### **Hydrolysis of Particulate BOD**

Hydrolysis is the biochemical process by which complex particulate organic matter is enzymatically broken down into simpler soluble compounds.

The reaction has the general chemical formula:

$$BODₚ → BODₛ$$

Rate Expression

$$r\_{hyd} = k\_{hyd} \cdot BOD\_p$$

**Examples of hydrolysis include:**

A) Hydrolysis of Cellulose (Vavilin et al.,1996).

This is the enzymatic cleavage of insoluble cellulose polymers $$(C₆H₁₀O₅)\_n$$ into soluble glucose $$(C₆H₁₂O₆)$$. This is mediated by cellulase enzymes. The reaction liberates fermentable sugars essential for downstream biological processes.

**Chemical Reaction:**

$$\text{(C}*6\text{H}*{10}\text{O}\_5\text{)}\_n + n \cdot \text{H}\_2\text{O} \rightarrow n \cdot \text{C}*6\text{H}*{12}\text{O}\_6$$

$$ \left(\mathrm{C\_6H\_{10}O\_5}\right)*n ;+; n,\mathrm{H\_2O} ;\longrightarrow; n,\mathrm{C\_6H*{12}O\_6} $

$$[(\mathrm{C\_6H\_{10}O\_5})*n + n,\mathrm{H\_2O} \longrightarrow n,\mathrm{C\_6H*{12}O\_6}]$$

(\left(\mathrm{C\_6H\_{10}O\_5}\right)\_n + n\,\mathrm{H\_2O} \to n\,\mathrm{C\_6H\_{12}O\_6}\))

$$(\left(\mathrm{C\_6H\_{10}O\_5}\right)\_n + n\,\mathrm{H\_2O} \to n\,\mathrm{C\_6H\_{12}O\_6}\))$$

Example Species::

* **Reactant:** Cellulose polymer $$(C₆H₁₀O₅)ₙ$$
* **Product:** Glucose $$(C₆H₁₂O₆)$$

**Rate Expression:**

$$r\_{\text{hyd, cellulose}} = k\_{\text{hyd, cellulose}} \cdot C\_{\text{cellulose}}$$

**Units:**

* **$$r\_{hyd,cellulose}:** mol·m⁻³·s⁻¹$$ glucose produced
* **$$k\_{hyd,cellulose}:** s⁻¹$$
* **$$C\_{cellulose}:** mol·m⁻³$$ cellulose

**The rate refers to:** This rate denotes the moles of glucose produced per m³ reactor volume per second.

Typical Rate Constant (20–35 °C):

* $$k\_{hyd, cellulose} ≈ 1.0×10⁻⁶ – 5×10⁻⁶ s⁻¹$$ (depending on temperature and inoculum)
* $$θ \_{cellulose}$$(temperature coefficient) = 1.07–1.09 (dimensionless)
  + *$$θ means: k\_T = k\_20 × θ^(T-20)$$*
  + Higher θ indicates stronger temp sensitivity

B) Hydrolysis of Proteins (Angelidaki and Ahring, 1994)

This is the protease-catalyzed hydrolysis of protein macromolecules $$(C₄H₇O₂N)\_n$$ to soluble amino acids such as alanine $$(C₄H₉O₃N)$$. This provides nitrogen and carbon for microbes

**Chemical Reaction:**

$$\text{(C}\_4\text{H}\_7\text{O}\_2\text{N})\_n + n \cdot \text{H}\_2\text{O} \rightarrow n \cdot \text{C}\_4\text{H}\_9\text{O}\_3\text{N}$$

**Example Species:**

* **Reactant:** Protein polymer ($$(C₄H₇O₂N)\_n$$)
* **Product:** Soluble Amino acids (e.g., $$C₄H₉O₃N$$)

**Rate Expression:**

$$r\_{\text{hyd, protein}} = k\_{\text{hyd, protein}} \cdot C\_{\text{protein}}$$

**Units:**

* $$r\_{hyd,protein}**:** mol·m⁻³·s⁻¹$$ amino acids produced
* $$k\_{hyd,protein}**:** s⁻¹$$
* $$C\_{protein}**:** mol·m⁻³$$ protein

**The rate refers to moles** of amino acids produced per cubic meter per second.

**Typical Rate Constant:**

* $$k\_{hyd, protein} ≈ 1.5×10⁻⁶ – 4×10⁻⁶ s⁻¹$$
* $$θ\_{protein} = 1.08–1.09$$

C) Hydrolysis of Lipids (Palatsi et al. ,2010)

This is the lipase-driven hydrolysis of triglycerides (e.g., triolein, $$C₅₇H₁₀₄O₆$$) yields glycerol ($$C₃H₈O₃$$) and fatty acids ($$C₁₈H₃₄O₂$$). This is a slower process, especially in low-temperature conditions.

**Chemical Reaction:**

$$\text{C}*{57}\text{H}*{104}\text{O}\_6 + 3 \cdot \text{H}\_2\text{O} \rightarrow \text{C}\_3\text{H}*8\text{O}3 + 3 \cdot \text{C}{18}\text{H}*{34}\text{O}\_2$$

$$ \mathrm{C\_{57}H\_{104}O\_6} ;+; 3,\mathrm{H\_2O} ;\longrightarrow; \mathrm{C\_3H\_8O\_3} ;+; 3,\mathrm{C\_{18}H\_{34}O\_2} $$

[\mathrm{C\_{57}H\_{104}O\_6}+3\cdot\mathrm{H\_2O}\longrightarrow\mathrm{C\_3H\_8O\_3}+3\cdot\mathrm{C\_{18}H\_{34}O\_2}]

**Example Species:**

* **Reactant:** Triglycerides ($$C₅₇H₁₀₄O₆$$)
* **Products:** Glycerol ($$C₃H₈O₃$$), Oleic acid ($$C₁₈H₃₄O₂$$)

**Rate Expression:**

$$r\_{\text{hyd, lipid}} = k\_{\text{hyd, lipid}} \cdot C\_{\text{lipid}}$$

**Units:**

* **$$r\_{hyd,lipid}:** mol·m⁻³·s⁻¹$$ glycerol produced
* **$$k\_{hyd,lipid}:** s⁻¹$$
* **$$C\_{lipid}:** mol·m⁻³$$ triglycerides

**The rate refers to:** Moles of glycerol formed per m³·s.

**Typical Rate Constant:**

* $$k\_{hyd,lipid} = 5×10⁻⁷ – 1×10⁻⁶ s⁻¹$$
* $$θ\_{lipid} = 1.06–1.09$$

D) Hydrolysis of Biomass (Batstone et al.,2002).

This is the autolytic lysis of decaying biomass (heterotrophic bacteria, C₅H₇O₂N), releasing soluble intermediates and gases $$(CO₂, NH₃, CH₄)$$.

**Chemical Reaction:**

$$\text{C}\_5\text{H}\_7\text{O}\_2\text{N} + 3 \cdot \text{H}\_2\text{O} \rightarrow 5 \cdot \text{CO}\_2 + \text{NH}\_3 + \text{CH}\_4$$

**Example Species:**

* **Reactant:** Active biomass $$(C₅H₇O₂N)$$ (heterotrophs)
* **Products:** $$CO₂$$, ammonia ($$NH₃$$), methane ($$CH₄$$)

**Rate Expression:**

$$r\_{\text{hyd, biomass}} = k\_{\text{hyd, biomass}} \cdot C\_{\text{biomass}}$$

**Units:**

* **$$r\_{hyd,biomass}:** mol·m⁻³·s⁻¹ CO₂$$produced
* **$$k\_{hyd,biomass}:** s⁻¹$$
* **$$C\_{biomass}:** mol·m⁻³$$ biomass

**The rate refers to:** The rate is moles of $$CO₂$$ released per m³·s.

**Typical Rate Constant:**

* $$k\_{hyd,biomass} = 1×10⁻⁷ – 1×10⁻⁶ s⁻¹$$
* $$θ\_{biomass} = 1.07–1.09$$

**Carbon Oxidation (Aerobic): Consolidated Reactions, Rates, and References**

Carbon oxidation is the microbial process in which heterotrophic bacteria consume biodegradable organic matter in the presence of oxygen to produce carbon dioxide, water, and new biomass.

The kinetics are generally modeled using **Monod kinetics**, which account for:

* substrate limitation (half-saturation for substrate)
* oxygen limitation (half-saturation for oxygen)

**Monod kinetics** means:

* As substrate concentration increases, the rate approaches a maximum asymptotically.
* As oxygen increases, the rate also approaches a maximum.
* The combined limitation is represented by the product of both limiting terms.

The general **Monod form** is:

$$r = \mu\_{\text{H}} \cdot \frac{C\_{\text{S}}}{K\_{\text{S}} + C\_{\text{S}}} \cdot \frac{C\_{\text{O}*2}}{K*{\text{O}} + C\_{\text{O}*2}} \cdot C*{\text{X,H}}$$

$$ r = \mu\_{\text{H}} \cdot \frac{C\_{\text{S}}}{K\_{\text{S}} + C\_{\text{S}}} \cdot \frac{C\_{\mathrm{O\_2}}}{K\_{\mathrm{O}} + C\_{\mathrm{O\_2}}} \cdot C\_{\text{X,H}} $$

* $$r$$ is expressed in **mol substrate degraded per m³·s**.
* Each specific reaction uses a different substrate $$C\_S$$.

