Let’s put this to use

### Various forms of the Microscopic Species A Mass Balance

<table>
<thead>
<tr>
<th>Five Microscopic species A mass balance—Six forms</th>
</tr>
</thead>
<tbody>
<tr>
<td>In terms of mass flux and mass concentrations $\rho \left( \frac{\partial \omega_A}{\partial t} + \nabla \cdot \omega_A \right) = -\nabla \cdot j_A + r_A$ $= \rho D_{AB} \nabla^2 \omega_A + r_A$</td>
</tr>
<tr>
<td>In terms of molar flux and molar concentrations $c \left( \frac{\partial x_A}{\partial t} + \nabla \cdot x_A \right) = -\nabla \cdot j_A + (x_B R_A - x_A R_B)$ $= cD_{AB} \nabla^2 x_A + (x_B R_A - x_A R_B)$</td>
</tr>
<tr>
<td>In terms of combined molar flux and molar concentrations $\frac{\partial c_A}{\partial t} = -\nabla \cdot \mathbf{N}_A + R_A$</td>
</tr>
</tbody>
</table>

(The $\mathbf{N}_A$ version, with Fick’s law substituted in, provides little advantage.)

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Various forms of Fick’s Law (and the species mass balances that employ them)

<table>
<thead>
<tr>
<th>Mass flux</th>
<th>Molar flux</th>
<th>Combined molar flux</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I_A = -\rho D_{AB} \nabla \omega_A$</td>
<td>$I_A^* = -c D_{AB} \nabla x_A$</td>
<td>$N_A = x_A (N_A + N_B) - c D_{AB} \nabla x_A$</td>
</tr>
</tbody>
</table>
Various quantities in diffusion and mass transfer

How much is present: \[ c_A = c_4 = \frac{1}{M_A} (\rho_A) = \frac{1}{M_A} (\rho \omega_A) \]

- \( I_A \) is \textit{mass} flux of species \( A \) relative to a mixture’s \textit{mass average velocity}, \( \bar{v} \)
  \[ I_A = \rho_A (\bar{v}_A - \bar{v}) \]
  \( I_A + I_B = 0 \), i.e. these fluxes are measured relative to the mixture’s center of mass

- \( I_A^* \) is \textit{molar} flux relative to a mixture’s \textit{molar average velocity}, \( \bar{v}^* \)
  \[ I_A^* = c_A (\bar{v}_A - \bar{v}^*) \]
  \( I_A^* + I_B^* = 0 \)

- \( N_A \) is \textit{mass} flux of species \( A \) in a mixture, i.e. average velocity of all molecules of species \( A \) within a small volume
  \( \bar{v} = \omega_A \bar{v}_A + \omega_B \bar{v}_B \) is mass average velocity; same velocity as in the microscopic momentum and energy balances
  \( \bar{v}^* = x_A \bar{v}_A + x_B \bar{v}_B \) is molar average velocity

Example: Heterogeneous catalysis in a reactor
An irreversible, instantaneous chemical reaction \((2A \rightarrow B)\) takes place at a catalyst surface in a reactor as shown. How might mass transfer affect the observed rate of reaction?

### Modeling Questions:

- Where does mass transfer take place?
- What is the concentration distribution like in the gas?
- Does the shape of the particles matter?
- What is the impact of the overall (bulk) flow?
- What should be our first modeling problem?
Example: Heterogeneous catalysis

An irreversible, instantaneous chemical reaction \((2A \rightarrow B)\)

More Modeling Questions:

How fast will this happen?
Does it depend on the reaction rate?
What else does it depend on?
What can we learn about the unit’s mass transfer character?

Example: Water (40°C, 1.0 atm) slowly and steadily evaporates into nitrogen (80°C, 1.0 atm) from the bottom of a cylindrical tank as shown in the figure below. A stream of dry nitrogen flows slowly past the open tank. The mole fraction of water in the gas at the top opening of the tank is 0.02. What is the rate of water evaporation?

