Concentration response to mass impulse: 1D

$$\frac{\partial(h\cdot C)}{\partial t}+\frac{\partial}{\partial x}(h\cdot v_x C)+\frac{\partial}{\partial y}(h\cdot v_y C)=$$

$$\frac{\partial}{\partial x}(h\cdot D_x\frac{\partial C}{\partial x})+\frac{\partial}{\partial y}(h\cdot D_y\frac{\partial C}{\partial y})$$

2D

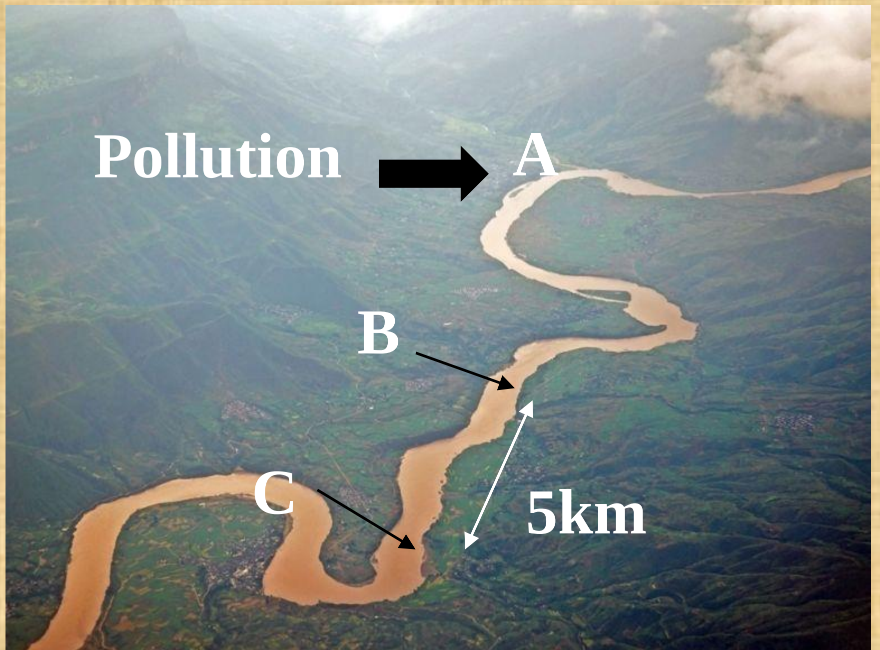
$$\frac{\partial C}{\partial t}+v_x\frac{\partial}{\partial x}C=D_x\frac{\partial^2 C}{\partial x^2}$$