Carbon Oxidation of Soluble Glucose *.*

* Glucose is oxidized by heterotrophs to yield $$CO₂$$.
* This reaction supplies energy for microbial growth.
* Monod kinetics describe dependence on glucose and oxygen.

**Chemical Reaction:**

$$\text{C}*6\text{H}*{12}\text{O}\_6 + 6 \cdot \text{O}\_2 \rightarrow 6 \cdot \text{CO}\_2 + 6 \cdot \text{H}\_2\text{O}$$

$$ \mathrm{C\_6H\_{12}O\_6} ;+; 6,\mathrm{O\_2} ;\longrightarrow; 6,\mathrm{CO\_2} ;+; 6,\mathrm{H\_2O} $$

[\mathrm{C\_6H\_{12}O\_6}+6\cdot\mathrm{O\_2}\longrightarrow6\cdot\mathrm{CO\_2}+6\cdot\mathrm{H\_2O}]

**Example species:**

* **Reactant substrate:** Glucose ($$C₆H₁₂O₆$$)
* **Oxidant:** Oxygen ($$O₂$$)
* **Products:** Carbon dioxide ($$CO₂$$), Water ($$H₂O$$)

**Kinetic Rate Expression (Monod)**

$$r\_{\text{ox,glucose}} = \mu\_{\text{H}} \cdot \frac{C\_{\text{glucose}}}{K\_{\text{S,glucose}} + C\_{\text{glucose}}} \cdot \frac{C\_{\text{O}*2}}{K*{\text{O}} + C\_{\text{O}*2}} \cdot C*{\text{X,H}}$$

$$r\_{\text{glucose}} = \mu\_H \cdot \frac{S\_{\text{glucose}}}{K\_{S,\text{glucose}} + S\_{\text{glucose}}} \cdot \frac{S\_{O\_2}}{K\_O + S\_{O\_2}} \cdot X\_H$$

**Units:**

* $$R\_glucose$$ : mol glucose oxidized per m³ per s
* $$K$$
* $$C$$

**Monod Kinetics Description:**

* Expresses **substrate and oxygen limitation**. Numerator mols refer to glucose (reactant).
* The first fraction models glucose availability.
* The second fraction models oxygen availability.
* $$X\_H$$ is active biomass concentration (heterotrophs).
* When $$glucose ≫ K\_S$$ , the substrate term $$≈1$$.
* When $$O₂ ≫ KO$$ , oxygen term ≈1.
* Both must be sufficient to achieve maximum rate.
* This is **double-substrate Monod kinetics**, i.e., both glucose and oxygen limit

**Typical Constants** Henze, M. et al. (1987).**:**

* $$r\_{ox,glucose}$$: Moles of **glucose degraded per cubic meter per second**
* $$\mu\_{\text{H}} = 3.5 \times 10^{-5} \ s^{-1}$$
  + Max growth rate of heterotrophs consuming glucose) (Maximum specific growth rate on glucose.) $$2e-5–5e-5 s^{-1}$$.
* $$K\_{\text{S,glucose}}= 2 \times 10^{-3} \ mol \cdot m^{-3}$$
  + (Half-saturation constant for glucose substrate). Mols refer to glucose. $$1e-3–5e-3 mol/m³$$
* $$K\_{\text{O}} = 1 \times 10^{-3} \ mol \cdot m^{-3}$$
  + (Half-saturation constant for dissolved oxygen) Mols refer to dissolved oxygen. $$1e-4–1e-3 mol/m³$$
* $$\theta\_{\text{H}} = 1.07$$
  + Temperature correction factor applying only to $$\mu\_{\text{H}}$$. Adjusts max growth rate. Applies to all carbonaceous substrate oxidations by heterotrophs.
* $$\mu\_{T} = \mu\_{20} \cdot \theta\_{\text{H}}^{(T - 20)}$$
  + T in °C.
  + Recommended range: $$10–35 °C$$.

Carbon Oxidation of Soluble Acetate

**Chemical Reaction:**

$$\text{C}\_2\text{H}\_4\text{O}\_2 + 2 \cdot \text{O}\_2 \rightarrow 2 \cdot \text{CO}\_2 + 2 \cdot \text{H}\_2\text{O}$$

$$\text{C}\_2\text{H}\_4\text{O}\_2 + 2 \cdot \text{O}\_2 \rightarrow 2 \cdot \text{CO}\_2 + 2 \cdot \text{H}\_2\text{O}$$

### **Example Species**

* **Substrate:** Acetic acid $$(C\_2H\_4O\_2)$$
* **Oxidant:** Oxygen $$(O\_2)$$.
* **Products:** Carbon dioxide $$(CO2)$$, water $$(H2 O)$$

**Rate Expression (Monod):**

$$r\_{\text{ox,acetate}} = \mu\_{\text{H}} \cdot \frac{C\_{\text{acetate}}}{K\_{\text{S,acetate}} + C\_{\text{acetate}}} \cdot \frac{C\_{\text{O}*2}}{K*{\text{O}} + C\_{\text{O}*2}} \cdot C*{\text{X,H}}$$

$$r\_{\text{acetate}} = \mu\_H \cdot \frac{S\_{\text{acetate}}}{K\_{S,\text{acetate}} + S\_{\text{acetate}}} \cdot \frac{S\_{O\_2}}{K\_O + S\_{O\_2}} \cdot X\_H$$

**Monod Kinetics Description:**

* Substrate limitation captured by $$K\_S,acetate$$.
* Oxygen limitation captured by $$K\_O$$.
* Same Monod principle as glucose.
* Substrate limitation (acetate) and oxygen limitation.

**Typical Constants** Reference: Henze et al. (1987)**:**

* $$r\_ox,acetate$$ = Moles acetate degraded per m³·s.**mol acetate oxidized per m³ per s**
* $$\mu\_{\text{H}} = 3.5 \times 10^{-5} \ s^{-1}$$
  + Max growth rate on acetate. 2×10−5 to 4×10−5 s−1
* $$K\_{\text{S,acetate}} = 1 \times 10^{-3} \ mol \cdot m^{-3}$$
  + Moles refer to acetate 5×10−4 to 2×10−3 mol·m−3
* $$K\_{\text{O}} = 1 \times 10^{-3} \ mol \cdot m^{-3}$$
  + Mols refer to oxygen 1 x 10 –4 to 1 x 10-3 mol.m-3
* $$\theta\_{\text{H}} = 1.07$$
  + Temperature coefficient for heterotrophs.

**Typical Ranges:**

* Same as glucose oxidation.

Reaction 3: Oxidation of Soluble Amino Acids (Alanine Example) Henze et al. (1987) Palatsi et al. (2010)

Aerobic oxidation of amino acids to CO2 and ammonia. Releases nitrogen for nitrification downstream.

**Chemical Reaction:**

\text{C}\_3\text{H}\_7\text{NO}\_2 + 3 \cdot \text{O}\_2 \rightarrow 3 \cdot \text{CO}\_2 + 3 \cdot \text{H}\_2\text{O} + \text{NH}\_3

$$ \mathrm{C\_3H\_7NO\_2} ;+; 3,\mathrm{O\_2} ;\longrightarrow; 3,\mathrm{CO\_2} ;+; 2,\mathrm{H\_2O} ;+; \mathrm{NH\_3} $$

[\mathrm{C\_3H\_7NO\_2}+3\cdot\mathrm{O\_2}\longrightarrow3\cdot\mathrm{CO\_2}+2\cdot\mathrm{H\_2O}+\mathrm{NH\_3}]

**Example Species:**

* **Reactant:** Alanine (C₃H₇NO₂)
* **Products:** CO₂, H₂O, NH₃

**Rate Expression**

r\_{\text{amino}} = \mu\_H \cdot \frac{S\_{\text{amino}}}{K\_{S,\text{amino}} + S\_{\text{amino}}} \cdot \frac{S\_{O\_2}}{K\_O + S\_{O\_2}} \cdot X\_H

$$ r\_{\text{amino}} = \mu\_{\text{H}} \cdot \frac{S\_{\text{amino}}}{K\_{\text{S,amino}} + S\_{\text{amino}}} \cdot \frac{S\_{\mathrm{O\_2}}}{K\_{\mathrm{O}} + S\_{\mathrm{O\_2}}} \cdot X\_{\text{H}} $$

**Explanation:**

* Double substrate Monod kinetics.
* Moles in rate refer to amino acid oxidized.

**Typical Constants: (Henze et al)**

* R =mol amino acids per m3 per second. r**ate of consumption of soluble amino acids** in mol\cdotpm−3⋅s−1.
* \mu\_H = 3.2 \times 10^{-5} s^{-1} 2×10−5 to *3.5×10−5* s*−1*
* K\_{S,\text{amino}} = 2 \times 10^{-3} mol·m^{-3} (moles anine) 1x10-3 to 3x10-3mol/m3
* K\_O = 1 \times 10^{-3} mol·m^{-3} (moles oxygen) 1x10-4 to 1x10-3 mol/m3
* \theta\_H = 1.07

Reaction 4: Oxidation of Soluble Lipids

**Description:**

Aerobic oxidation of long-chain fatty acids. Slow due to lower solubility and need for prior emulsification.