Modeling Inspiration:

There may be a stagnant region between the source and sink that must be traversed.
An irreversible, instantaneous chemical reaction \((2A \rightarrow B)\) takes place at a catalyst surface, as shown. The reaction is "diffusion-limited," however, because the rate of completion of the reaction is determined by the rate of diffusion through the "film" near the catalyst surface. Calculate the steady state composition distribution in the film \((x_d(z))\).
Which approach is best for solving the model?

Solve

See hand notes for the start (Example 3) Solution assigned in HW4a
Problem Summary: Heterogeneous Chemical Reaction

- One-dimensional (1D)
- Steady
- Use molar flux (due to reaction)
- Use combined molar flux \( N_A \); we can draw modeling simplifications about \( N_B \) due to fast reaction
- Needed stoichiometry
- Boundary conditions: concentrations known (fast reaction \( \Rightarrow A \) disappears at surface.)

Example: Heterogeneous catalysis

An irreversible, instantaneous chemical reaction \((2A \rightarrow B)\) takes place at a catalyst surface, as shown. The reaction is “diffusion-limited,” however, because the rate of completion of the reaction is determined by the rate of diffusion through the “film” near the catalyst surface. Calculate the steady state composition distribution in the film \((x(t))\).

Could we have used \( f_A \) instead?

Various forms of Fick’s Law

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## 1D Steady Diffusion—Heterogeneous Chemical Reaction

### Equation of Species Mass Balance in Terms of Molar Quantities

<table>
<thead>
<tr>
<th>Equation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( J^*_A )</td>
<td>Molar flux relative to a mixture's molar average velocity ( v^* )</td>
</tr>
<tr>
<td>( \dot{N}_A )</td>
<td>Rate of production of moles of ( A ) by homogeneous chemical reaction per volume</td>
</tr>
</tbody>
</table>

#### Definition:

- **Fick's law:**
  \( J^*_A = c x_A (v_A - v^*) \)

- **Microscopic species A mass balance:**
  \( c \left( \frac{\partial x_A}{\partial t} + v^* \cdot \nabla x_A \right) = c D_{AB} \nabla^2 x_A + \left( x_B R_A - x_A R_B \right) \)

#### Could we have used \( J_A \) instead?

### Various Forms of Fick's Law

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1D Steady Diffusion—Heterogeneous Chemical Reaction

### Equation of Species Mass Balance

#### In Cartesian, cylindrical, and spherical coordinates for three-valued fluid:

Tomato sauce: mixed tomato sauce with fluid.

- \( \frac{\partial \omega_i}{\partial t} + \nabla \cdot (\rho \mathbf{v}_\text{m} \omega_i) = - \nabla \cdot (\rho D_{i,j} \nabla \omega_j) + r_i \)

#### In Cartesian, cylindrical, and spherical coordinates for three-valued fluid:

- \( \frac{\partial \omega_i}{\partial t} + \nabla \cdot (\rho \mathbf{v}_\text{m} \omega_i) = - \nabla \cdot (\rho D_{i,j} \nabla \omega_j) + r_i \)

#### Microscopic species A mass balance:

- \( \dot{j}_A = \rho \omega_A (\mathbf{v}_\text{m} - \mathbf{v}) \)

- Fick’s law:

- \( \dot{j}_A = - \rho D_{AB} \nabla \omega_A \)

- Microscopic species A mass balance:

- \( \rho \left( \frac{\partial \omega_A}{\partial t} + \mathbf{v} \cdot \nabla \omega_A \right) = \rho D_{AB} \nabla^2 \omega_A + r_A \)

### Flux choice

- **Molar** because there is a reaction
- **Combined molar** because the convection is only due to diffusion

### Problem Summary: Heterogeneous Chemical Reaction

- One-dimensional (1D)
- Steady
- Use molar flux (due to reaction)
- Use combined molar flux \( N_A \); we can draw modeling simplifications about \( N_B \) due to fast reaction)
- Needed stoichiometry
- Boundary conditions: concentrations known (fast reaction \( A \) disappears at surface).

