Chapter 6
Dynamical Systems

Discrete Mathematics II/Mathematical Modelling

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1. **A dynamical system model of CO_2 concentration in greenhouses**

2. **Numerical methods**

Microclimate forecasting and control in greenhouses

Figure: Greenhouses.

- Optimum growing environment;
- Longer growing season;
- Garden in any weather condition;
- Protection from pests;
- ...

Greenhouse elements and functions

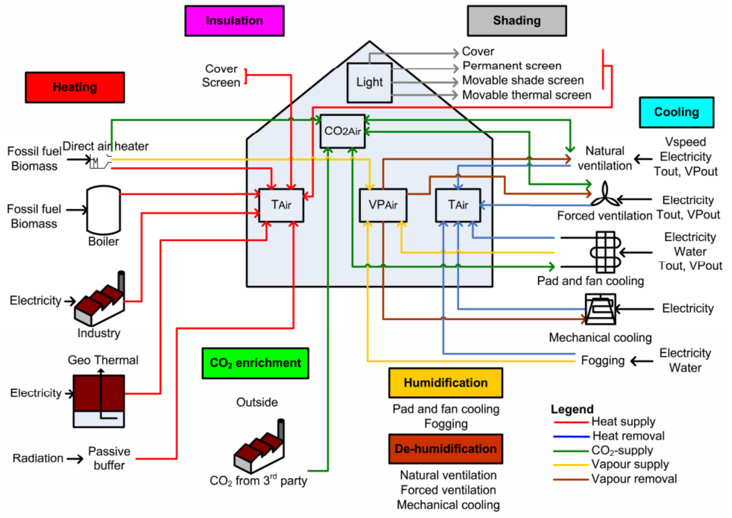


Figure: Greenhouse elements and functions.

CO_2 flow and the photosynthesis of plants

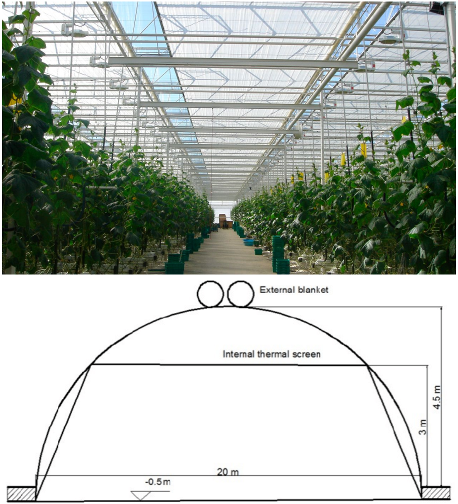


Figure: Internal thermal screen that divides the air in a greenhouse into two compartments: above and below the thermal screen.

CO_2 flow and the photosynthesis of plants

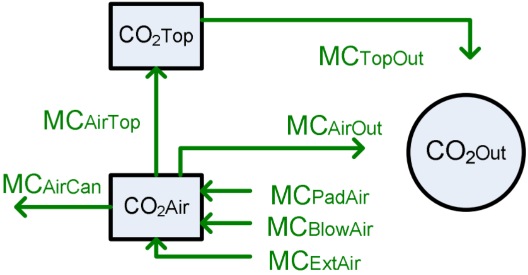


Figure: CO_2 flow in a greenhouse.

- Top/Air: the compartment above/below the thermal screen;
- Out/Ext: outside the greenhouse/external source;
- $Blow/Pad$: the direct air heater/pad and fan;
- Can: the canopy inside the greenhouse;
- MC_{AB}: the net CO_2 flux from A to B.

CO_2 flow and the photosynthesis of plants

Balance laws:

$$\begin{aligned} cap_{CO_2\,Air}\dot{CO_2}_{Air} &= MC_{BlowAir} + MC_{ExtAir} + MC_{PadAir} \\ &\quad - MC_{AirCan} - MC_{AirTop} - MC_{AirOut}. \quad (1) \end{aligned}$$

$$cap_{CO_2\,Top}\dot{CO_2}_{Top} = MC_{AirTop} - MC_{TopOut}. \quad (2)$$

- $cap_{CO_2\,Top/Air}$: capacity of the compartment above/below the thermal screen to store CO_2 (m);
- $\dot{CO_2}_{Top/Air}$: the rate change of CO_2 concentration in the compartment above/below the thermal screen in time (mg m^{-3} s^{-1});
- MC_{AB}: the net CO_2 flux from A to B (mg m^{-2} s^{-1}).

CO_2 flow and the photosynthesis of plants

$$MC_{BlowAir} = \eta_{HeatCO_2} H_{BlowAir} = \frac{\eta_{HeatCO_2} U_{Blow} P_{Blow}}{A_{Flr}}. \quad (3)$$

- η_{HeatCO_2}: the amount of CO_2 released when 1 Joule sensible energy is produced by the direct air heater (mg $\{CO_2\}$ J^{-1});
- $H_{BlowAir}$: the heat flux from the direct air heater to the greenhouse air (W m^{-2});
- U_{Blow}: the control valve of the direct air heater ranging in $[0, 1]$;
- P_{Blow}: the heat capacity of the direct air heater (W);
- A_{Flr}: the area of the greenhouse floor (m^2).

CO_2 flow and the photosynthesis of plants

$$MC_{ExtAir} = \frac{U_{ExtCO_2}\phi_{ExtCO_2}}{A_{Flr}}. \qquad (4)$$

- U_{ExtCO_2}: the control valve of the external CO_2 source ranging in $[0, 1]$;
- ϕ_{ExtCO_2}: the capacity of the external CO_2 source (mg s^{-1}).