**Chemical Reaction:**

\text{C}*{18}\text{H}*{34}\text{O}\_2 + 26 \cdot \text{O}\_2 \rightarrow 18 \cdot \text{CO}\_2 + 17 \cdot \text{H}\_2\text{O}

$$ 2,\mathrm{C\_{18}H\_{34}O\_2} ;+; 51,\mathrm{O\_2} ;\longrightarrow; 36,\mathrm{CO\_2} ;+; 34,\mathrm{H\_2O} $$

[2\cdot\mathrm{C\_{18}H\_{34}O\_2}+51\cdot\mathrm{O\_2}\longrightarrow36\cdot\mathrm{CO\_2}+34\cdot\mathrm{H\_2O}]

**Example Species:**

* **Reactant:** Oleic acid (C₁₈H₃₄O₂)
* **Products:** CO₂, H₂O

**Rate Expression:**

r\_{\text{lipid}} = \mu\_H \cdot \frac{S\_{\text{lipid}}}{K\_{S,\text{lipid}} + S\_{\text{lipid}}} \cdot \frac{S\_{O\_2}}{K\_O + S\_{O\_2}} \cdot X\_H

$$ r\_{\text{lipid}} = \mu\_{\text{H}} \cdot \frac{S\_{\text{lipid}}}{K\_{\text{S,lipid}} + S\_{\text{lipid}}} \cdot \frac{S\_{\mathrm{O\_2}}}{K\_{\mathrm{O}} + S\_{\mathrm{O\_2}}} \cdot X\_{\text{H}} $$

**Explanation:**

* Moles refer to lipid oxidized.
* Rate limited by lipid hydrolysis and oxygen.

Constants

* R\_ox,lipid = mol amino acids per m3 per second . The *moles again refer to the reactant substrate* (soluble lipids).
* \mu\_H = 1.8 \times 10^{-5} {s^{-1}). Lower due to solubility. 1×10−5 to 2.0×10−5 s*−*−1
* K\_{S,\text{lipid}} = 1 \times 10^{-3} mol·m^{-3}. MOls lipid
  + 5×10−4 to 1.5×10−3 mol·m−3
* K\_O = 1 \times 10^{-3} mol·m^{-3}. Moles oxygen.
  + 1×10−4 to 1×10−3 mol·m−3
* \theta\_H = 1.07. temperature factor.

**References:**

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### **PAC Adsorption**

**Chemical Reaction**

Contaminants adsorb onto powdered activated carbon (PAC) surfaces via Langmuir isotherm equilibrium, improving settling and reducing soluble organics.

Chemical – physical removal of organics. Dissolved contaminant are adsorbed onto PAC particles:

Contaminant + PAC ↔ Surface Complex

**Rate Expression**

r\_{ads} = k\_{ads} \cdot PAC \cdot \frac{C}{1 + K\_{ads} \cdot C}

[;r\_{\mathrm{ads}}=k\_{\mathrm{ads}}\cdot\mathrm{PAC}\cdot\frac{C}{1+K\_{\mathrm{ads}}\cdot C};]

**Constants (SI Units)**  
 Site-specific (system and contaminant dependent)

k\_ads: system-specific, typical ≈1×10^-4 m³/kg⋅s

K\_ads: varies (e.g., 1–10 m³/kg)

Source: Kuo et al. (2012)

## **Methanogenesis (Optional)**

Methanogenesis is the final biochemical step in anaerobic digestion. In this reaction, acetate and hydrogen are converted into methane and carbon dioxide by obligate anaerobic archaea called methanogens (Zeikus, 1977). I

1. **Acetoclastic Methanogenesis:**

The acetoclastic pathway converts acetate to methane and carbon dioxide, while the hydrogenotrophic pathway combines hydrogen with carbon dioxide to form methane.

**Chemical Reaction (**Acetoclastic Pathway:)

\text{CH}\_3\text{COO}^{-} + \text{H}^{+} \rightarrow \text{CH}\_4 + \text{CO}\_2

$$ \mathrm{CH\_3COO^-} + \mathrm{H^+} ;\longrightarrow; \mathrm{CH\_4} + \mathrm{CO\_2} $$

[\mathrm{CH\_3COO^-}+\mathrm{H^+}\longrightarrow\mathrm{CH\_4}+\mathrm{CO\_2}]

**Reactants:**

* Acetate (CH3COO^-)
* Hydrogen (H2)
* Carbon dioxide (CO2)

**Products:**

* Methane (CH4)
* Carbon dioxide (CO2)
* Water (H2O)

**Rate Expression:**

r\_{\text{meth,acetate}} = \mu\_{\text{meth}} \cdot \frac{S\_{\text{acetate}}}{K\_{\text{S,acetate}} + S\_{\text{acetate}}} \cdot X\_{\text{meth}}

$$ r\_{\text{meth,acetate}} = \mu\_{\text{meth}} \cdot \frac{S\_{\text{acetate}}}{K\_{\text{S,acetate}} + S\_{\text{acetate}}} \cdot X\_{\text{meth}} $$

For acetoclastic pathway, r\_meth,acetate refers to mol methane generated.

**Typical Constants:**

* Units: mol methane produced per m3 per second.
* mu\_meth ranges 1e-6 to 5e-6 per second (Zeikus, 1977).
* mu\_meth,H2 ranges 1e-6 to 4e-6 per second (Angelidaki & Sanders, 2004).
* K\_S,acetate ranges 5e-4 to 2e-3 mol per m3 (Batstone et al., 2002).
* K\_S,H2 ranges 1e-5 to 1e-4 mol per m3 (Batstone et al., 2002).
* theta\_meth typically 1.03 to 1.06 per °C between 20 and 40 °C (Batstone et al., 2002).

1. Hydrogenotrophic Pathway:

**Chemical Reaction:**

4 \cdot \text{H}\_2 + \text{CO}\_2 \rightarrow \text{CH}\_4 + 2 \cdot \text{H}\_2\text{O}

$$ 4,\mathrm{H\_2} + \mathrm{CO\_2} ;\longrightarrow; \mathrm{CH\_4} + 2,\mathrm{H\_2O} $$

[;4\cdot\mathrm{H\_2}+\mathrm{CO\_2}\longrightarrow\mathrm{CH\_4}+2\cdot\mathrm{H\_2O};]

### **Example Species**

**Reactants:**

* Acetate (CH3COO^-)
* Hydrogen (H2)
* Carbon dioxide (CO2)

**Products:**

* Methane (CH4)
* Carbon dioxide (CO2)
* Water (H2O)

**Rate Expression:**

r\_{\text{meth,H2}} = \mu\_{\text{meth,H2}} \cdot \frac{S\_{\text{H2}}}{K\_{\text{S,H2}} + S\_{\text{H2}}} \cdot X\_{\text{meth}}

$$ r\_{\text{meth,H2}} = \mu\_{\text{meth,H2}} \cdot \frac{S\_{\mathrm{H\_2}}}{K\_{\text{S,H2}} + S\_{\mathrm{H\_2}}} \cdot X\_{\text{meth}} $$

These equations use **Monod kinetics** (Batstone et al., 2002):

* **mu\_meth** is the maximum specific growth rate of methanogens on acetate.
* **mu\_meth,H2** is the maximum specific growth rate on hydrogen.
* **S\_acetate** is the substrate concentration of acetate in mol per m3.
* **S\_H2** is the substrate concentration of hydrogen gas in mol per m3.
* **K\_S,acetate** and **K\_S,H2** are the half-saturation constants.
* **X\_meth** is the methanogen biomass concentration in kg per m3.  
   The rate expression predicts methane production based on substrate availability and microbial density. The moles in the numerator refer to the **reactant consumed** (acetate or hydrogen), and the resulting methane produced is stoichiometrically related.

**Units**

* Units: mol methane produced per m3 per second.
* For acetoclastic pathway, r\_meth,acetate refers to mol methane generated.
* For hydrogenotrophic pathway, r\_meth,H2 refers to mol methane generated.

### **Constants and References**

* mu\_meth: Maximum specific growth rate on acetate = 3e-6 per second (Batstone et al., 2002).
* mu\_meth,H2: Maximum specific growth rate on hydrogen = 2e-6 per second (Batstone et al., 2002).
* K\_S,acetate: Half-saturation constant for acetate = 1e-3 mol per m3. This mol refers to acetate (Batstone et al., 2002).
* K\_S,H2: Half-saturation constant for hydrogen = 5e-5 mol per m3. This mol refers to hydrogen (Batstone et al., 2002).
* theta\_meth: Temperature coefficient = 1.04 per °C (applies to mu\_meth and mu\_meth,H2) (Batstone et al., 2002).

### **Typical Ranges of Constants**

* mu\_meth ranges 1e-6 to 5e-6 per second (Zeikus, 1977).
* mu\_meth,H2 ranges 1e-6 to 4e-6 per second (Angelidaki & Sanders, 2004).
* K\_S,acetate ranges 5e-4 to 2e-3 mol per m3 (Batstone et al., 2002).
* K\_S,H2 ranges 1e-5 to 1e-4 mol per m3 (Batstone et al., 2002).
* theta\_meth typically 1.03 to 1.06 per °C between 20 and 40 °C (Batstone et al., 2002).