**Example:** Heterogeneous catalysts

- An irreversible, instantaneous chemical reaction (\( 2A \rightarrow B \)) takes place at a catalyst surface, as shown. The reaction is “diffusion-limited,” however, because the rate of completion of the reaction is determined by the rate of diffusion through the “film” near the catalyst surface. Calculate the steady state composition distribution in the film \( x_A(x) \)
Example: Mass transfer in Distillation

In general, the molar flow rates in the enriching ($L, V$) and stripping ($\text{\textit{L}}_{\text{t}}, \text{\textit{V}}_{\text{t}}$) sections are not equal.

This is only true if every time a mole of vapor is condensed, a mole of liquid is vaporized (Constant Molal Overflow)

**Constant Molal Overflow (CMO)**

1. The heat of vaporization per mole $\lambda$ is constant (independent of concentration)
2. Specific heat changes are small compared to latent heat changes
3. The column is adiabatic
4. The saturated liquid and vapor lines on an enthalpy-composition diagram (in molar units) are parallel

Wankat, pp110-1
Diffusion Lectures 7 & 8 Modeling 1D Steady Diffusion

1D Steady Diffusion—Equimolar Counter Diffusion

**Example:** Distillation (continued)

“This is only true if every time a mole of vapor is condensed, a mole of liquid is vaporized (Constant Molal Overflow)”

This condition is met by equimolar counter diffusion.

\[ \psi_A = -\psi_B \]
\[ N_A = -N_B \]

\[ N_A + N_B = c \psi^* \]
\[ \psi^* = 0 \]

---

1D Steady Diffusion—Equimolar Counter Diffusion

**Example:** Mass transfer in distillation (continued)

Equimolar Counter Diffusion

A distillation column is separating two components \(A\) and \(B\) at steady state. In the vapor phase the two components are moving in equimolar counter diffusion. What are the molar fluxes of \(A\) and \(B\)? What is the concentration distribution in the region of the equimolar counter diffusion?

Wankat, pp110-1
Which approach is best for solving the model?

Various forms of Fick's Law (and the species mass balances that employ them):

- Mol flux: \( j_a = -D_{ab} \frac{\partial c_b}{\partial x} \)
- Molar flux: \( j_a = -D_{ab} \frac{\partial x_b}{\partial x} \)
- Combined flux: \( j_a = x_a (\Delta x_a + \Delta x_b) - \Delta D_{ab} \Delta x_a \)

Solve
See hand notes for the start (Example 4) Solution assigned in HW4a

Which approach is best for solving the model?

Solve

Could we have used \( J_A \) instead?

Various forms of Fick’s Law

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</table>

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1D Steady Diffusion—Equimolar Counter Diffusion

**Equation of Species Mass Balance in Terms of Molar Quantities**

In Cartesian coordinates, the time rate of change of mass balance for species \( i \) is given by:

\[
\frac{\partial}{\partial t} \left( \rho c_i \right) + \nabla \cdot (\rho v_i c_i) = \frac{\partial}{\partial t} \left( \rho \frac{\partial c_i}{\partial x} \right) + \rho v_i \frac{\partial c_i}{\partial x} + \rho R_{i,A} - \rho R_{i,B}
\]

where \( \rho \) is the density, \( c_i \) is the molar concentration of species \( i \), \( v_i \) is the species concentration-averaged velocity, \( R_{i,A} \) is the rate of production of moles of \( A \) by homogeneous chemical reaction per volume, and \( R_{i,B} \) is the rate of production of moles of \( B \) by homogeneous chemical reaction per volume.