CO_2 flow and the photosynthesis of plants

$$\begin{aligned} MC_{PadAir} &= f_{Pad}(CO_{2\,Out} - CO_{2\,Air}) \\ &= \frac{U_{Pad}\phi_{Pad}(CO_{2\,Out} - CO_{2\,Air})}{A_{Flr}}. \end{aligned} \quad (5)$$

- f_{Pad}: the ventilation flux due to the pad and fan system (m s^{-1});
- U_{Pad}: the control valve of the pad and fan system ranging in $[0, 1]$;
- ϕ_{Pad}: the capacity of the air flux through the pad (m^3 s^{-1}).

CO_2 flow and the photosynthesis of plants

$$MC_{AirTop} = f_{ThScr}(CO_{2\,Air} - CO_{2\,Top}), \tag{6}$$

$$\begin{aligned} f_{ThScr} &= U_{ThScr}K_{ThScr}|T_{Air} - T_{Top}|^{\frac{2}{3}} \\ &\quad + (1 - U_{ThScr})\left[\frac{g(1 - U_{ThScr})}{2\rho_{Air}^{Mean}}|\rho_{Air} - \rho_{Top}|\right]^{\frac{1}{2}}. \end{aligned}$$

- f_{ThScr}: the air flux through the thermal screen (m s^{-1});
- U_{ThScr}: the control of the thermal screen ranging in $[0, 1]$;
- K_{ThScr}: the screen flux coefficient determining the permeability of the screen (m K$^{-\frac{2}{3}}$ s^{-1});
- g: the gravitational acceleration (m s^{-2});
- $\rho_{Air/Top}$: the density of the greenhouse air below/above the thermal screen (kg m^{-3});
- ρ_{Air}^{Mean}: the mean density of the greenhouse air (kg m^{-3});
- $T_{Air/Top}$: the temperature below/above the thermal screen (K).

CO_2 flow and the photosynthesis of plants

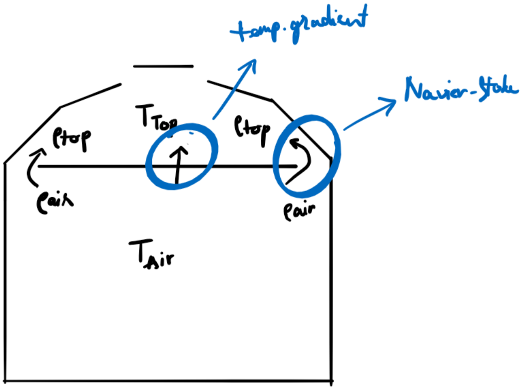


Figure: Air flow through the thermal screen.

CO_2 flow and the photosynthesis of plants

$$MC_{AirOut} = (f_{VentSide} + f_{VentForced})(CO_{2\,Air} - CO_{2\,Out}). \quad (7)$$

- $f_{VentSide}$: the rate for the sidewall ventilation system (m s^{-1});
- $f_{VentForced}$: the rate for the forced ventialtion system (m s^{-1}).

CO_2 flow and the photosynthesis of plants

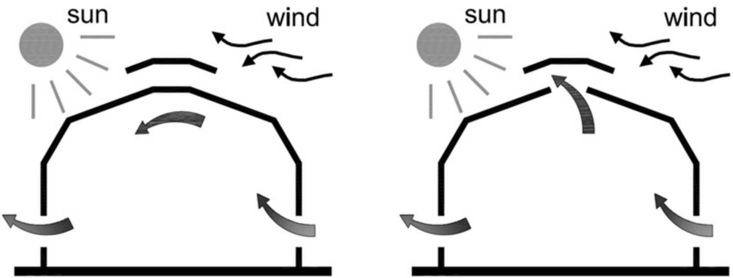
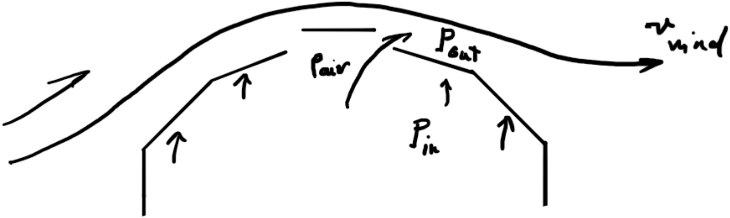


Figure: Without/With Chimney's effect.

CO_2 flow and the photosynthesis of plants



Bernoulli: $P_{out} - P_{In} = \frac{1}{2} \rho_{air} \cdot v_{wind}^2$

Figure: Air flow through the roof opening.

CO_2 flow and the photosynthesis of plants

$$f_{VentRoofSide} =$$

$$\frac{C_d}{A_{Flr}} \left[\frac{U_{Roof}^2 U_{Side}^2 A_{Roof}^2 A_{Side}^2}{U_{Roof}^2 A_{Roof}^2 + U_{Side}^2 A_{Side}^2} \cdot \frac{2gh_{SideRoof}(T_{Air} - T_{Out})}{T_{Air}^{Mean}} + \left(\frac{U_{Roof} A_{Roof} + U_{Side} A_{Side}}{2} \right)^2 C_w v_{Wind}^2 \right]^{\frac{1}{2}}.$$

- $f_{VentRoofSide}$: the ventilation rate through both the roof and side vents (m s^{-1});
- $C_{d/w}$: discharge/global wind pressure coefficient depending on the greenhouse shape and the use of an outdoor thermal screen (-);
- $U_{Roof/Side}$: the control of the roof/side openings ranging in [0,1];
- $A_{Roof/Side}$: the roof/side opening area (m^2);
- $h_{SideRoof}$: the vertical distance between mid-points of side wall and roof ventilation openings (m);
- T_{Air}^{Mean}: the mean temperature between the indoor and outdoor temperatures (K); v_{Wind}: wind speed (m s^{-1}).