### **References**

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**Nitrification**

Nitrification is the aerobic, chemoautotrophic biological oxidation of ammonium to nitrate. It is a two-step process mediated by specialized bacterial guilds. I

1. Ammonia Oxidation (Nitrosomonas)

Ammonia oxidation is the first step in nitrification and is carried out by **ammonia-oxidizing bacteria (AOB)** such as *Nitrosomonas europaea* (Prosser, 1989). T**Chemical Reaction**

\text{NH}\_4^{+} + 1.5 \cdot \text{O}\_2 \rightarrow \text{NO}\_2^{-} + 2 \cdot \text{H}^{+} + \text{H}\_2\text{O}

$$ 2,\mathrm{NH\_4^+} + 3,\mathrm{O\_2} ;\longrightarrow; 2,\mathrm{NO\_2^-} + 4,\mathrm{H^+} + 2,\mathrm{H\_2O} $$

[2\cdot\mathrm{NH\_4^+}+3\cdot\mathrm{O\_2}\longrightarrow2\cdot\mathrm{NO\_2^-}+4\cdot\mathrm{H^+}+2\cdot\mathrm{H\_2O}]

**Example Species:**

* Reactant: Ammonium ion (NH4+)
* Products: Nitrite ion (NO2-), protons (H+), water (H2O)

**Rate Expression**

r\_{\text{nit,amm}} = \mu\_{\text{AOB}} \cdot \frac{S\_{\text{NH4}}}{K\_{\text{S,NH4}} + S\_{\text{NH4}}} \cdot \frac{S\_{\text{O2}}}{K\_{\text{S,O2}} + S\_{\text{O2}}} \cdot X\_{\text{AOB}}

$$ r\_{\text{nit,amm}} = \mu\_{\text{AOB}} \cdot \frac{S\_{\text{NH4}}}{K\_{\text{S,NH4}} + S\_{\text{NH4}}} \cdot \frac{S\_{\mathrm{O\_2}}}{K\_{\text{S,O2}} + S\_{\mathrm{O\_2}}} \cdot X\_{\text{AOB}} $$

* **Explanation of Rate Expression:**  
   This is a **double Monod expression**, reflecting substrate limitation by **ammonium** and **oxygen**:
* mu\_AOB is the **maximum specific growth rate of AOB** (per second), reflecting how fast AOB can grow when both substrates are abundant.
  + Typical range: 2e-6 to 6e-6 per second.
  + *Reference*: Henze et al. (2000).
* S\_NH4 is the ammonium concentration in mol per cubic meter.
* K\_S,NH4 is the **half-saturation constant for ammonium** in mol per cubic meter.
  + It is the concentration at which the growth rate is half of mu\_AOB.
  + Typical range: 1e-4 to 4e-4 mol/m3.
  + *Reference*: Henze et al. (2000).
* S\_O2 is the dissolved oxygen concentration in mol per cubic meter.
* K\_S,O2,AOB is the **oxygen half-saturation constant** in mol per cubic meter.
  + Reflects oxygen affinity of AOB.
  + Typical range: 2e-5 to 1e-4 mol/m3.
  + *Reference*: Henze et al. (2000).
* X\_AOB is the active biomass concentration of AOB in kg/m3.
* **The moles in the rate r refer to moles of ammonium oxidized per cubic meter per second.**

**Units of Reaction Rate:**  
mol NH4+ oxidized / m3 / second

**Constants:**

* mu\_AOB: maximum growth rate = 4e-6 per second (Henze et al., 2000).
* K\_S,NH4: half-saturation ammonium = 2e-3 mol per m3 (refers to ammonium).
* K\_S,O2: oxygen half-saturation = 2e-4 mol per m3 (refers to O2).
* theta\_AOB: temperature coefficient = 1.07 per °C (Henze et al., 2000).

**Typical Ranges of Constants:**

* mu\_AOB: 2e-6 to 5e-6 per second. Henze et al. (2000)
* K\_S,NH4: 1e-3 to 3e-3 mol per m3. Henze et al. (2000)
* K\_S,O2: 1e-4 to 3e-4 mol per m3. Henze et al. (2000)
* theta\_AOB: 1.06 to 1.08 per °C over 15–35 °C. Blackburne et al. (2007)

**Temperature Correction and Correlation:**  
 theta\_AOB applies to mu\_AOB. For example, at 25 °C, mu\_AOB increases by factor of 1.07^(25–20) = approx 1.40 (Henze et al., 2000).

1. **Nitrite Oxidation (Nitrobacter)**

Nitrite oxidation is the second nitrification step, converting nitrite to nitrate.

**Chemical Reaction**

\text{NO}\_2^{-} + 0.5 \cdot \text{O}\_2 \rightarrow \text{NO}\_3^{-}

$$ 2,\mathrm{NO\_2^-} + \mathrm{O\_2} ;\longrightarrow; 2,\mathrm{NO\_3^-} $$

[2\cdot\mathrm{NO\_2^-}+\mathrm{O\_2}\longrightarrow2\cdot\mathrm{NO\_3^-}]

**Example Species:**

* Reactant: Nitrite ion (NO2-)
* Product: Nitrate ion (NO3-)

**Rate Expression**

r\_{\text{nit,nitrite}} = \mu\_{\text{NOB}} \cdot \frac{S\_{\text{NO2}}}{K\_{\text{S,NO2}} + S\_{\text{NO2}}} \cdot \frac{S\_{\text{O2}}}{K\_{\text{S,O2,NOB}} + S\_{\text{O2}}} \cdot X\_{\text{NOB}}

$$ r\_{\text{nit,nitrite}} = \mu\_{\text{NOB}} \cdot \frac{S\_{\mathrm{NO\_2}}}{K\_{\text{S,NO2}} + S\_{\mathrm{NO\_2}}} \cdot \frac{S\_{\mathrm{O\_2}}}{K\_{\text{S,O2,NOB}} + S\_{\mathrm{O\_2}}} \cdot X\_{\text{NOB}} $$

**Explanation of Rate Expression:**  
 Monod-type kinetics: This is a Monod model describing substrate-limited growth:

* mu\_NOB: maximum specific growth rate of nitrite oxidizers. Maximum specific growth rate of Nitrobacter (per second). It represents the rate of biomass growth under non-limiting conditions.
* S\_NO2: nitrite concentration in mol per m3.
* K\_S,NO2: Half-saturation constant for nitrite (mol per cubic meter), referring to the nitrite concentration at which the reaction proceeds at half the maximum rate.
* S\_O2: Dissolved oxygen concentration in mol per cubic meter.
* K\_S,O2,NOB: Half-saturation constant for oxygen (mol per cubic meter), referring to the oxygen concentration for half-maximal activity.
* X\_NOB: Biomass concentration of Nitrobacter in kg per cubic meter.

**Units of Reaction Rate:**  
 mol NO2- oxidized per m3 per second. The moles in the rate (r) refer specifically to moles of nitrite oxidized per unit volume per time.

**Constants**

* mu\_NOB: 3e-6 per second (Henze et al., 2000).
* K\_S,NO2: 1e-3 mol per m3 (refers to nitrite).
* K\_S,O2,NOB: 1e-4 mol per m3 (refers to O2).
* theta\_NOB: 1.06 per °C (Henze et al., 2000).

**Typical Ranges of Constants:**

* mu\_NOB: 1e-6 to 4e-6 per second. Reference: Henze et al. (2000)
* K\_S,NO2: 5e-4 to 2e-3 mol per m3. Reference: Henze et al. (2000)
* K\_S,O2,NOB: 5e-5 to 2e-4 mol per m3. Reference: Henze et al. (2000)
* theta\_NOB: 1.05–1.07 per °C. Reference: Siegrist & Gujer (1995)

**Temperature Correction and Correlation:**  
 theta\_NOB applies to mu\_NOB. For 30 °C, mu\_NOB is multiplied by 1.06^(30–20) = ~1.79.

### **References:**

* Prosser, J.I. (1989). Autotrophic nitrification in bacteria. *Advances in Microbial Physiology*.
* Henze, M. et al. (2000). *Activated Sludge Model No.1*. IWA Publishing.
* Blackburne, R. et al. (2007). Partial nitrification to nitrite using low dissolved oxygen concentration as the main selection factor. *Biodegradation*.
* Siegrist, H., Gujer, W. (1995). *Nitrogen removal in activated sludge systems*. Water Science and Technology.

**Denitrification**

Denitrification is critical for nitrogen removal and climate considerations (due to N₂O emissions). It is the stepwise biological reduction of oxidized nitrogen compounds (primarily nitrate and nitrite) into gaseous nitrogen forms (N₂O and ultimately N₂ gas) and is responsible for removing bioavailable nitrogen from wastewater.

1. Reaction 1 – Nitrate Reduction to Nitrite

This reaction reduces nitrate (NO3-) to nitrite (NO2-) under anoxic conditions. Facultative anaerobic heterotrophic bacteria couple the oxidation of organic carbon to the reduction of nitrate. The enzyme involved is nitrate reductase (Nar). This is often the fastest step of denitrification.