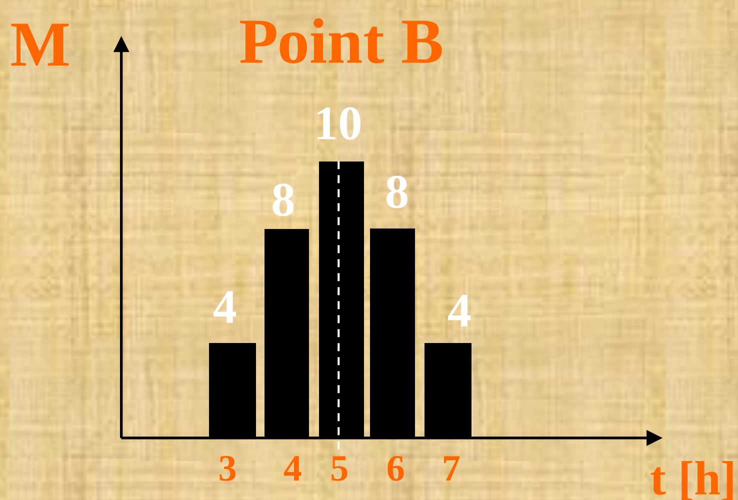
1D

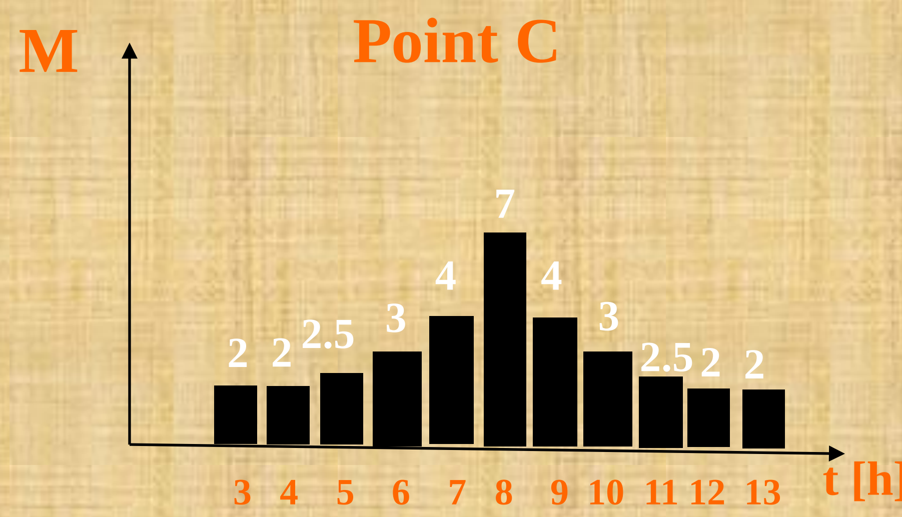
Basic eq. of 1D transport

C…concentration,
v…velocity,
D…turbulent diff. coeff.

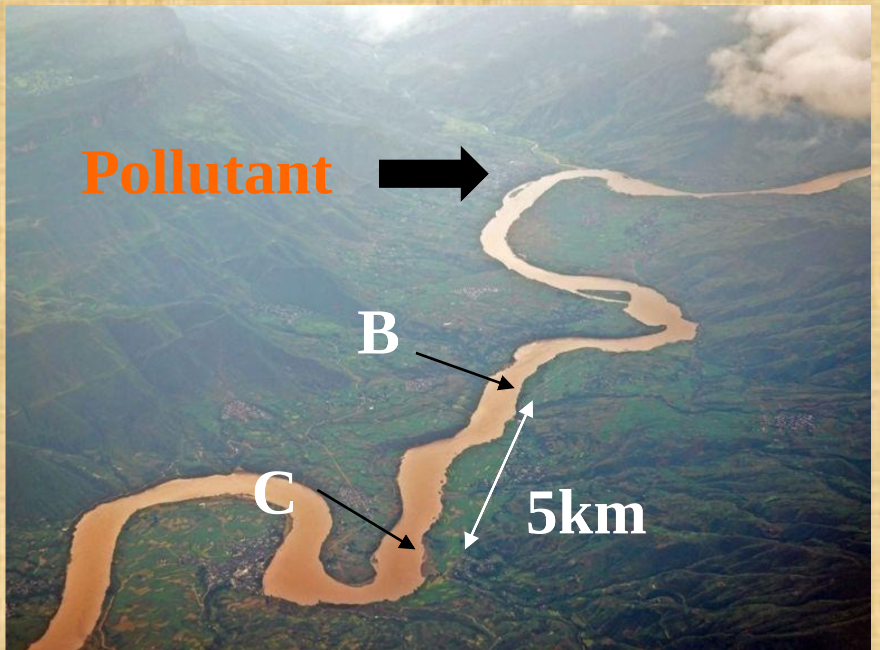
How to calculate D (diffusion)?