CO_2 flow and the photosynthesis of plants

Insect-screen effect:

$$\eta_{InsScr} = \zeta_{InsScr}(2 - \zeta_{InsScr}).$$

- η_{InsScr}: reduction factor (-);
- ζ_{InsScr}: the screen porosity i.e. the area of holes per unit area of the insect screen (-).

Greenhouse leakage:

$$f_{leakage} = \begin{cases} 0.25 \cdot c_{leakage}, & v_{Wind} < 0.25, \\ v_{Wind} \cdot c_{leakage}, & v_{Wind} \geq 0.25. \end{cases}$$

- $f_{leakage}$: the leakage rate depending on wind speed (m s^{-1});
- $c_{leakage}$: the leakage coefficient depending on the greenhouse type (-).

CO_2 flow and the photosynthesis of plants

If $\eta_{Side} \geq \eta_{Side\_Thr}$,

$$f_{VentSide} = \eta_{InsScr} f_{VentRoofSide}(A_{Roof} = 0) + 0.5 f_{leakage}.$$

Otherwise,

$$\begin{aligned} f_{VentSide} = \eta_{InsScr} & [U_{ThScr} f_{VentRoofSide}(A_{Roof} = 0) \\ & + (1 - U_{ThScr}) f_{VentRoofSide} \eta_{Side}] + 0.5 f_{leakage}. \end{aligned}$$

- η_{Side}: the ratio between the side vents area and total ventilation area (-);
- η_{Side_Thr}: the threshold value above which no chimney effect is assumed to occur (-).

CO_2 flow and the photosynthesis of plants

$$f_{VentForced} = \frac{\eta_{InsScr} U_{VentForced} \phi_{VentForced}}{A_{Flr}}.$$

- $U_{VentForced}$: the control valve of the forced ventilation ranging in $[0, 1]$;
- $\phi_{VentForced}$: the air flow capacity of the forced ventilation system (m^3 s^{-1})

CO_2 flow and the photosynthesis of plants

$$MC_{TopOut} = f_{VentRoof}(CO_{2\,Top} - CO_{2\,Out}). \tag{8}$$

$$f_{VentRoof} = \frac{C_d U_{Roof} A_{Roof}}{2A_{Flr}} \left[\frac{g h_{Roof}(T_{Air} - T_{Out})}{2T_{Air}^{Mean}} + C_w v_{Wind}^2 \right]^{\frac{1}{2}}.$$

- h_{Roof}: the vertical dimension of a single ventilation opening (m).

CO_2 flow and the photosynthesis of plants

$$MC_{AirCan} = M_{CH_2O} h_{C_{Buf}} (P - R). \tag{9}$$

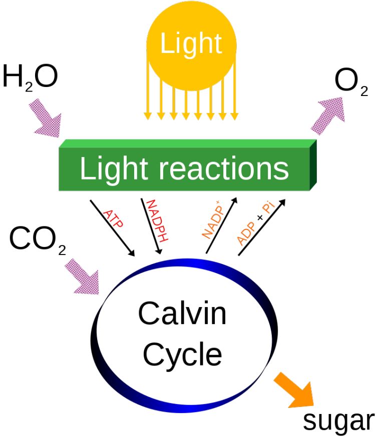
- M_{CH_2O}: the molar mass of CH_2O (mg μmol^{-1});
- $h_{C_{Buf}}$: the inhibition of the photosynthesis rate by saturation of the leaves with carbohydrates (-), where

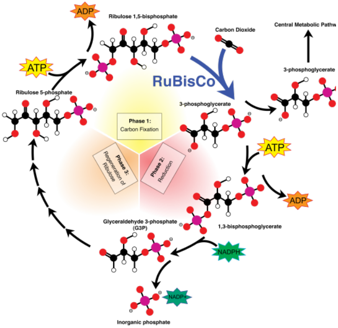
$$h_{C_{Buf}} = \begin{cases} 0, & C_{Buf} > C_{Buf}^{Max}, \\ 1, & C_{Buf} \leq C_{Buf}^{Max}; \end{cases}$$

- C_{Buf}/C_{Buf}^{Max}: the capacity/maximum capacity of carbonhydrates storage in the canopy buffer (mg $\{CH_2O\}$ m^{-2});
- P/R: the photosynthesis/photorespiration rate of the canopy during the photosynthesis process (μmol $\{CO_2\}$ m^{-2} s^{-1}).

CO_2 flow and the photosynthesis of plants

One leaf:





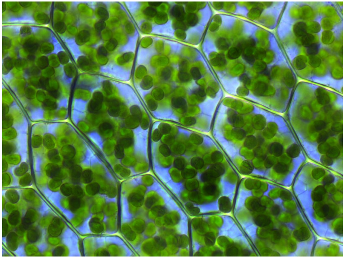


Figure: Photosynthesis - Calvin Cycle - Chloroplast.

CO_2 flow and the photosynthesis of plants

CO_2 diffusion:

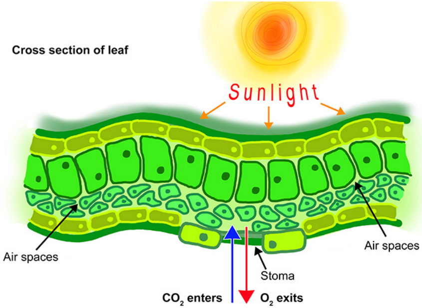


Figure: CO_2 diffuses into leaf cells through stomata.