**Reference:** Payne, 1981; Tiedje, 1982.

**Chemical Reaction**

NO\_{3}^{-} + 2 \cdot H^{+} + 2 \cdot e^{-} \rightarrow NO\_{2}^{-} + H\_{2}O

$$ \mathrm{NO\_3^-} + 2,\mathrm{H^+} + 2,\mathrm{e^-} ;\longrightarrow; \mathrm{NO\_2^-} + \mathrm{H\_2O} $$

[\mathrm{NO\_3^-}+2\cdot\mathrm{H^+}+2\cdot\mathrm{e^-}\longrightarrow\mathrm{NO\_2^-}+\mathrm{H\_2O}]

### **Example Species:**

**Reactants:**

* Nitrate (NO3-)
* Acetate (CH3COO-)

**Products:**

* Nitrite (NO2-)
* Water (H2O)

**Rate Expression**

r\_{NO3^{-}} = \mu\_{max} \cdot \frac{S\_{NO3^{-}}}{K\_{S,NO3^{-}} + S\_{NO3^{-}}} \cdot \frac{S\_{COD}}{K\_{S,COD} + S\_{COD}} \cdot X\_{DEN}

$$ r\_{\mathrm{NO\_3^-}} = \mu\_{\max} \cdot \frac{S\_{\mathrm{NO\_3^-}}}{K\_{\text{S,NO3^-}} + S\_{\mathrm{NO\_3^-}}} \cdot \frac{S\_{\text{COD}}}{K\_{\text{S,COD}} + S\_{\text{COD}}} \cdot X\_{\text{DEN}} $$

Explanation of Rate Expression

This is a Monod-based model describing the specific nitrate consumption rate.

* r\_NO3- represents the moles of nitrate consumed per cubic meter reactor volume per second.
* S\_NO3- is the nitrate concentration in mol per cubic meter.
* S\_COD is the readily biodegradable chemical oxygen demand concentration in mol C per cubic meter.
* mu\_max is the maximum specific growth rate of denitrifying biomass.
* K\_S,NO3- is the half-saturation constant for nitrate.
* K\_S,COD is the half-saturation constant for COD.
* X\_DEN is the biomass concentration in kg per cubic meter.

Units of r\_NO3-:  
 mol nitrate consumed per cubic meter reactor volume per second.

The "mol" refers to moles of nitrate removed.

### **Constants**

* mu\_max: maximum growth rate of denitrifiers. Typical range: 0.12 to 0.25 per hour (converted approximately to 3.3e-5 to 6.9e-5 per second). This is the biological maximum rate under optimal substrate and temperature conditions. (Reference: Tiedje, 1982)
* K\_S,NO3-: half-saturation constant for nitrate. Range: 0.1 to 0.5 grams nitrogen per cubic meter. This corresponds to approximately 7e-3 to 3.5e-2 mol nitrate per cubic meter. This is the concentration at which nitrate reduction rate is 50% of mu\_max. (Reference: van Loosdrecht et al., 2002)
* K\_S,COD: half-saturation constant for COD. Range: 20 to 50 grams COD per cubic meter, equivalent to 0.625 to 1.56 mol C per cubic meter. (Reference: Henze et al., 2000)
* theta\_mu: temperature coefficient. Typical value: 1.07. This means that the rate increases by about 7% per degree Celsius. (Reference: Henze et al., 2000)

### **Temperature Correction**

Temperature correction applies to mu\_max. It is described by the Arrhenius relationship:

\mu\_{T} = \mu\_{20} \cdot \theta^{(T - 20)}

where theta is 1.07, T is the reactor temperature in degrees Celsius, and mu\_20 is the reference rate at 20 degrees Celsius.

1. Reaction 2 – Nitrite Reduction to Nitric Oxide

This step of denitrification reduces nitrite (NO2-) to nitric oxide (NO).

**Reference:** Tiedje, 1982; van Loosdrecht et al., 2002.

**Chemical Reaction:**

NO\_{2}^{-} + 2 \cdot H^{+} + e^{-} \rightarrow NO + H\_{2}O

[\mathrm{NO\_2^-}+2\cdot\mathrm{H^+}+\mathrm{e^-}\longrightarrow\mathrm{NO}+\mathrm{H\_2O}]

### **Example Species:**

**Reactants:**

* Nitrite (NO2-)
* Acetate (CH3COO-) as electron donor

**Products:**

* Nitric oxide (NO)
* Water (H2O)

**Rate Expression**

r\_{NO2^{-}} = \mu\_{max} \cdot \frac{S\_{NO2^{-}}}{K\_{S,NO2^{-}} + S\_{NO2^{-}}} \cdot \frac{S\_{COD}}{K\_{S,COD} + S\_{COD}} \cdot X\_{DEN}

$$ r\_{\mathrm{NO\_2^-}} = \mu\_{\max} \cdot \frac{S\_{\mathrm{NO\_2^-}}}{K\_{\text{S,NO2^-}} + S\_{\mathrm{NO\_2^-}}} \cdot \frac{S\_{\text{COD}}}{K\_{\text{S,COD}} + S\_{\text{COD}}} \cdot X\_{\text{DEN}} $$

### **Explanation of Rate Expression**

This is a Monod model describing nitrite reduction rate.

* r\_NO2- is the moles of nitrite reduced per cubic meter reactor volume per second.
* S\_NO2- represents the nitrite concentration in mol per cubic meter.
* S\_COD is the concentration of soluble readily biodegradable organic carbon (acetate) in mol C per cubic meter.
* mu\_max is the maximum specific growth rate of nitrite-reducing denitrifying biomass.
* K\_S,NO2- is the half-saturation constant for nitrite.
* K\_S,COD is the half-saturation constant for COD.
* X\_DEN is the active biomass concentration in kg per cubic meter.

**Units of r\_NO2-:**  
 mol nitrite consumed per cubic meter per second.

Here the “mol” refers to moles of nitrite removed.

### **Constants** Reference: Henze et al., 2000.

* mu\_max: maximum growth rate of nitrite-reducing bacteria.
  + Typical range: 0.08 to 0.20 per hour (2.2e-5 to 5.6e-5 per second)
  + Reference: Tiedje, 1982.
* K\_S,NO2-: half-saturation constant for nitrite.
  + Range: 0.05 to 0.3 grams N per cubic meter (~3.6e-3 to 2.1e-2 mol per cubic meter).
  + Reference: van Loosdrecht et al., 2002.
* K\_S,COD: half-saturation constant for COD.
  + Range: 20 to 50 grams COD per cubic meter (~0.625 to 1.56 mol C per cubic meter).
  + Reference: Henze et al., 2000.
* theta\_mu: temperature coefficient (applies to mu\_max).
  + Value: 1.07 (meaning ~7% increase in rate per °C).

### **H. Temperature Correction**

Temperature correction uses the Arrhenius relation

\mu\_{T} = \mu\_{20} \cdot \theta^{(T - 20)}

* mu\_20 is the reference maximum growth rate at 20 °C.
* theta is 1.07.
* T is the operating temperature (°C).

## Reaction 3: Nitric Oxide Reduction to Nitrous Oxide

This step reduces nitric oxide (NO) to nitrous oxide (N2O).

**Reference:** Tiedje, 1982; Richardson et al., 2001.

**Chemical Reaction**

2 \cdot NO + 2 \cdot H^{+} + 2 \cdot e^{-} \rightarrow N\_{2}O + H\_{2}O

$$ 2,\mathrm{NO} + 2,\mathrm{H^+} + 2,\mathrm{e^-} ;\longrightarrow; \mathrm{N\_2O} + \mathrm{H\_2O} $$

[2\cdot\mathrm{NO}+2\cdot\mathrm{H^+}+2\cdot\mathrm{e^-}\longrightarrow\mathrm{N\_2O}+\mathrm{H\_2O}]

### **Example Species**

**Reactants:**

* Nitric oxide (NO)
* Acetate (CH3COO-) as electron donor

**Products:**

* Nitrous oxide (N2O)
* Water (H2O)

**Rate Expression:**

r\_{NO} = \mu\_{max} \cdot \frac{S\_{NO}}{K\_{S,NO} + S\_{NO}} \cdot \frac{S\_{COD}}{K\_{S,COD} + S\_{COD}} \cdot X\_{DEN}

$$ r\_{\mathrm{NO}} = \mu\_{\max} \cdot \frac{S\_{\mathrm{NO}}}{K\_{\text{S,NO}} + S\_{\mathrm{NO}}} \cdot \frac{S\_{\text{COD}}}{K\_{\text{S,COD}} + S\_{\text{COD}}} \cdot X\_{\text{DEN}} $$

### **Explanation of Rate Expression:**

This is a Monod-type expression describing NO reduction:

* r\_NO is the moles of nitric oxide consumed per cubic meter per second.
* S\_NO is nitric oxide concentration (mol per cubic meter).
* S\_COD is soluble readily biodegradable organic carbon (mol C per cubic meter).
* mu\_max is the maximum specific growth rate of NO-reducing denitrifiers.
* K\_S,NO is the half-saturation constant for NO.
* K\_S,COD is the half-saturation constant for COD.
* X\_DEN is active denitrifying biomass concentration (kg per cubic meter).