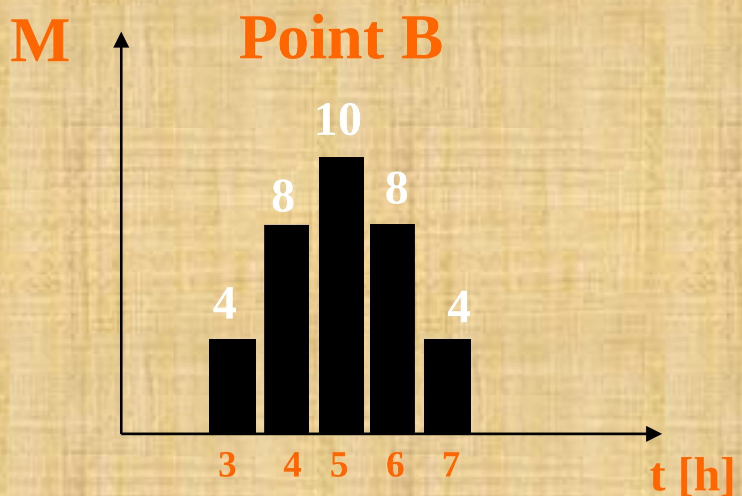


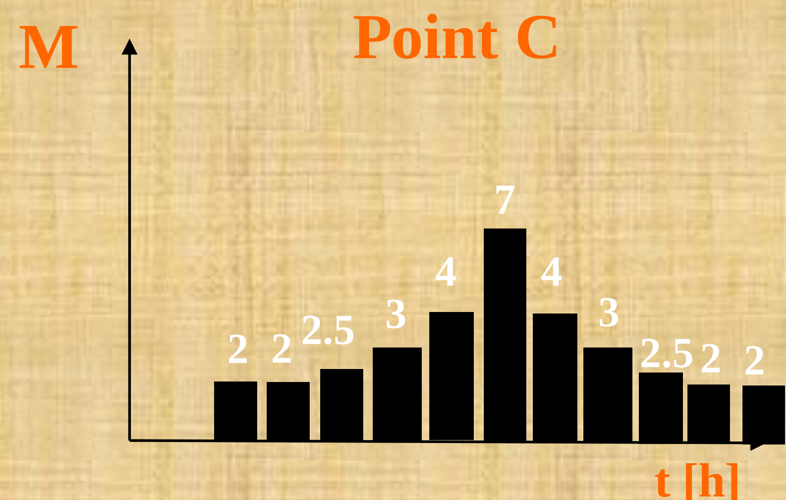


How to calculate D (diffusion)?

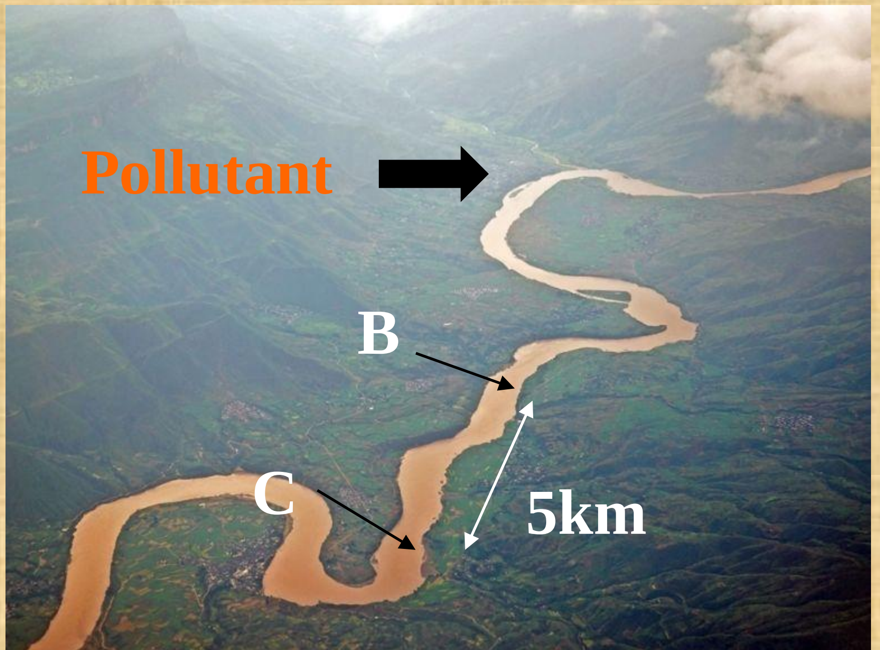


First step:
Is this conservative?