CO_2 flow and the photosynthesis of plants

Fick's law:

$$P = \frac{CO_{2\,Air} - CO_{2\,Stom}}{Res}.$$

- $CO_{2\,Stom}$: the amount of CO_2 in the chloroplasts (μmol m^{-3});
- Res: the resistance to CO_2 diffusion (s m^{-1}).

Carbon fixation:

$$2H_2O \to 4e^- + 4H^+ + O_2$$
$$CO_2 + 4e^- + 4H^+ \to CH_2O + H_2O$$

Michaelis–Menten kinetic model

$$P = \frac{P_{Max}}{1 + \dfrac{CO_{2\,0.5}}{CO_{2\,Stom}}}.$$

- P_{Max}: the photosynthesis rate at saturating $CO_{2\,Stom}$ (μmol $\{CO_2\}$ m^{-2} s^{-1});
- $CO_{2\,0.5}$: the amount of $CO_{2\,Stom}$ such that $P = P_{Max}/2$ (μmol m^{-3}).

CO_2 flow and the photosynthesis of plants

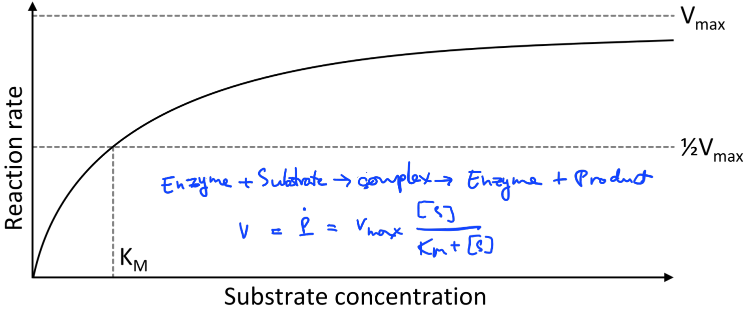


Figure: Michaelis–Menten kinetic model.

Solve for $CO_{2\,Stom}$, P satisfies

$$ResP^2 - (CO_{2\,Air} + CO_{2\,0.5} + ResP_{Max})P + CO_{2\,Air}P_{Max} = 0.$$

Only P that $P \to P_{Max}$ as $CO_{2,Air} \to +\infty$.

CO_2 flow and the photosynthesis of plants

<u>P_{Max} and the Arrhenius model:</u>

$$k(T) = k(T_0)e^{-\frac{H_a}{R}\left(\frac{1}{T}-\frac{1}{T_0}\right)}.$$

- T: the temperature of the leaf (K);
- T_0: a specific temperature of the leaf that we know the reaction rate (K);
- $K(T)$: the reaction rate (-);
- H_a: the activation energy (J mol^{-1});
- R: the ideal gas constant (J mol^{-1} K^{-1}).

CO_2 flow and the photosynthesis of plants

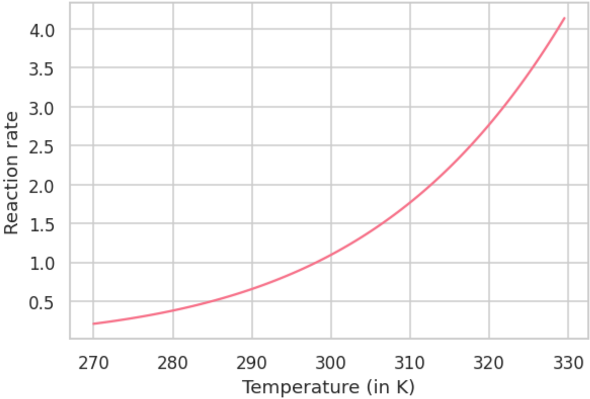


Figure: Arrhenius model with $T_0 = 298.15$, $k(T_0) = 1$, $H_a = 37000$.

CO_2 flow and the photosynthesis of plants

Enzyme activity:

$$f(T) = \frac{1 + e^{-\frac{H_d}{R}\left(\frac{1}{T_0} - \frac{1}{\frac{H_d}{S}}\right)}}{1 + e^{-\frac{H_d}{R}\left(\frac{1}{T} - \frac{1}{\frac{H_d}{S}}\right)}}.$$

- $f(T)$: the enzyme activity rate (-);
- H_d: the deactivation energy (J mol^{-1});
- S: the entropy term (J mol^{-1} K^{-1}).

CO_2 flow and the photosynthesis of plants

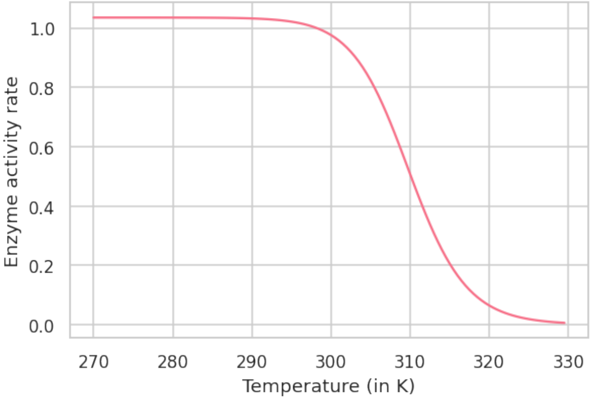


Figure: Enzyme activity model with $H_d = 220000$ and $S = 710$.