**Molar Flux**

\( J_A^* \)

**Molar Flux relative to a mixture's molar average velocity \( v^* \)**

**Definition:**

\( J_A^* = c x_A (v_A - v^*) \)

**Fick’s Law:**

\( J_A^* = -c D_A \nabla x_A \)

**Microscopic Species A Mass Balance:**

\[ c \left( \frac{\partial x_A}{\partial t} + u^* \cdot \nabla x_A \right) = c D_A \nabla^2 x_A + (x_BR_A - x_AR_B) \]

(The two fluxes are the same for equimolar counter diffusion)

**Could we have used \( J_A \) instead?**

**Various Forms of Fick’s Law**

- **Mass Flux:**
  \[ j_A = -\rho D_A \nabla c_A \]

- **Molar Flux:**
  \[ J_A = -c D_A \nabla x_A \]

- **Combined Molar Flux:**
  \[ N_A = x_A (N_A + N_B) - c D_A \nabla x_A \]

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**1D Steady Diffusion—Equimolar Counter Diffusion**

**Equation of Species Mass Balance** in Cartesian, spherical, and cylindrical coordinates for these solutions of (Laplace). Two cases are presented: the general case, wherein the flux with respect to the mass average velocity, \( \mathbf{v} \) is given in Eq. (1); and the case used here, \( \mathbf{v}^* \), wherein the flux is with respect to an average velocity, \( \mathbf{v}^* \).

**Definition:**
Fick’s law:

\[
\mathbf{j}_A = \rho \omega_A \mathbf{v}_A - \rho \mathbf{v}
\]

**Microscopic species A mass balance:**

\[
\rho \left( \frac{\partial \omega_A}{\partial t} + \mathbf{v} \cdot \nabla \omega_A \right) = \rho D_{AB} \mathbf{v}^2 \omega_A + r_A
\]

\( r_A \equiv \text{rate of production of mass of } A \text{ by homogeneous chemical reaction per volume} \)

**Problem Summary:** Equimolar Counter Diffusion

- One-dimensional (1D)
- Steady
- Use molar flux (due to equimolar counter diffusion specified)
- Use combined molar flux \( N_A \) or \( \mathbf{j}_A \)
- Boundary conditions: concentrations known over a known distance

**Flux choice**

Choose:
- **Molar** because equimolar motion was specified
- **Combined molar and molar** are the same when \( \mathbf{v}^* = 0 \) (\( N_A = \mathbf{j}_A \))

\[
\mathbf{j}_A = c \mathbf{v}_A (\mathbf{v}_A - \mathbf{v}^*)
\]

These two molar fluxes are the same when \( \mathbf{v}^* = 0 \).
Problems Summary

1. Unimolecular mass transfer (evaporating tank, Ex 1)

✓ 2. Heterogeneous chemical reaction (catalytic converter, Ex 3, convection only due to diffusion)

✓ 3. Equimolar counter diffusion (distillation, $\nu^* = 0$, $(N_A = \int_A)$ Ex 4)

4. Homogeneous chemical reaction

We did this earlier → Could we have taken a different approach?
Example: Water (40°C, 1.0 atm) slowly and steadily evaporates into nitrogen (40°C, 1.0 atm) from the bottom of a cylindrical tank as shown in the figure below. A stream of dry nitrogen flows slowly past the open tank. The mole fraction of water in the gas at the top opening of the tank is 0.02. What is the rate of water evaporation?

Could we have used $J_A$ instead?
Equation of Species Mass Balance in Terms of Molar quantities

\[ J_A^* = \frac{N_A}{v_{f*}} \]

Fick's law:

\[ I_A = c x_A (v_A - v^*) \]

Microscopic species A mass balance:

\[ c \left( \frac{\partial x_A}{\partial t} + v^* \cdot \nabla x_A \right) = c D_{AB} \nabla^2 x_A + (x_B R_A - x_A R_B) \]

(Let's explore \( v^* \) in some limits)

\[ R_A = \text{rate of production of moles of } A \text{ by homogeneous chemical reaction per volume} \]

Could we have used \( I_A \) instead of \( N_A \)?

Definition:

\[ I_A = c x_A (v_A - v^*) \]

When is \( v^* = 0? \)

- \( B \) is stagnant \( \Rightarrow v_B = 0 \).
- If \( A \) is dilute, \( x_A \approx 0 \).
- then, \( v^* \approx 0 \).