How to calculate D (diffusion)?

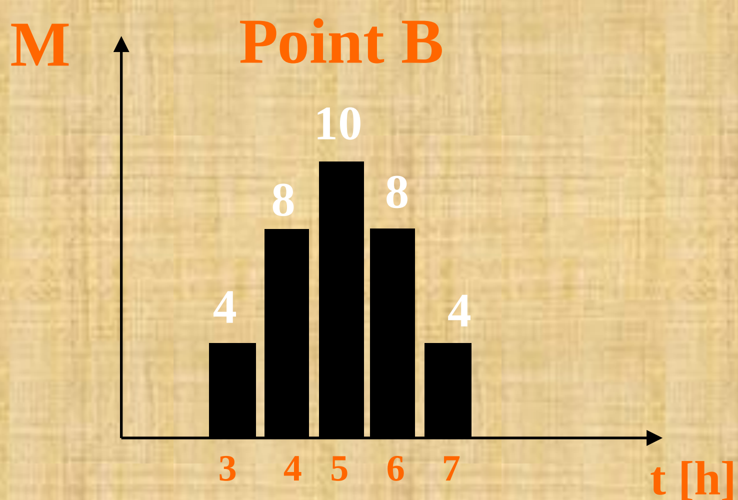


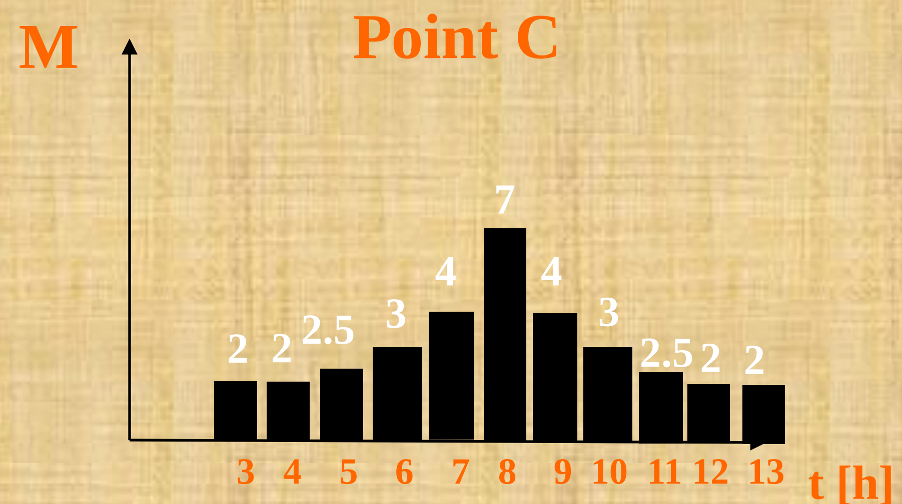
$$\sigma^2 = M((\xi - M(\xi))^2)$$

$$\sigma_x = \sqrt{2Dt}$$

$$\Downarrow$$

$$D = \frac{1}{2}\frac{\partial \sigma^2}{\partial t}$$





An impulse-response function describes the evolution of the variable of interest along a specified time horizon after a shock in a given moment (1D).