CO_2 flow and the photosynthesis of plants

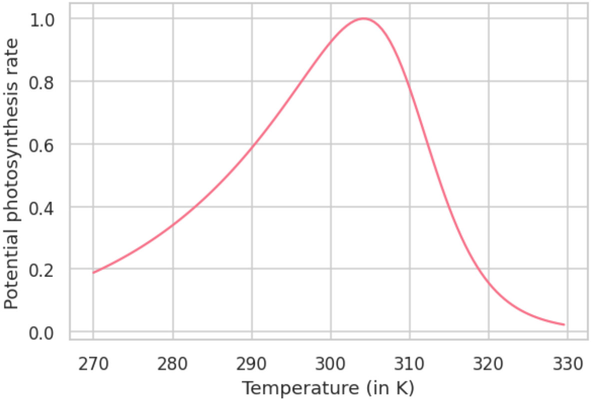


Figure: (Potential photosynthesis rate $P_{Max}(T) = k(T)f(T)$ (normalized).

CO_2 flow and the photosynthesis of plants

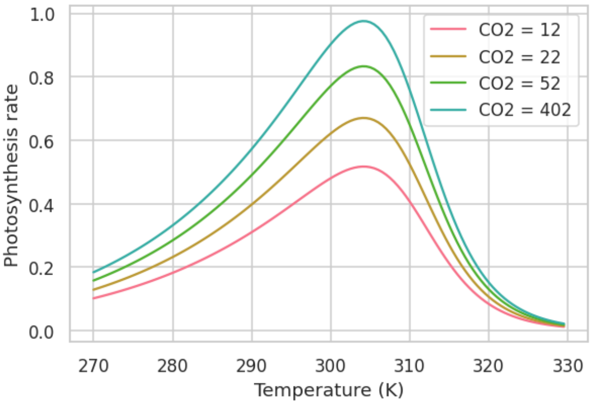


Figure: Photosynthesis rate with different value of CO_2 in the greenhouse air and resistance $Res = 2.5$ (normalized).

CO_2 flow and the photosynthesis of plants

Canopy:

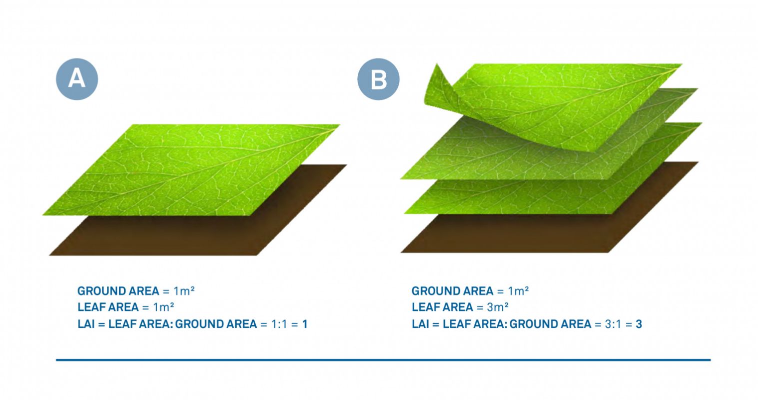


Figure: Leaf area index.

CO_2 flow and the photosynthesis of plants

P_{Max} and the Arrhenius model:

$$k(T) = LAI \cdot k(T_0) \cdot e^{-\frac{H_a}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)}.$$

- T: the temperature of the canopy (K);
- T_0: a specific temperature of the canopy that we know the reaction rate (K);
- $k(T)$: the reaction rate of the canopy at T (-);
- $k(T_0)$: the reaction rate in the stroma of a leaf at T_0 (-).

CO_2 flow and the photosynthesis of plants

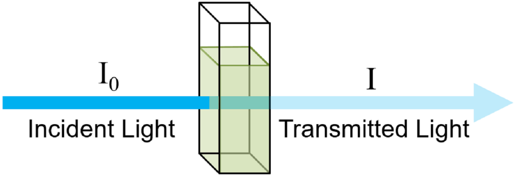
Michaelis–Menten model:

$$P_{Max}(L,T) = \frac{P_{MLT} \cdot P_{Max}(T)}{1 + \dfrac{L_{0.5}}{L}}.$$

- L: the photosynthetically active radiation absorbed by the canopy (μmol {photons} m^{-2} s^{-1});
- $L_{0.5}$: the photosynthetically active radiation at which $P_{Max}(L,T) = P_{MLT} \cdot P_{Max}(T)/2$ (μmol {photons} m^{-2} s^{-1});
- P_{MLT}: the value of P_{Max} at saturation L and optimum T (μmol $\{CO_2\}$ m^{-2} s^{-1}).

CO_2 flow and the photosynthesis of plants

Beer's law:



$$I = \frac{I_0.K.e^{-K.LAI}}{1-m}.$$

- K: the extinction coefficient in between 0.7-1.0 if the leaves are not inclined. Otherwise 0.3-0.5;
- I: the L measured at the ground surface (μmol {photons} m^{-2} s^{-1});
- I_0: the L measured above the canopy (μmol {photons} m^{-2} s^{-1});
- m: the transmittance of the leaves, which set as default 0.1.

CO_2 flow and the photosynthesis of plants

Absorbed L:

$$L = L_0 \left(1 - \frac{K.e^{-K.LAI}}{1-m} \right).$$

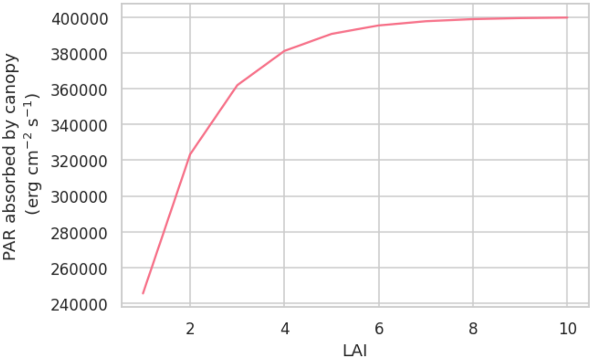


Figure: Dependence of PAR on LAI.