### **Units and Interpretation:**

**Units of r\_NO:**  
 mol nitric oxide reduced per cubic meter per second.

“mol” refers to moles of NO removed.

### **Constants:**

* mu\_max:
  + Maximum growth rate of NO reducers.
  + Typical range: 0.05 to 0.15 per hour (1.4e-5 to 4.2e-5 per second).
  + Reference: Richardson et al., 2001.
* K\_S,NO:
  + Half-saturation for NO.
  + Range: 1e-6 to 5e-6 mol per cubic meter.
  + Reference: Richardson et al., 2001.
* K\_S,COD:
  + Half-saturation for COD.
  + Range: 0.625 to 1.56 mol C per cubic meter.
  + Reference: Henze et al., 2000.
* theta\_mu:
  + Temperature coefficient for mu\_max.
  + Value: 1.06.
  + Reference: Tiedje, 1982.

### **Temperature Correction**

Temperature adjustment uses Arrhenius-type relationship:

\mu\_{T} = \mu\_{20} \cdot \theta^{(T - 20)}

* mu\_20: reference mu\_max at 20 °C.
* theta: 1.06.
* T: actual temperature (°C)

### **Reference for this Reaction:**

* Tiedje J.M. (1982). Denitrification.
* Richardson D.J. et al. (2001). *Biochimica et Biophysica Acta*.
* Henze M. et al. (2000). *Activated Sludge Models*.

### **Reference for this Reaction**

* Payne W.J. (1981). *Denitrification*. Wiley-Interscience.
* Tiedje J.M. (1982). Denitrification. *Antonie van Leeuwenhoek*.
* Henze M. et al. (2000). *Activated Sludge Models*. IWA.
* van Loosdrecht M.C.M. et al. (2002). *Biological Wastewater Treatment*. IWA.

### **Reference for this Reaction**

* Tiedje J.M. (1982). Denitrification. *Antonie van Leeuwenhoek*.
* van Loosdrecht M.C.M. et al. (2002). *Biological Wastewater Treatment*. IWA.
* Henze M. et al. (2000). *Activated Sludge Models*. IWA.

Reaction 4: Nitrous Oxide Reduction to Nitrogen Gas

This final denitrification step converts nitrous oxide (N2O) into dinitrogen gas (N2), completing the nitrogen removal process.(Tiedje, 1982; Richardson et al., 2009).

### **Chemical Reaction**

N\_{2}O + 2 \cdot H^{+} + 2 \cdot e^{-} \rightarrow N\_{2} + H\_{2}O

$$ \mathrm{N\_2O} + 2,\mathrm{H^+} + 2,\mathrm{e^-} ;\longrightarrow; \mathrm{N\_2} + \mathrm{H\_2O} $$

[\mathrm{N\_2O}+2\cdot\mathrm{H^+}+2\cdot\mathrm{e^-}\longrightarrow\mathrm{N\_2}+\mathrm{H\_2O}]

### **Example Species**

**Reactants:**

* Nitrous oxide (N2O)
* Acetate (CH3COO-) as electron donor

**Products:**

* Dinitrogen gas (N2)
* Water (H2O)

### **Rate Expression**

r\_{N2O} = \mu\_{max} \cdot \frac{S\_{N2O}}{K\_{S,N2O} + S\_{N2O}} \cdot \frac{S\_{COD}}{K\_{S,COD} + S\_{COD}} \cdot X\_{DEN}

$$ r\_{\mathrm{N\_2O}} = \mu\_{\max} \cdot \frac{S\_{\mathrm{N\_2O}}}{K\_{\text{S,N2O}} + S\_{\mathrm{N\_2O}}} \cdot \frac{S\_{\text{COD}}}{K\_{\text{S,COD}} + S\_{\text{COD}}} \cdot X\_{\text{DEN}} $$

**Explanation of Rate Expression**

This Monod-type expression models N2O reduction:

* r\_N2O is the moles of N2O consumed per cubic meter per second.
* S\_N2O is nitrous oxide concentration (mol per cubic meter).
* S\_COD is soluble readily biodegradable carbon (mol C per cubic meter).
* mu\_max is the maximum growth rate of N2O reducers.
* K\_S,N2O is the half-saturation constant for N2O.
* K\_S,COD is the half-saturation constant for COD.
* X\_DEN is active denitrifying biomass concentration (kg per cubic meter).

### **Units and Interpretation**

Units of r\_N2O:  
 mol nitrous oxide reduced per cubic meter per second.

**Constants**

* mu\_max:
  + Maximum specific growth rate of N2O reducers.
  + Typical range: 0.03 to 0.12 per hour (8.3e-6 to 3.3e-5 per second).
  + Reference: Richardson et al., 2009.
* K\_S,N2O:
  + Half-saturation constant for N2O.
  + Range: 5e-7 to 1e-6 mol per cubic meter.
  + Reference: Richardson et al., 2009.
* K\_S,COD:
  + Half-saturation for COD.
  + Range: 0.625 to 1.56 mol C per cubic meter.
  + Reference: Henze et al., 2000.
* theta\_mu:
  + Temperature coefficient for mu\_max.
  + Value: 1.07.
  + Reference: Tiedje, 1982.

### **Temperature Correction**

Temperature dependence is described by:

\mu\_{T} = \mu\_{20} \cdot \theta^{(T - 20)}

* mu\_20: Reference mu\_max at 20 °C.
* theta: 1.07.
* T: Temperature (°C).

Combined References

1. Henze, M., Grady, C.P.L., Gujer, W., Marais, G.v.R., & Matsuo, T. (2000). *Activated Sludge Models ASM1, ASM2, ASM2d and ASM3*. IWA Publishing. Link
2. Tchobanoglous, G., Burton, F.L., Stensel, H.D., et al. (2014). *Wastewater Engineering: Treatment and Resource Recovery*, 5th Ed. McGraw-Hill.
3. Richardson, D.J., Felgate, H., Watmough, N.J., Thomson, A.J., & Baggs, E.M. (2009). Mitigating the environmental impact of nitrous oxide. *Nature Reviews Microbiology*, 7(7), 527–536. DOI
4. Grady, C.P.L., Daigger, G.T., Love, N.G., & Filipe, C.D.M. (1999). *Biological Wastewater Treatment*. CRC Press.
5. Pochana, K., & Keller, J. (1999). Study of factors affecting simultaneous nitrification and denitrification (SND). *Water Science & Technology*, 39(6), 61–68. DOI
6. Metcalf & Eddy (2014). *Wastewater Engineering: Treatment and Reuse*. McGraw-Hill.
7. Knowles R. (1982). *Denitrification*. Microbiological Reviews.
8. Payne W. J. (1981). *Denitrification*. Wiley-Interscience.
9. Tiedje J. M., et al. (1982). *Denitrification: ecological niches, competition and survival.* Antonie van Leeuwenhoek.

### **Reference for this Reaction**

* Payne W.J. (1981). *Denitrification*. Wiley-Interscience.
* Tiedje J.M. (1982). Denitrification. *Antonie van Leeuwenhoek*.
* Henze M. et al. (2000). *Activated Sludge Models*. IWA.
* van Loosdrecht M.C.M. et al. (2002). *Biological Wastewater Treatment*. IWA.

### **Reference for this Reaction**

* Tiedje J.M. (1982). Denitrification. *Antonie van Leeuwenhoek*.
* van Loosdrecht M.C.M. et al. (2002). *Biological Wastewater Treatment*. IWA.
* Henze M. et al. (2000). *Activated Sludge Models*. IWA.

## **Combined Variable List**

Below is a **merged variable index** for all denitrification reactions:

* S\_NO3: Nitrate concentration (mol/m³)
* S\_NO2: Nitrite concentration (mol/m³)
* S\_N2O: Nitrous oxide concentration (mol/m³)
* S\_COD: Readily biodegradable carbon (mol C/m³)
* X\_DEN: Active denitrifying biomass (kg/m³)
* μ\_max: Maximum specific growth rate (s⁻¹)
* K\_S,NO3: Half-saturation constant for nitrate (mol/m³)
* K\_S,NO2: Half-saturation constant for nitrite (mol/m³)
* K\_S,N2O: Half-saturation constant for nitrous oxide (mol/m³)
* K\_S,COD: Half-saturation constant for COD (mol/m³)
* θ: Temperature correction coefficient (dimensionless)
* T: Temperature (°C)
* r\_NO3: Rate of nitrate reduction (mol/m³·s)
* r\_NO2: Rate of nitrite reduction (mol/m³·s)
* r\_N2O: Rate of nitrous oxide reduction (mol/m³·s)

**Acetogenesis**

Acetogenesis is the conversion of volatile fatty acids (VFAs) such as propionate and butyrate into acetate, CO2, and hydrogen gas. (Batstone et al., 2002).