Under simplified conditions (regular geometry, and constant diff. coefficient: Analytical solution of 1D transport eq. can be found:

$$\frac{\partial C}{\partial t} + v_x \frac{\partial}{\partial x} C = D_x \frac{\partial^2 C}{\partial x^2}$$

$$C = \frac{G}{2A\sqrt{D_x \Pi t}} \exp\left(\frac{-(x - v_x t)^2}{4 D_x t} \right)$$

$C=C(x,t)$…concentration response to mass impulse (at x distance from pollution, in time t,
G…mass [g] of pollution (mass impulse),
D_x…longitudinal diffusion coeff.
x…distance from pollution,
t…time,
A…cross-section area (A=const)
v_x…velocity along river (assumed to be constant in time)

1D concentration response functions

Input: pollutant concentration is time dependent (time serie)

Solution is based on the eq:

$$C = \frac{G}{2A\sqrt{D_x \Pi t}} \exp\left(\frac{-(x - v_x t)^2}{4 D_x t} \right)$$

The input load [g/s] is given: $\dot{M}_i$ **i=1,…n for each time interval**

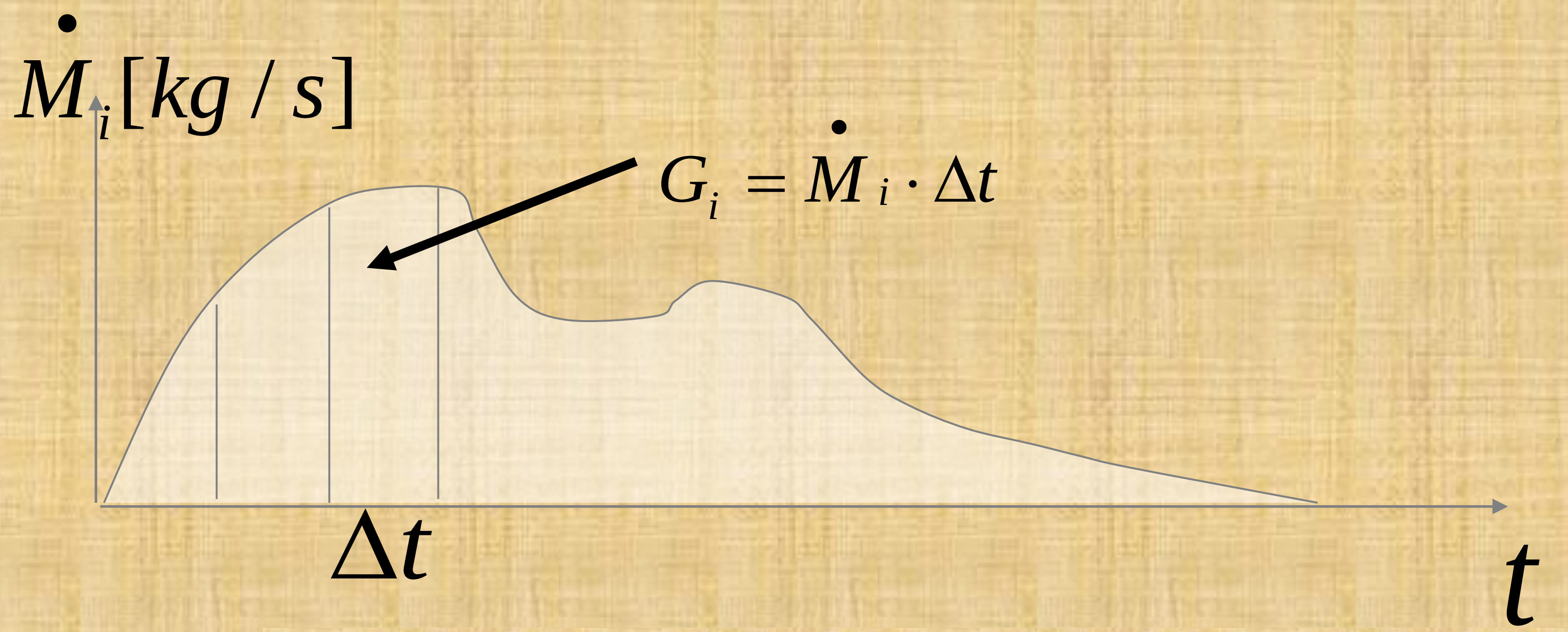
Then $G_i = \dot{M}_i \cdot \Delta t$ **The input load time serie is segmented into time intervals**

if $\Delta t \to 0, \;\; n \to \infty$

Drawing board!