CO_2 flow and the photosynthesis of plants

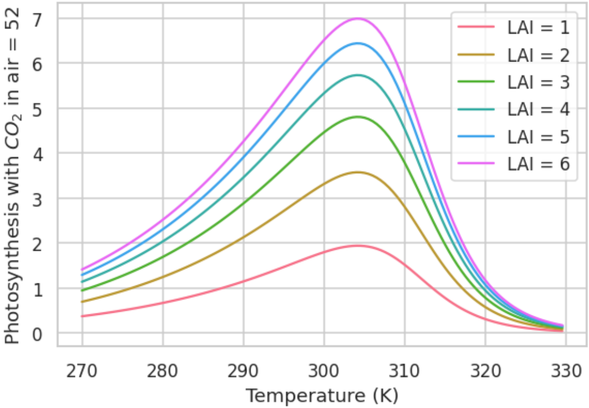


Figure: Photosynthesis with fixed $CO_{2\,Air}$ and different LAI.

Forward Euler method

First-order differential equation:

$$\begin{cases} \dot{x} = f(t, x), \\ x(t_0) = x_0. \end{cases} \tag{10}$$

Taylor expansion:

$$\begin{aligned} x(t+h) &= x(t) + \dot{x}(t)h + O(h^2) \\ &= x(t) + f(t, x(t))h + O(h^2). \end{aligned} \tag{11}$$

Forward Euler method

Forward Euler formula:

$$x_{n+1} = x_n + f(t_n, x_n)h, \tag{12}$$

where

$$x_n := x(t_n) \quad n = 0, 1, 2, \ldots$$

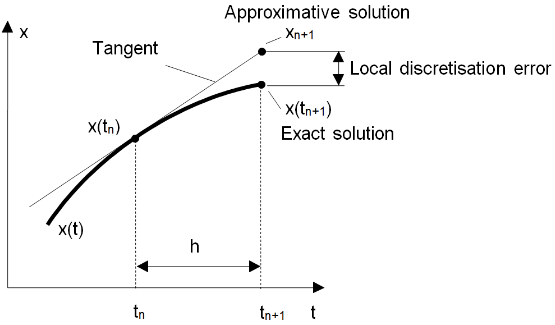


Figure: Forward Euler numerical scheme.

Forward Euler method

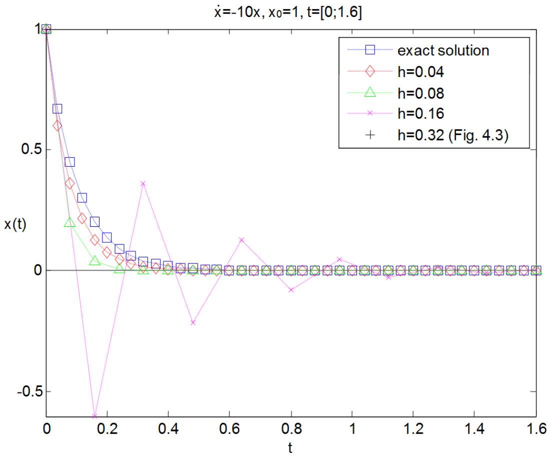


Figure: Example $\dot{x} = -10x$, $x_0 = 1$ with different $h < 0.32$.

Forward Euler method

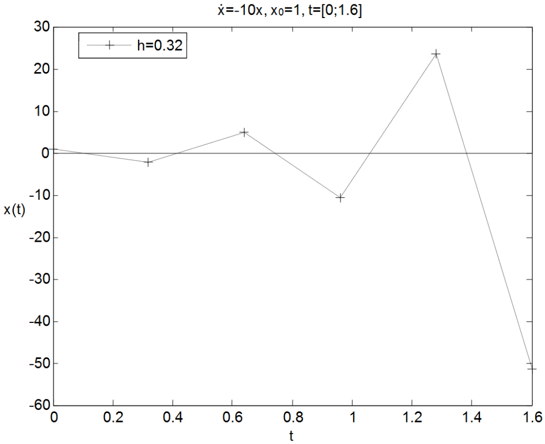


Figure: Example $\dot{x} = -10x$, $x_0 = 1$ with $h = 0.32$.

Forward Euler method

Test equation:

$$\begin{cases} \dot{x} = \alpha x, \quad \alpha \in \mathbb{R}, \\ x(t_0) = x_0. \end{cases} \tag{13}$$

Applying the Forward Euler method

$$x_{n+1} = (1+\alpha h)x_n = (1+\alpha h)^2 x_{n-1} = \cdots = (1+\alpha h)^{n+1} x_0. \tag{14}$$

Stability condition:

$$|1 + \alpha h| < 1. \tag{15}$$

Forward Euler method

Stability function and stability region:

$$x_{n+1} = \Phi(\alpha h)x_n. \tag{16}$$

Then $\Phi = \Phi(z)$ for $z \in \mathbb{C}$ is called stability function and the region

$$\{z \in \mathbb{C} : |\Phi(z)| < 1\} \tag{17}$$

is called the stability region for the numerical scheme.

A-stable numerical scheme: A numerical scheme is A-stable if its stability region contains the left half complex plane.

L-stable numerical scheme: A numerical scheme is L-stable if it is A-stable and $\Phi(z) \to 0$ as $z \to \infty$.

Forward Euler method

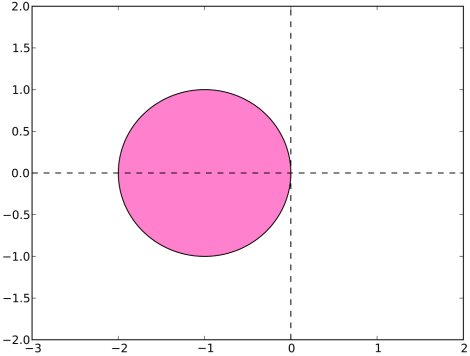


Figure: Stability region of Forward Euler $\{z \in \mathbb{C} : |1+z| < 1\}$.