\( I_A \) and \( N_A \) are equal for stagnant \( B \), dilute \( A \)
Could we have used $j_A$ instead?

Various forms of Fick's Law (and the species mass balances that employ them)

**Mass flux**

$$j_A = -\rho D_{AB} \omega_A$$

**Molar flux**

$$j_A^\text{m} = -\rho D_{AB} \omega_A$$

**Combined molar flux**

$$N_A = x_A (N_A + N_B) - cD_{AB} \omega_A$$

---

1D Steady Diffusion—Unimolecular Mass Transfer (film theory)

**Equation of Species Mass Balance**

$${\partial \omega_A \over \partial t} + \nabla \cdot (\rho \omega_A \mathbf{v}) = \rho D_{AB} \nabla^2 \omega_A + r_A$$

- $\omega_A$: concentration of species A
- $\rho$: density
- $\mathbf{v}$: mixture's mass average velocity
- $D_{AB}$: diffusion coefficient of species A in species B
- $r_A$: rate of production of mass of A by homogeneous chemical reaction per volume

**Microscopic species A mass balance**

$$\rho \left( {\partial \omega_A \over \partial t} + \mathbf{v} \cdot \nabla \omega_A \right) = \rho D_{AB} \nabla^2 \omega_A + r_A$$

**Fick's law**

$$j_A = \rho \omega_A (\mathbf{v} - \mathbf{u})$$

---

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Diffusion Lectures 7 & 8 Modeling 1D Steady Diffusion

1D Steady Diffusion—Unimolecular Mass Transfer (film theory)

\[ j_A: \text{ Mass flux relative to a mixture's mass average velocity } v \]

**Definition:**
\[ j_A = \rho \omega_A (v_A - v) \]

**Fick's law:**
\[ j_A = -\rho D_{AB} \nabla \omega_A \]

**Microscopic species A mass balance:**
\[ \rho \left( \frac{\partial \omega_A}{\partial t} + v \cdot \nabla \omega_A \right) = \rho D_{AB} \nabla^2 \omega_A + r_A \]

\[ r_A = \text{ rate of production of mass of } A \text{ by homogeneous chemical reaction per volume} \]

**Problem Summary:** Unimolecular Mass Transfer (film theory)

- One-dimensional (1D)
- Steady
- Use molar flux
- Use combined molar flux \( N_A \)
- Boundary conditions: concentrations known over a known distance

**Flux choice**
Choose:
- **Molar** because mole fractions specified
- **Combined molar and molar** are the same when \( B \) is stagnant and \( A \) is dilute (implies \( v^* = 0 \))
Gas Absorption

While a chemical plant would not exist without the chemical reactors, the biggest expense (the biggest equipment) will often be the separation equipment, distillation columns and gas absorption columns.

- Packed column (tower)
- Liquid poured into top trickles down through packing
- Gas pumped into bottom flows upward
- Analysis involves both fluid mechanics (determines cross-sectional area) and mass transfer (determines height)
Gas Absorption

Exiting liquid stream contains high concentrations of the impurity. This is later "stripped" by heating the liquid so that the impurity bubbles out.

The "swing" in temperature may sometimes be replaced by a "swing" in pressure (lowers costs)

Gas Absorption Packing

High fluid flow trades off with high interfacial area (both are desired)

6 types of random packing; cheaper, common

Structured packing; pricey, more efficient (up to 30% more efficient); fluids move past each other with less bypassing
Gas Absorption - the liquids

What are the gases to be absorbed? What are the liquids that absorb them?

Choice depends on the concentrations in the feed gas mixture and on the desired percent removal.

**High concentration (10-50%):** dissolve in a nonvolatile, nonreactive liquid, aka **physical solvent** (less common, but simpler).

**Lower concentration (1-10%):** use liquid capable of fast, reversible chemical reaction with the gas to be removed, aka **chemical solvent** (20X more common, but complex).