Convolution integral for the response function of an input pollutant time series:

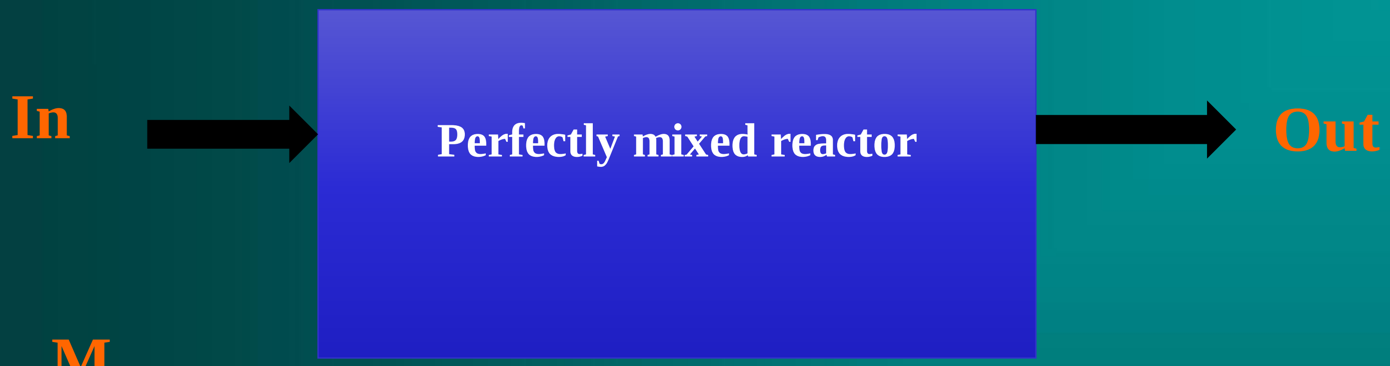
$$C = \sum_{i=1}^{n} \frac{\dot{M}_i \Delta t}{2A(\Pi D_x (t-(i-1)\Delta t))^{1/2}} \exp\left(\frac{-(x - v_x (t-(i-1)\Delta t))^2}{4D_x (t-(i-1)\Delta t)}\right)$$

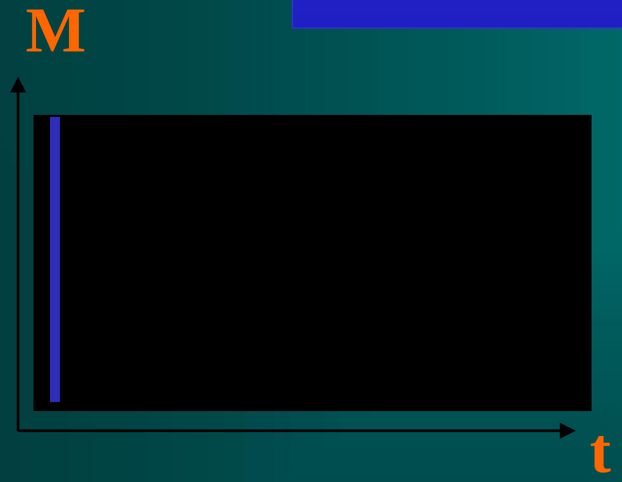


The term convolution refers to both the **result function and to the process of computing it**. It is defined as the integral of the product of the two functions after one is reversed and shifted. The integral is evaluated for all values of shift, producing the convolution function

