beta\rho^2/\mu^2 \times 10^{-9}$<br>(1/K · m <sup>3</sup> ) |
|------------|--------------------------------|---------------------|-------------------------------|------------------------------------------|------------------|---------------------------------------------|------|----------------------------------------------------------------|
| Water      |                                |                     |                               |                                          |                  |                                             |      |                                                                |
| 273        | 999.3                          | 4226                | 1794                          | 1.795                                    | 0.558            | 0.132                                       | 13.6 |                                                                |
| 293        | 998.2                          | 4182                | 993                           | 0.995                                    | 0.597            | 0.143                                       | 6.96 | 2.035                                                          |
| 313        | 992.2                          | 4175                | 658                           | 0.663                                    | 0.633            | 0.153                                       | 4.33 | 8.833                                                          |
| 333        | 983.2                          | 4181                | 472                           | 0.480                                    | 0.658            | 0.160                                       | 3.00 | 22.75                                                          |
| 353        | 971.8                          | 4194                | 352                           | 0.362                                    | 0.673            | 0.165                                       | 2.57 | 46.68                                                          |
| 373        | 958.4                          | 4211                | 278                           | 0.290                                    | 0.682            | 0.169                                       | 1.72 | 85.09                                                          |
| 473        | 862.8                          | 4501                | 139                           | 0.161                                    | 0.665            | 0.171                                       | 0.94 | 517.2                                                          |
| 573        | 712.5                          | 5694                | 92.2                          | 0.129                                    | 0.564            | 0.139                                       | 0.93 | 1766.0                                                         |

$T = 273 \text{ K} \rightarrow \mu_w = 1794 \text{ Pa} \cdot \text{s}$   
 $T = 293 \text{ K} \rightarrow \mu_w = 993 \text{ Pa} \cdot \text{s}$   
{ Interpolación }  
 $\mu_w = 1153,2 \text{ Pa} \cdot \text{s} = 1,15 \text{ cP}$

# Cálculo de difusividad en fase líquida (I)

Solución:

Ecuación de Wilke-Chang

$$D_{BW} = 7,4 \cdot 10^{-8} T \frac{\sqrt{\Phi_W M_W}}{\mu_W [V_B^{0,6}]}$$

$\text{cm}^2 \cdot \text{s}^{-1}$

$$M_W = 18 \frac{\text{g}}{\text{mol}} \quad \Phi_W = 2,6$$

$$\mu_W = 1,15 \text{ cP}$$

B → Cl<sub>2</sub>  
W → Agua

| Término  | Definición                                              | Unidades                            |
|----------|---------------------------------------------------------|-------------------------------------|
| $M_W$    | Peso molecular del agua                                 | $\text{g} \cdot \text{mol}^{-1}$    |
| $\Phi_W$ | Factor de asociación del disolvente -agua- (2,6)        | -                                   |
| $\mu_W$  | Viscosidad del agua                                     | cP                                  |
| $V_B$    | Volumen molar del soluto a su temperatura de ebullición | $\text{cm}^3 \cdot \text{mol}^{-1}$ |
| T        | Temperatura                                             | K                                   |

**Table 24.4** Molecular volumes at normal boiling point for some commonly encountered compounds

| Compound                        | Molecular volume,<br>in $\text{cm}^3/\text{g mol}$ | Compound                           | Molecular volume,<br>in $\text{cm}^3/\text{g mol}$ |
|---------------------------------|----------------------------------------------------|------------------------------------|----------------------------------------------------|
| Hydrogen, H <sub>2</sub>        | 14.3                                               | Nitric oxide, NO                   | 23.6                                               |
| Oxygen, O <sub>2</sub>          | 25.6                                               | Nitrous oxide, N <sub>2</sub> O    | 36.4                                               |
| Nitrogen, N <sub>2</sub>        | 31.2                                               | Ammonia, NH <sub>3</sub>           | 25.8                                               |
| Air                             | 29.9                                               | Water, H <sub>2</sub> O            | 18.9                                               |
| Carbon monoxide, CO             | 30.7                                               | Hydrogen sulfide, H <sub>2</sub> S | 32.9                                               |
| Carbon dioxide, CO <sub>2</sub> | 34.0                                               | Bromine, Br <sub>2</sub>           | 53.2                                               |
| Carbonyl sulfide, COS           | 51.5                                               | Chlorine, Cl <sub>2</sub>          | 48.4                                               |
| Sulfur dioxide, SO <sub>2</sub> | 44.8                                               | Iodine, I <sub>2</sub>             | 71.5                                               |