Backward Euler method

Backward Euler formula:

$$x_{n+1} = x_n + f(t_n, x_{n+1})h, \tag{18}$$

where

$$x_n := x(t_n) \quad n = 0, 1, 2, \ldots$$

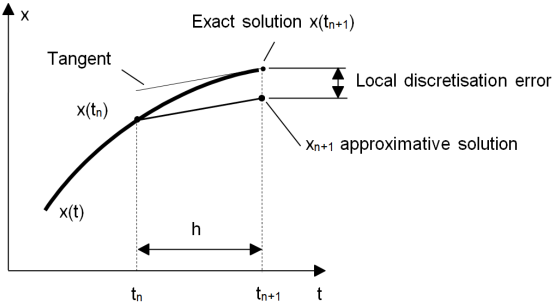


Figure: Backward Euler numerical scheme.

Backward Euler method

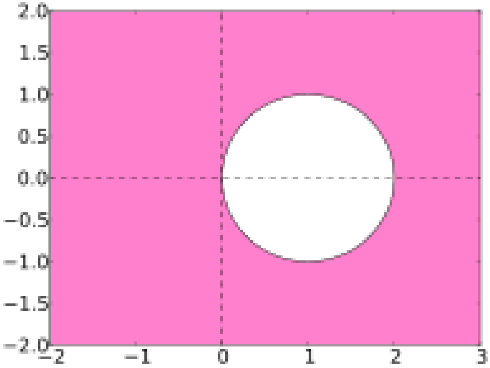


Figure: Stability region of Backward Euler $\{z \in \mathbb{C} : \dfrac{1}{|1-z|} < 1\}$.

Newton–Raphson scheme

$$f(x) = 0, \tag{19}$$

where $f = (f_1, \dots, f_N)$ is differentiable and $x = (x_1, \dots, x_N)$.

Newton iteration formula:

$$x_{n+1} = x_n - J(x_n)^{-1} f(x_n), \tag{20}$$

where

$$J(x) \coloneqq \begin{pmatrix} \dfrac{\partial f_1}{\partial_{x_1}} & \cdots & \dfrac{\partial f_1}{\partial_{x_N}} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial f_N}{\partial_{x_1}} & \cdots & \dfrac{\partial f_N}{\partial_{x_N}}. \end{pmatrix} \tag{21}$$

Newton–Raphson scheme

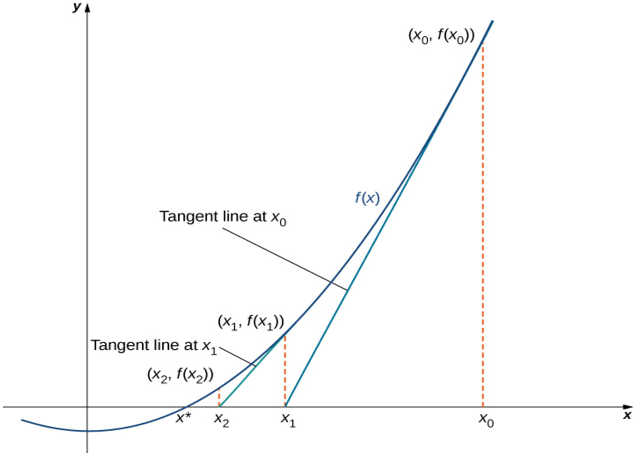


Figure: Newton iteration scheme.

Newton–Raphson scheme

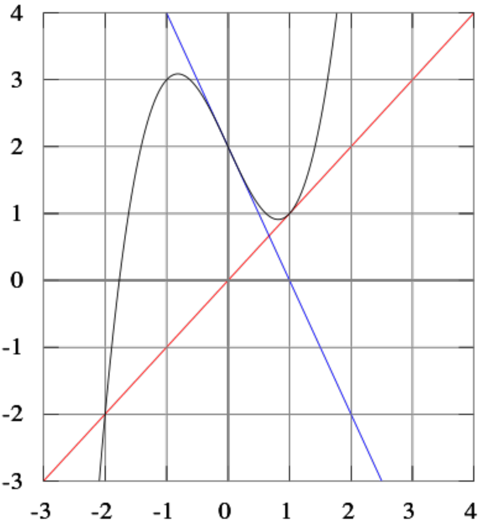


Figure: Intersection of two tangent line at 0 and 1 of $f(x) = x^3 - 2x + 2$.

Explicit Midpoint Runge–Kutta method

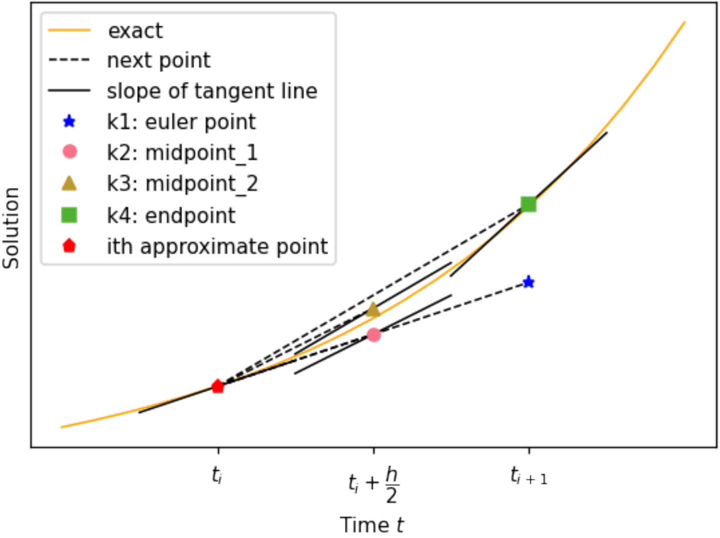


Figure: Improvement of Forward Euler.