**Very low concentration (<1%):** use an adsorbent that reacts irreversibly (this is expensive; may produce solid waste).

Some depend on the solubility of the gas.

Most react chemically with the components of the gas.

---

Gas Absorption Tower Design

A type of “differential contacting”

**Design:** Diameter, Height

- **Diameter:** constrained by the fluid mechanics of the gas and liquid flowing past each other; complicated; described by largely empirical correlations (use turnkey procedure).
- **Height:** must be sufficient to attain the separation desired; depends on how solubility depends on concentration (linear or nonlinear isotherm, dilute (easy), not dilute (hard)).
Gas Absorption Tower Design

A type of “differential contacting”

**Design:** Diameter, Height

- **Diameter:** constrained by the fluid mechanics of the gas and liquid flowing past each other; complicated; described by largely empirical correlations (use turnkey procedure)
- **Height:** must be sufficient to attain the separation desired; depends on how solubility depends on concentration (linear or nonlinear isotherm, dilute (easy), not dilute (hard))

*Can be modeled.*

---

**Column height** must be sufficient to attain the separation desired.

We need a *model* of how the separation is achieved to produce the design equations for the height of the column.

- A model that *works* will reveal what the physics of the unit is.
- Models that *only partially work* also reveal important aspects of the physics.
The packed column is designed to create interfacial area between the liquid and gas.

We focus on the liquid-gas interface where the mass transfer takes place.

**Idealize** the entire device as comprising only the appropriate amount of this interface, with mass transfer taking place.

**Retain the role of the column**, by forcing the appropriate concentrations of species $A$ enter and exit the column.
A gas absorption column is operating at steady state. The gas stream is composed of component $A$ and an inert carrier gas $I$. The liquid stream is chemical absorbent $B$. Component $A$ diffuses across the gas-liquid interface until it reacts with $B$. What are the molar fluxes of $A$ and $B$? What is the concentration distribution in the region in which $A$ diffuses into liquid $B$?
Model of Gas Absorption in a Column

- Liquid $B$ attracts $A$; the concentration of $A$ increases as the liquid passes through the column.

$L, G$  
$X_{A1}, Y_{A1}$  
$A$-free molar flow rates  
Molar ratios of $A$

1D Steady Diffusion—Gas Absorption with Chemical Solvent

Example: Heterogeneous catalysis

Use a “penetration model”

The action of the chemical solvent $B$ (absorbent) modeled as a homogeneous chemical reaction taking place in the penetration region.

$A + B \rightarrow AB$

$R_A = -k_1c_A$
1D Steady Diffusion—Gas Absorption with Chemical Solvent

Which approach is best for solving the model?

Various forms of Fick’s Law and the species mass balances that employ them:

Mass flux: \( \dot{m}_A = -D_A \frac{\partial C_A}{\partial z} \)

Molar flux: \( \dot{n}_A = -D_A \frac{\partial Y_A}{\partial z} \)

Volumetric flux: \( \dot{V}_A = \frac{\dot{n}_A}{\rho_A} = \frac{-D_A}{\rho_A} \frac{\partial C_A}{\partial z} \)

Slow-moving region into which \( A \) “penetrates”

Liquid \( A, B \) (well mixed)

The chemical solvent (absorbent) appears as a homogeneous chemical reaction in the penetration region.

1D Steady Diffusion—Gas Absorption with Chemical Solvent

Which approach is best for solving the model?

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See hand notes for the start (Example 5)
Solution assigned in HW4a

1D Steady Diffusion—Gas Absorption with Chemical Solvent

Problem Summary: Gas Absorption with Chemical Solvent

- One-dimensional (1D)
- Steady
- Use molar flux (due to reaction)
- Use combined molar flux $N_A$
- Needed stoichiometry and rate equation
- Boundary conditions: concentrations known ($A$ disappears at penetration length)

The chemical solvent (absorbent) appears as a homogeneous chemical reaction in the penetration region.
Could we have used $J_A$ instead?