$$V_B = 48,4 \frac{\text{cm}^3}{\text{mol}}$$

# Cálculo de difusividad en fase líquida (I)

Solución:

Ecuación de Wilke-Chang

$$D_{BW} = 7,4 \cdot 10^{-8} T \frac{\sqrt{\Phi_W M_W}}{\mu_W [V_B^{0,6}]}$$

$M_W = 18 \frac{\text{g}}{\text{mol}} \quad \Phi_W = 2,6$   
 $\mu_W = 1,15 \text{ cP} \quad V_B = 48,4 \frac{\text{cm}^3}{\text{mol}}$

B → Cl<sub>2</sub>  
W → Agua

| Término  | Definición                                              | Unidades                           |
|----------|---------------------------------------------------------|------------------------------------|
| $M_W$    | Peso molecular del agua                                 | g·mol <sup>-1</sup>                |
| $\Phi_W$ | Factor de asociación del disolvente -agua- (2,6)        | -                                  |
| $\mu_W$  | Viscosidad del agua                                     | cP                                 |
| $V_B$    | Volumen molar del soluto a su temperatura de ebullición | cm <sup>3</sup> ·mol <sup>-1</sup> |
| T        | Temperatura                                             | K                                  |

$$D_{BW} = 7,4 \cdot 10^{-8} \cdot 289 \cdot \frac{\sqrt{2,6 \cdot 18 \frac{\text{g}}{\text{mol}}}}{1,15 \text{ cP} \cdot [48,4^{0,6}]} = 1,24 \cdot 10^{-5} \frac{\text{cm}^2}{\text{s}}$$

# Cálculo de difusividad en fase líquida (I)

Solución:

Ecuación de Wilke-Chang

$$D_{BW} = 7,4 \cdot 10^{-8} T \frac{\sqrt{\Phi_W M_W}}{\mu_W [V_B^{0,6}]}$$

$\text{cm}^2 \cdot \text{s}^{-1}$

$$M_W = 18 \frac{\text{g}}{\text{mol}} \quad \Phi_W = 2,6$$

$$\mu_W = 1,15 \text{ cP} \quad V_B = 48,4 \frac{\text{cm}^3}{\text{mol}}$$

$$D_{BW} = 1,24 \cdot 10^{-5} \frac{\text{cm}^2}{\text{s}}$$

$$\text{Error} = \frac{1,26 \cdot 10^{-5} \frac{\text{m}^2}{\text{s}} - 1,24 \cdot 10^{-5} \frac{\text{cm}^2}{\text{s}}}{1,26 \cdot 10^{-5} \frac{\text{cm}^2}{\text{s}}} \cdot 100 = 1,81 \%$$

B → Cl<sub>2</sub>  
W → Agua

| Término  | Definición                                              | Unidades                            |
|----------|---------------------------------------------------------|-------------------------------------|
| $M_W$    | Peso molecular del agua                                 | $\text{g} \cdot \text{mol}^{-1}$    |
| $\Phi_W$ | Factor de asociación del disolvente -agua- (2,6)        | -                                   |
| $\mu_W$  | Viscosidad del agua                                     | cP                                  |
| $V_B$    | Volumen molar del soluto a su temperatura de ebullición | $\text{cm}^3 \cdot \text{mol}^{-1}$ |
| T        | Temperatura                                             | K                                   |