**Chemical Reaction:**

C3H6O2 + 2 \cdot H2O \rightarrow C2H4O2 + CO2 + 3 \cdot H2

[\mathrm{C\_3H\_6O\_2}+2\cdot\mathrm{H\_2O}\longrightarrow\mathrm{C\_2H\_4O\_2}+\mathrm{CO\_2}+3\cdot\mathrm{H\_2}]

**Example Species:**

**Reactants:**

* Propionate: C3H6O2
* Butyrate: C4H8O2
* Water: H2O

**Products:**

* Acetate: C2H4O2
* Hydrogen: H2
* Carbon dioxide: CO2
* Biomass (generic): C5H7O2N

**Rate Expression:**

r\_{acet} = \mu\_{acet} \cdot \frac{S\_{VFA}}{K\_{S,VFA} + S\_{VFA}} \cdot X\_{acet}

[r\_{\mathrm{acet}}=\mu\_{\mathrm{acet}}\cdot\frac{S\_{\mathrm{VFA}}}{K\_{\mathrm{S,VFA}}+S\_{\mathrm{VFA}}}\cdot X\_{\mathrm{acet}}]

**Units and Moles Clarification:**

* Units of r\_acet: mol·m^-3·s^-1
* The moles refer to **moles of volatile fatty acids consumed** per cubic meter per second.
* This includes all short-chain VFAs (e.g., propionate, butyrate), generally expressed as an acetate-equivalent mass.

**Constants and Typical Ranges**

**μ\_acet**

* Maximum specific growth rate of acetogenic bacteria
* Typical range: 0.1 – 0.5 1/day
* Reference: Batstone et al. (2002)

**K\_S,VFA**

* Half-saturation constant for volatile fatty acids
* Typical range: 5.0 × 10^-4 – 1.0 × 10^-3 mol·m^-3
* Reference: Batstone et al. (2002)

**b\_acet**

* Decay rate of acetogenic biomass
* Typical range: 0.02 – 0.06 1/day
* Reference: Batstone et al. (2002)

**Temperature Correction Details**

**θ\_acet**

* Temperature coefficient for μ\_acet
* Typical value: 1.03 – 1.06 (dimensionless)
* Applies specifically to μ\_acet
* Temperature range: 15–35 °C
* Reference: Batstone et al. (2002)

## **References (Combined)**

* Batstone, D. J., Keller, J., Angelidaki, I., Kalyuzhnyi, S. V., Pavlostathis, S. G., Rozzi, A., Sanders, W. T., Siegrist, H., & Vavilin, V. A. (2002). The IWA Anaerobic Digestion Model No. 1 (ADM1). *Water Science & Technology*, 45(10), 65–73. <https://iwa-network.org/publications/anaerobic-digestion-model-no-1-adm1/>
* Appels, L., Baeyens, J., Degrève, J., & Dewil, R. (2008). Principles and potential of the anaerobic digestion of waste-activated sludge. *Progress in Energy and Combustion Science*, 34(6), 755–781. <https://doi.org/10.1016/j.pecs.2008.06.002>
* McCarty, P. L., & Smith, D. P. (1986). Anaerobic wastewater treatment. *Environmental Science and Technology*, 20(12), 1200–1206. <https://pubs.acs.org/doi/10.1021/es00154a001>

**Acidogenesis:**

Acidogenesis is the second stage of anaerobic digestion, following hydrolysis. In this process, fermentative acidogenic bacteria convert soluble organic monomers (such as glucose, amino acids, and fatty acids) into volatile fatty acids (VFAs) including acetate, propionate, and butyrate, as well as CO₂, H₂, and small amounts of alcohols.

**Chemical Reaction:**

C6H12O6 \rightarrow C2H4O2 + CO2 + H2

[\mathrm{C\_6H\_{12}O\_6}\longrightarrow\mathrm{C\_2H\_4O\_2}+\mathrm{CO\_2}+\mathrm{H\_2}]

This represents glucose conversion to acetic acid, CO₂, and hydrogen.

### **Example Species**

* **Reactant:** Glucose – C6H12O6
* **Products:**
  + Acetic Acid – C2H4O2
  + Carbon Dioxide – CO2
  + Hydrogen – H2

Note: Depending on substrate, VFAs can also include propionic acid (C3H6O2) and butyric acid (C4H8O2).

**Rate Expression**

Monod-type kinetics are used to describe acidogenesis. The general form is:

r\_acid = \mu\_acid \cdot \frac{S}{K\_S + S} \cdot X

[r\_{\mathrm{acid}}=\mu\_{\mathrm{acid}}\cdot\frac{S}{K\_S+S}\cdot X]

Where (Batstone et al. ,2002):

* r\_acid is the acidogenesis rate, expressed in **mol of substrate converted per m³ reactor volume per second** (mol·m⁻³·s⁻¹).
* **Moles refer to reactant glucose (C6H12O6) degraded per unit time.**
* S is substrate concentration (mol·m⁻³).
* X is active biomass concentration (mol biomass equivalents·m⁻³).

This rate accounts for substrate limitation but does not explicitly include hydrogen partial pressure inhibition in this form (though some models add a hydrogen inhibition term).

**Maximum specific growth rate (mu\_acid):**

* Value: 0.8 day⁻¹
* SI Units: 9.26 × 10⁻⁶ s⁻¹
* Refers to: Maximum conversion rate per unit biomass
* Source: Batstone et al., 2002

**Half-saturation constant (K\_S):**

* Value: 50 mg COD·L⁻¹ (0.050 kg COD·m⁻³)
* Refers to: Concentration of soluble substrate at which rate is half maximal
* Source: Batstone et al., 2002

**Yield coefficient (Y):**

* Value: 0.1 mol biomass·mol substrate⁻¹
* Refers to: Moles of biomass generated per mole of glucose degraded
* Source: Batstone et al., 2002

**Decay coefficient (b):**

* Value: 0.02 day⁻¹
* SI Units: 2.31 × 10⁻⁷ s⁻¹
* Refers to: Biomass decay rate
* Source: Batstone et al., 2002

**Theta (Temperature Correction Factor):**

* Value: 1.07 per °C
* Refers to: Correction applied to μ\_acid per degree deviation from 35 °C
* Typical operational range: 15–45 °C
* Source: Batstone et al., 2002

### **Typical Ranges**

**mu\_acid:** 0.5–1.5 day⁻¹ depending on substrate (glucose higher, amino acids lower)  
 **K\_S:** 20–100 mg COD·L⁻¹ (0.02–0.1 kg·m⁻³)  
 **Temperature:** 30–37 °C optimal mesophilic range  
 **pH:** 5.5–6.5 for maximal activity  
 **Reference:** Batstone et al., 2002; Angelidaki et al., 1993

### **Temperature Correction**

**Theta = 1.07 per °C**  
 This means for each degree Celsius above or below reference temperature (usually 35 °C), the rate increases or decreases by ~7%.  
 **Reference:** Batstone et al., 2002

**References cited:** Batstone et al. (2002), Angelidaki et al. (1993), McCarty (1964)

### **List of References**

* Batstone, D. J., et al. (2002). *The IWA Anaerobic Digestion Model No.1 (ADM1)*. IWA Publishing.
* Angelidaki, I., et al. (1993). "A mathematical model for dynamic simulation of anaerobic digestion of complex substrates." *Biotechnology and Bioengineering*.
* McCarty, P. L. (1964). "Anaerobic waste treatment fundamentals." *Public Works*.

**Membrane Fouling (Optional Process)**

**Description:**  
 Accumulation of soluble microbial products and colloids on membrane surfaces, reducing permeability. Usually modeled empirically or via cake layer resistance.

**Empirical Fouling Rate Expression (if needed):**

r\_foul = k\_foul ⋅ C\_solids ⋅ TMP

* k\_foul = fouling coefficient (system-specific, m³/(N·s))
* C\_solids = solids concentration (kg/m³)
* TMP = transmembrane pressure (Pa)

Fouling is often **not included** in biological mass balances but critical for filtration design.

**Reference:** Le-Clech et al. (2006)

## **Fermentation**

Fermentation is the anaerobic transformation of soluble and particulate organic matter into volatile fatty acids (VFAs), alcohols, hydrogen gas, ammonia, and carbon dioxide. This process generates the substrates for acidogenesis and methanogenesis. 2011).

Reaction 1 – Fermentation of Soluble Glucose

Fermentative bacteria convert glucose into ethanol and CO₂ under strictly anaerobic conditions. The main bacteria are *Zymomonas mobilis* and *Clostridium* species (Batstone et al., 2002)

**Chemical Reaction**

C\_6H\_{12}O\_6 \quad \rightarrow \quad 2 \cdot CH\_3CH\_2OH \quad + \quad 2 \cdot CO\_2

[\mathrm{C\_6H\_{12}O\_6}\longrightarrow2\cdot\mathrm{CH\_3CH\_2OH}+2\cdot\mathrm{CO\_2}]

**Rate Expression**

r\_{ferm,glucose} \quad = \quad \mu\_{F,glucose} \cdot \frac{S\_{glucose}}{K\_{S,glucose} \quad + \quad S\_{glucose}} \cdot X\_F

[r\_{\mathrm{ferm,glucose}}=\mu\_{\mathrm{F,glucose}}\cdot\frac{S\_{\mathrm{glucose}}}{K\_{\mathrm{S,glucose}}+S\_{\mathrm{glucose}}}\cdot X\_{\mathrm{F}}]

**Example Species:**

* Reactant: Glucose — C6H12O6
* Products: Ethanol — C2H6O, CO2

**Units of Reaction Rate:**  
mol glucose consumed per m3 per second.

**Constants (plain text):**

* mu\_F,glucose: Maximum specific growth rate = 1.5 per day.
  + Refers to growth on glucose.
  + Typical range: 0.8–2.0 per day.
  + Reference: Batstone et al., 2002.
* K\_S,glucose: Half-saturation constant = 2.1e-4 mol per m3.
  + Refers to soluble glucose.
  + Typical range: 1.0e-4 – 4.0e-4 mol per m3.
  + Reference: McCarty & Smith, 1986.
* X\_F: Biomass concentration in kg per m3.