Explicit Midpoint Runge–Kutta method

Explicit Midpoint method:

Step 1. Compute the slope at x_n

$$k_1 = f(t_n, x_n). \tag{22}$$

Step 2. Compute the slope at the midpoint

$$k_2 = f(t_n + \frac{1}{2}h, x_n + \frac{1}{2}hk_1). \tag{23}$$

Step 3. Compute x_{n+1}

$$x_{n+1} = x_n + hk_2. \tag{24}$$

Explicit Midpoint Runge–Kutta method

Proof for multi-variate scalar case of f:

$$k_1 = f(t_n, x_n). \tag{25}$$

$$k_2 = f(t_n + \alpha h, x_n + \beta h k_1). \tag{26}$$

$$x_{n+1} = x_n + a h k_1 + b h k_2. \tag{27}$$

Explicit Midpoint Runge–Kutta method

Taylor expansion:

$$
\begin{aligned}
f(t_n+\alpha h, x_n+\beta h k_1) &= f(t_n,x_n)+\alpha h\frac{\partial f}{\partial t}(t_n,x_n) \\
&\quad +\beta h k_1\frac{\partial f}{\partial x}(t_n,x_n)+O(h^2)
\end{aligned} \tag{28}
$$

Substituting in (25)-(27)

$$
\begin{aligned}
x_{n+1} &= x_n+(a+b)hf(t_n,x_n) \\
&\quad +bh^2\left(\alpha\frac{\partial f}{\partial t}+\beta f\frac{\partial f}{\partial x}\right)(t_n,x_n)+O(h^3).
\end{aligned} \tag{29}
$$

Explicit Midpoint Runge–Kutta method

Taylor expansion:

$$
\begin{aligned}
x(t_{n+1}) &= x(t_n) + h\dot{x}(t_n) + \frac{h^2}{2}\ddot{x}(t_n) + O(h^3) \\
&= x(t_n) + hf(t_n, x_n) \\
&\qquad + \frac{h^2}{2}\left(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial x}\right)(t_n, x_n) + O(h^3). \qquad (30)
\end{aligned}
$$

From (29)

$$a + b = 1, \quad \alpha b = \frac{1}{2}, \quad \beta b = \frac{1}{2}. \qquad (31)$$

Choose $a = 0, b = 1, \alpha = \beta = \dfrac{1}{2}$.

Explicit order-4 Runge–Kutta method

Explicit order-4 Runge–Kutta method:

Step 1. Compute the slope at x_n

$$k_1 = f(t_n, x_n). \tag{32}$$

Step 2. Compute the slope at the midpoint from k_1

$$k_2 = f(t_n + \frac{1}{2}h, x_n + \frac{1}{2}hk_1). \tag{33}$$

Step 3. Compute the slope at the midpoint from k_2

$$k_3 = f(t_n + \frac{1}{2}h, x_n + \frac{1}{2}hk_2). \tag{34}$$

Step 4. Compute the slope at the endpoint from k_3

$$k_4 = f(t_n + h, x_n + hk_3). \tag{35}$$

Step 5. Compute x_{n+1}

$$x_{n+1} = x_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4). \tag{36}$$

Explicit Runge–Kutta method

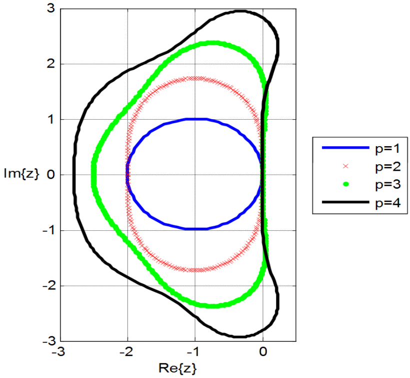


Figure: Stability region of Runge–Kutta of order $1 \leq p \leq 4$ where $\Phi(z) = \sum_{i=0}^{p} \frac{z^i}{i!}$.

Explicit Runge–Kutta method

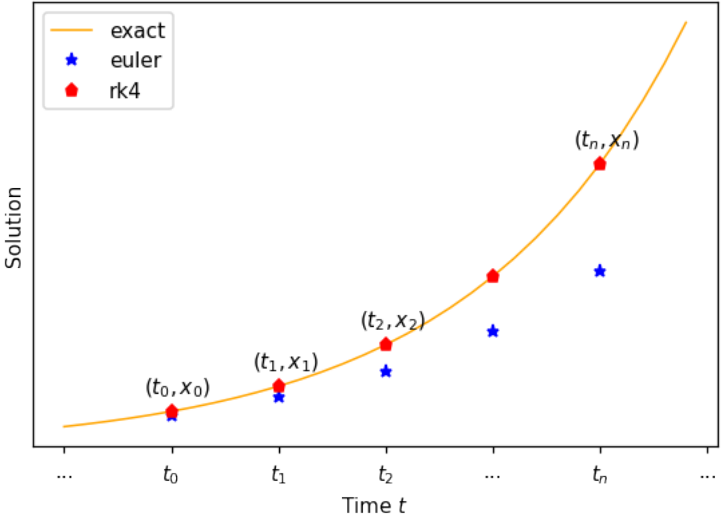


Figure: Forward Euler and Runge–Kutta of order 4.