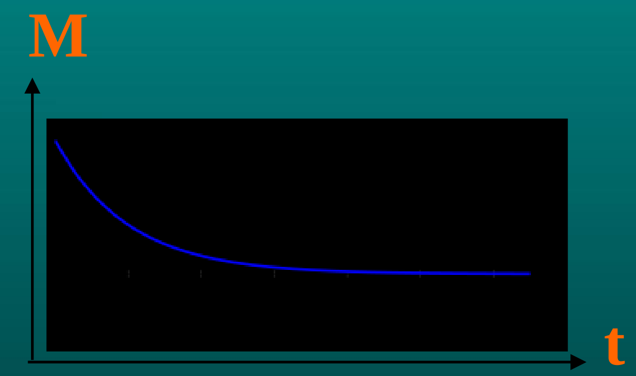
Reactor theory

The Case of sudden impulse (0D)



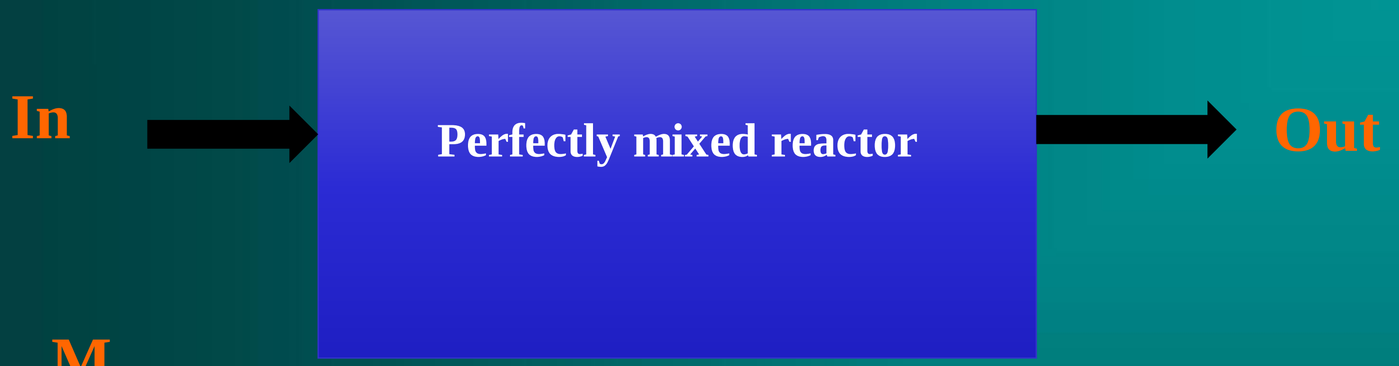


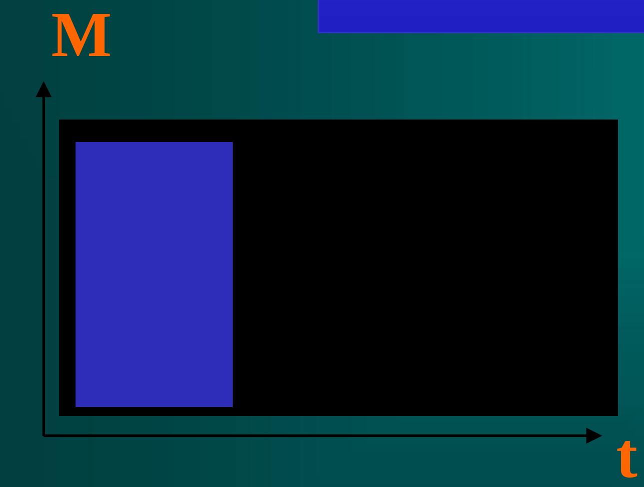
Dirac impulse

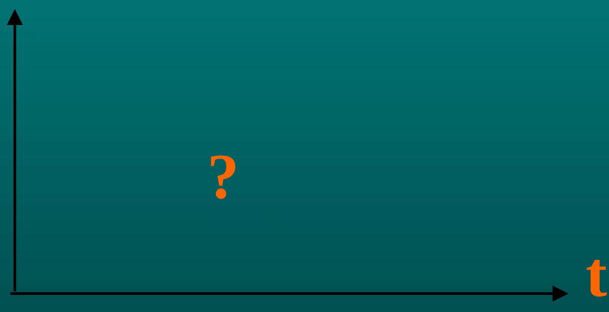


Impulse response function

The Case of a wide pulse (0D)