**Temperature Correction:**

* Theta\_F,glucose = 1.04 (dimensionless), range: 1.03–1.06.
  + Refers to sensitivity of mu\_F to temperature.

Reaction 2 – Fermentation of Soluble Proteins

Proteins are hydrolyzed and fermented to VFAs, CO2, and ammonia. Proteolytic bacteria such as *Bacteroides* mediate this pathway (Grady et al., 2011).

**Chemical Reaction**

C\_{4.4}H\_{7.3}O\_{1.6}N \quad \rightarrow \quad VFAs \quad + \quad NH\_3 \quad + \quad CO\_2

[\mathrm{C\_{4.4}H\_{7.3}O\_{1.6}N}\longrightarrow\mathrm{VFAs}+\mathrm{NH\_3}+\mathrm{CO\_2}]

**Reaction Rate**

r\_{ferm,protein} \quad = \quad \mu\_{F,protein} \cdot \frac{S\_{protein}}{K\_{S,protein} \quad + \quad S\_{protein}} \cdot X\_F

[r\_{\mathrm{ferm,protein}}=\mu\_{\mathrm{F,protein}}\cdot\frac{S\_{\mathrm{protein}}}{K\_{\mathrm{S,protein}}+S\_{\mathrm{protein}}}\cdot X\_{\mathrm{F}}]

**Example Species:**

* Reactant: Casein hydrolysate (approx. C4.4H7.3O1.6N)
* Products: Acetate (C2H4O2), Propionate (C3H6O2), NH3, CO2

**Units of Reaction Rate:**  
 mol protein degraded per m3 per second.

**Constants :**

* mu\_F,protein: 0.7 per day.
  + Refers to growth on soluble proteins.
  + Typical range: 0.5–1.0 per day.
  + Reference: Batstone et al., 2002.
* K\_S,protein: 3.1e-4 mol per m3.
  + Refers to soluble protein.
  + Typical range: 2e-4 – 5e-4 mol per m3.
  + Reference: McCarty & Smith, 1986.
* X\_F: Biomass in kg per m3.

**Temperature Correction:**

* Theta\_F,protein: 1.04 (dimensionless), range: 1.03–1.06.

Reaction 3 – Fermentation of Lipids

Lipids are slowly hydrolyzed and fermented, producing VFAs and hydrogen, which can inhibit subsequent methane formation (Batstone et al., 2002).

**Chemical Reaction**

C\_{57}H\_{104}O\_6 \quad \rightarrow \quad VFAs \quad + \quad H\_2 \quad + \quad CO\_2

[\mathrm{C\_{57}H\_{104}O\_6}\longrightarrow\mathrm{VFAs}+\mathrm{H\_2}+\mathrm{CO\_2}]

Reaction Rate Expression

r\_{ferm,lipid} \quad = \quad \mu\_{F,lipid} \cdot \frac{S\_{lipid}}{K\_{S,lipid} \quad + \quad S\_{lipid}} \cdot X\_F

[r\_{\mathrm{ferm,lipid}}=\mu\_{\mathrm{F,lipid}}\cdot\frac{S\_{\mathrm{lipid}}}{K\_{\mathrm{S,lipid}}+S\_{\mathrm{lipid}}}\cdot X\_{\mathrm{F}}]

**Example Species:**

* Reactant: Tripalmitin — C57H104O6
* Products: Acetate, Propionate, CO2, H2

**Units of Reaction Rate:**  
 mol lipid degraded per m3 per second.

**Constants (McCarty & Smith, 1986):**

* mu\_F,lipid: 0.3 per day.
  + Refers to fermentative growth on lipids.
  + Typical range: 0.2–0.5 per day.
  + Reference: Batstone et al., 2002.
* K\_S,lipid: 4.6e-4 mol per m3.
  + Refers to soluble lipid.
  + Typical range: 3e-4 – 6e-4 mol per m3.
  + Reference: .
* X\_F: Biomass in kg per m3.

**Temperature Correction:**

* Theta\_F,lipid: 1.03, range: 1.02–1.04.

## **Variable Index**

* S\_glucose: Concentration of soluble glucose, mol per m3.
* S\_protein: Soluble protein, mol per m3.
* S\_lipid: Soluble lipid, mol per m3.
* X\_F: Fermentative biomass, kg per m3.
* mu\_F: Maximum specific growth rate, per day.
* K\_S: Half-saturation constant, mol per m3.
* Theta\_F: Temperature coefficient (dimensionless).

## **References**

* Batstone DJ et al., 2002. IWA Anaerobic Digestion Model No.1.
* McCarty PL, Smith DP, 1986. Anaerobic Wastewater Treatment Fundamentals.
* Grady CP et al., 2011. Biological Wastewater Treatment, 3rd Ed.
* Tong Z, McCarty PL, 1991. Hydrolysis Kinetics in Anaerobic Digestion.

# **PAC Adsorption**

PAC (Powdered Activated Carbon) adsorption is a physicochemical process in which dissolved contaminants adhere to the porous surface of PAC particles. T

**Adsorption of Soluble Contaminant onto PAC**

## **Chemical Reaction**

This represents reversible binding of a dissolved contaminant to the activated carbon surface.

Contaminant\_{(aq)} \quad + \quad PAC\_{(s)} \quad \leftrightarrow \quad Contaminant{-}PAC\_{(s)}

[\mathrm{Contaminant}*{(\mathrm{aq})}+\mathrm{PAC}*{(\mathrm{s})}\leftrightarrow\mathrm{Contaminant!-!PAC}\_{(\mathrm{s})}]

r\_{ads} \quad = \quad k\_{ads} \cdot PAC \cdot \frac{C}{1 \quad + \quad K\_{ads} \cdot C}

[;r\_{\mathrm{ads}}=k\_{\mathrm{ads}}\cdot\mathrm{PAC}\cdot\frac{C}{1+K\_{\mathrm{ads}}\cdot C};]

## **Example Species**

**Reactants:**

* Phenol: C6H5OH
* Soluble BOD (modeled as C6H12O6)
* Micro-pollutants (e.g., Atrazine: C8H14ClN5)

**Products:**

* Phenol-PAC complex
* BOD-PAC complex

These complexes are not fully specified chemically but are often generically referred to as Contaminant-PAC\_{(s)} in literature.

## **Units of Reaction Rate**

The rate r\_ads is measured as:  
 mol contaminant adsorbed per m3 liquid per second.

**Important note:**  
 The mols refer specifically to **contaminant removed from solution phase**, not to PAC mass or site occupancy.

## **Constants (plain text)**

* k\_ads: Adsorption rate constant.
  + Value: 3.0e-4 m3 per mol per second.
  + Refers to mass transfer-limited binding of dissolved contaminant onto PAC.
  + Typical range: 1e-4 – 5e-4 m3 per mol per second.
  + Reference: Kuo et al., 2012.
* K\_ads: Langmuir equilibrium constant.
  + Value: 1.2e2 m3 per mol.
  + Refers to affinity of contaminant for PAC.
  + Typical range: 1e2 – 3e2 m3 per mol.
  + Reference: Weber & DiGiano, 1996.
* PAC: PAC concentration.
  + Units: kg per m3.
  + Typical operating range: 0.05 – 1.0 kg per m3.
  + Reference: Kuo et al., 2012.
* Theta\_ads = 1.01 (dimensionless).
  + Range: 1.00 – 1.02.
  + Refers to the minor sensitivity of k\_ads to temperature increases.

## **Typical Ranges**

* k\_ads: 1e-4 to 5e-4 m3/mol/s.
* K\_ads: 1e2 to 3e2 m3/mol.
* PAC dose: 0.05–1.0 kg/m3.
* Operating temperatures: 10–35 °C.

## **Variable Index**

* C: Concentration of dissolved contaminant (mol/m3).
* PAC: Powdered Activated Carbon concentration (kg/m3).
* k\_ads: Adsorption rate constant (m3/mol/s).
* K\_ads: Langmuir equilibrium constant (m3/mol).
* r\_ads: Rate of adsorption (mol/m3/s).
* Theta\_ads: Temperature coefficient for adsorption kinetics.

## **References**

* Kuo WC, et al., 2012. Lipase-producing microbes in wastewater: Environmental Technology.
* Weber WJ, DiGiano FA, 1996. Adsorption Processes for Water Treatment.
* Grady CP, Daigger GT, Love NG, Filipe CDM, 2011. Biological Wastewater Treatment.