## Cálculo de difusividad en fase líquida (II)

*En ocasiones se añade benceno al etanol para su desnaturalización. Estimar el coeficiente de difusión en fase líquida de benceno en etanol y de etanol en benceno a 288 K utilizando la ecuación de Wilke-Chang. Se conoce que a la temperatura solicitada los valores de la viscosidad dinámica son  $\mu_{\text{C}_6\text{H}_6}=0,75$  cP,  $\mu_{\text{C}_2\text{H}_5\text{OH}}=1,3$  cP, así como que los valores de los volúmenes molares del soluto a su temperatura de ebullición son  $V_{\text{B,C}_6\text{H}_6}=95,8$  cm<sup>3</sup>/mol,  $V_{\text{B,C}_2\text{H}_5\text{OH}}=59,2$  cm<sup>3</sup>/mol.*

# Cálculo de difusividad en fase líquida (II)

## Anexo

### 24.2 The Diffusion Coefficient 417

**Table 24.5** Atomic volumes for complex molecular volumes for simple substances<sup>†</sup>

| Element                       | Atomic volume,<br>in cm <sup>3</sup> /g mol | Element                                      | Atomic volume,<br>in cm <sup>3</sup> /g mol |
|-------------------------------|---------------------------------------------|----------------------------------------------|---------------------------------------------|
| Bromine                       | 27.0                                        | Oxygen, except as noted below                | 7.4                                         |
| Carbon                        | 14.8                                        | Oxygen, in methyl esters                     | 9.1                                         |
| Chlorine                      | 21.6                                        | Oxygen, in methyl ethers                     | 9.9                                         |
| Hydrogen                      | 3.7                                         | Oxygen, in higher ethers<br>and other esters | 11.0                                        |
| Iodine                        | 37.0                                        | Oxygen, in acids                             | 12.0                                        |
| Nitrogen, double bond         | 15.6                                        | Sulfur                                       | 25.6                                        |
| Nitrogen, in primary amines   | 10.5                                        |                                              |                                             |
| Nitrogen, in secondary amines | 12.0                                        |                                              |                                             |

<sup>†</sup>G. Le Bas, *The Molecular Volumes of Liquid Chemical Compounds*, Longmans, Green & Company, Ltd., London, 1915.

corrections are recommended:

|                                            |             |
|--------------------------------------------|-------------|
| for three-membered ring, as ethylene oxide | deduct 6    |
| for four-membered ring, as cyclobutane     | deduct 8.5  |
| for five-membered ring, as furan           | deduct 11.5 |
| for pyridine                               | deduct 15   |
| for benzene ring                           | deduct 15   |
| for naphthalene ring                       | deduct 30   |
| for anthracene ring                        | deduct 47.5 |

Recommended values of the association parameter,  $\Phi_B$ , are given below for a few common solvents.

| Solvent                                                     | $\Phi_B$           |
|-------------------------------------------------------------|--------------------|
| Water                                                       | 2.26 <sup>17</sup> |
| Methanol                                                    | 1.9                |
| Ethanol                                                     | 1.5                |
| Benzene, ether, heptane,<br>and other unassociated solvents | 1.0                |

If data for computing the molar volume of solute at its normal boiling point,  $V_A$ , are not available, Tyn and Calus<sup>18</sup> recommend the correlation

$$V_A = 0.285V_c^{1.048}$$

where  $V_c$  is the critical volume of species A in cm<sup>3</sup>/g. mol. Values of  $V_c$  are tabulated in Reid, Prausnitz, and Sherwood.<sup>19</sup>

<sup>17</sup> The correction of  $\Phi_B$  is recommended by R. C. Reid, J. M. Prausnitz, and T. K. Sherwood, *The Properties of Gases and Liquids*, Third Edition, McGraw-Hill Book Company, New York, 1977, p. 578.