**Various forms of Fick's Law**

**Mass flux**

$$j_{\text{m}} = -D_{\text{m}} \frac{\partial c}{\partial x}$$

**Molar flux**

$$j_A = -cD_{AB} \frac{\partial x_A}{\partial x}$$

**Combined molar flux**

$$N_A = x_A (N_A + N_B) - cD_{AB} \frac{\partial x_A}{\partial x}$$

---

**1D Steady Diffusion—Gas Absorption with Chemical Solvent**

**Equation of Species Mass Balance in Terms of Molar quantities**

If source, absorption, or chemical reaction considered to be at edge of column.

**Fick's law:**

$$c \frac{\partial x_A}{\partial t} + v_f \cdot \nabla x_A = cD_{AB} \nabla^2 x_A + (x_B \dot{R}_A - x_A \dot{R}_B)$$

**Microscopic species A mass balance:**

$$c \left( \frac{\partial x_A}{\partial t} + v' \cdot \nabla x_A \right) = cD_{AB} \nabla^2 x_A + (x_B \dot{R}_A - x_A \dot{R}_B)$$

$R_A$ ≈ rate of production of moles of A by homogeneous chemical reaction per volume
Could we have used $j_A$ instead?

**Various forms of Fick's Law**

- **Mass flux**: $j_A = -ho D_{AA} F \omega_A$
- **Molar flux**: $J_A = -c D_{AA} F x_A$
- **Combined molar flux**: $N_A = x_A (N_A + 2 x_B) - c D_{AA} F x_A$

**Equation of Species Mass Balance**

- Macroscopic species mass balance in a mixture of mass flux: $\omega_A$
- Microscopic species mass balance in a column of fluid: $x_A$

**Fick's law**

- Definition: $j_A = \rho \omega_A (\bar{v} - v)$
- Fick's law: $j_A = -\rho D_{AA} \bar{v} \omega_A$

Microscopic species A mass balance:

$$\rho \left( \frac{\partial \omega_A}{\partial t} + \bar{v} \cdot \nabla \omega_A \right) = \rho D_{AA} \bar{v} \omega_A + r_A$$

$r_A \equiv$ rate of production of mass of $A$ by homogeneous chemical reaction per volume

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**Problem Summary: Gas Absorption with Chemical Solvent**

- One-dimensional (1D)
- Steady
- Use molar flux (due to reaction)
- Use combined molar flux \( N_A \)
- Needed stoichiometry and rate equation
- Boundary conditions: concentrations known (\( A \) disappears at penetration length)

**Flux choice**

Choose:
- **Molar** because there is a reaction
- **Combined molar** because the convection is only due to diffusion

**Example:** Heterogeneous catalysis

Model of Gas Absorption in a Column

Gas contains \( A \), which depletes as the gas passes through the column.

Liquid attracts \( A \); the concentration of \( A \) increases as the liquid passes through the column.

**1D Steady Diffusion, Problems Summary**

1. Unimolecular mass transfer (evaporating tank, Ex 1; evaporating droplet, Ex 2)
   - Subcase: stagnant \( B \), dilute \( A \), \( y^* \approx 0 \), \( (N_A \approx J_A) \)

2. Heterogeneous chemical reaction (catalytic converter, Ex 3, convection only due to diffusion)

3. Equimolar counter diffusion (distillation, \( y^* = 0 \), \( (N_A = J_A) \) Ex 4)

4. Homogeneous chemical reaction (gas absorption by chemical solvent, Ex 5, convection only due to diffusion)
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Aside:

The **film model** and the **penetration model** will both appear again.

They are used as framings for **lumped-parameter mass transfer models** in complex unit operations. They differ in how they predict the mass transfer coefficient (**linear-driving-force model**) varies with diffusion coefficient.

**Film:**

$$k_c \propto D_{AB}^{1/2}$$

**Penetration:**

$$k_c \propto D_{AB}$$