## Cálculo de difusividad en fase líquida (II)

Solución:

Ecuación de Wilke-Chang

$$D_{BW} = 7,4 \cdot 10^{-8} T \frac{\sqrt{\Phi_W M_W}}{\mu_W [V_B^{0,6}]} \text{ cm}^2\text{s}^{-1}$$

| Término  | Definición                                              | Unidades                          |
|----------|---------------------------------------------------------|-----------------------------------|
| $M_W$    | Peso molecular del disolvente                           | $\text{g}\cdot\text{mol}^{-1}$    |
| $\Phi_W$ | Factor de asociación del disolvente                     | -                                 |
| $\mu_W$  | Viscosidad del disolvente                               | cP                                |
| $V_B$    | Volumen molar del soluto a su temperatura de ebullición | $\text{cm}^3\cdot\text{mol}^{-1}$ |
| T        | Temperatura                                             | K                                 |

\*  $\Phi_W = 2,6$ ;  $\Phi_{disol\ org} = 1$ ;  $\Phi_{Alcoholes} = 1,5$ ; \*\*  $\Phi_W = 2,26$ ;

# Cálculo de difusividad en fase líquida (II)

Solución:

B → Benceno  
W → Etanol

$$D_{BW} = 7,4 \cdot 10^{-8} T \frac{\sqrt{\Phi_W M_W}}{\mu_W [V_B^{0,6}]}$$

cm<sup>2</sup>·s<sup>-1</sup>

$$T = 288 \text{ K} \quad M_W = 46 \frac{\text{g}}{\text{mol}} \quad \Phi_W = 1,5$$

$$\mu_W = 1,3 \text{ cP} \quad V_{B,\text{benceno}} = 95,8 \text{ cm}^3/\text{mol}$$

| Término  | Definición                                              | Unidades                           |
|----------|---------------------------------------------------------|------------------------------------|
| $M_W$    | Peso molecular del disolvente                           | g·mol <sup>-1</sup>                |
| $\Phi_W$ | Factor de asociación del disolvente                     | -                                  |
| $\mu_W$  | Viscosidad del disolvente                               | cP                                 |
| $V_B$    | Volumen molar del soluto a su temperatura de ebullición | cm <sup>3</sup> ·mol <sup>-1</sup> |
| T        | Temperatura                                             | K                                  |

$$D_{BW} = 7,4 \cdot 10^{-8} \cdot 288 \cdot \frac{\sqrt{1,5 \cdot 46 \frac{\text{g}}{\text{mol}}}}{1,3 \text{ cP} \cdot [95,8^{0,6}]} = 8,81 \cdot 10^{-6} \frac{\text{cm}^2}{\text{s}}$$

# Cálculo de difusividad en fase líquida (II)

Solución:

Ecuación de Wilke-Chang

$$D_{BW} = 7,4 \cdot 10^{-8} T \frac{\sqrt{\Phi_W M_W}}{\mu_W [V_B^{0,6}]} \text{ cm}^2 \cdot \text{s}^{-1}$$

$$T = 288 \text{ K} \quad M_W = 78 \frac{\text{g}}{\text{mol}} \quad \Phi_W = 1$$

$$\mu_W = 0,75 \text{ cP} \quad V_{B,\text{etanol}} = 59,2 \text{ cm}^3/\text{mol}$$

$$D_{BW} = 7,4 \cdot 10^{-8} \cdot 288 \cdot \frac{\sqrt{1,0 \cdot 78 \frac{\text{g}}{\text{mol}}}}{0,75 \text{ cP} \cdot [59,2^{0,6}]} = 2,17 \cdot 10^{-5} \frac{\text{cm}^2}{\text{s}}$$

B → Etanol  
W → Benceno

| Término  | Definición                                              | Unidades                            |
|----------|---------------------------------------------------------|-------------------------------------|
| $M_W$    | Peso molecular del disolvente                           | $\text{g} \cdot \text{mol}^{-1}$    |
| $\Phi_W$ | Factor de asociación del disolvente                     | -                                   |
| $\mu_W$  | Viscosidad del disolvente                               | cP                                  |
| $V_B$    | Volumen molar del soluto a su temperatura de ebullición | $\text{cm}^3 \cdot \text{mol}^{-1}$ |
| T        | Temperatura                                             | K                                   |