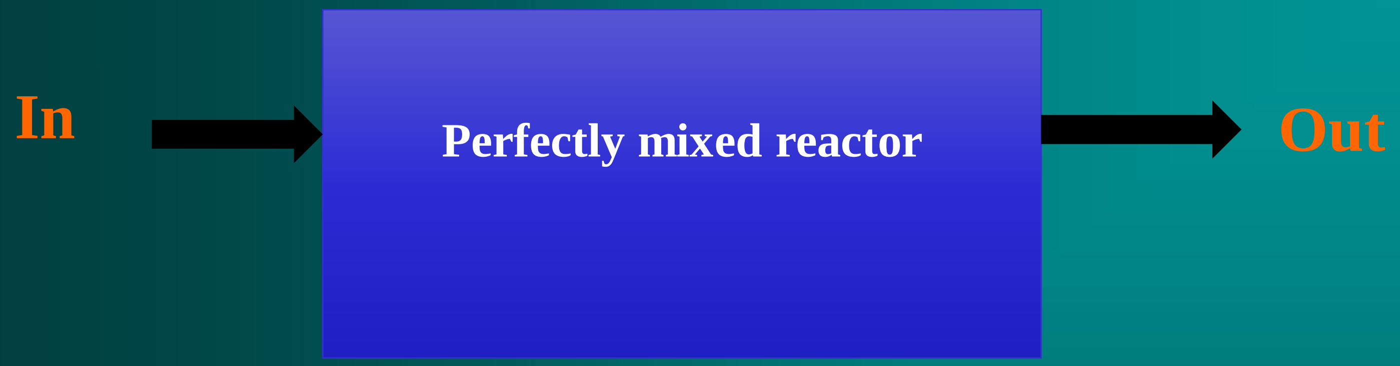


Wide pulse

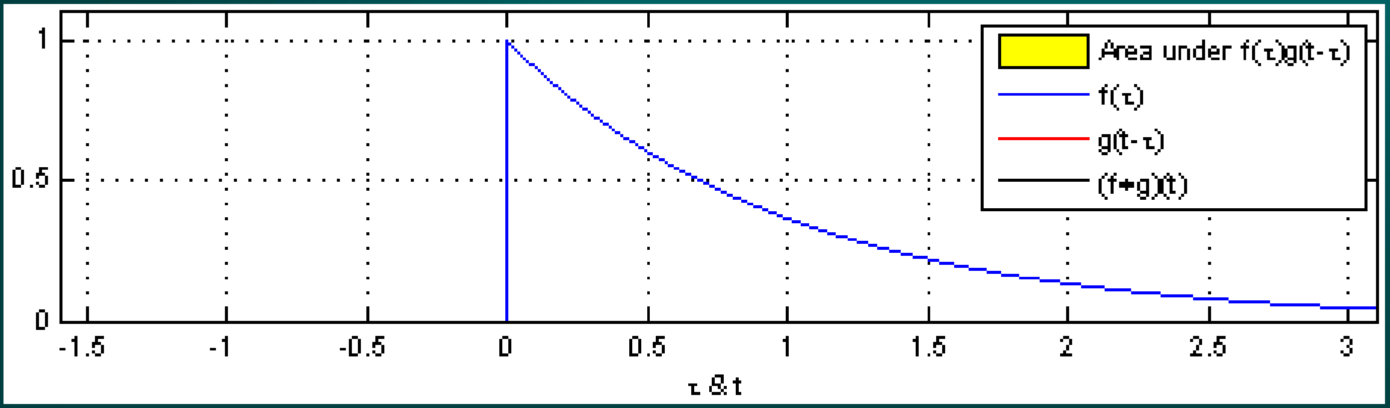
Response function g(t)=?

Convolution integral !

The Case of a wide pulse (0D)

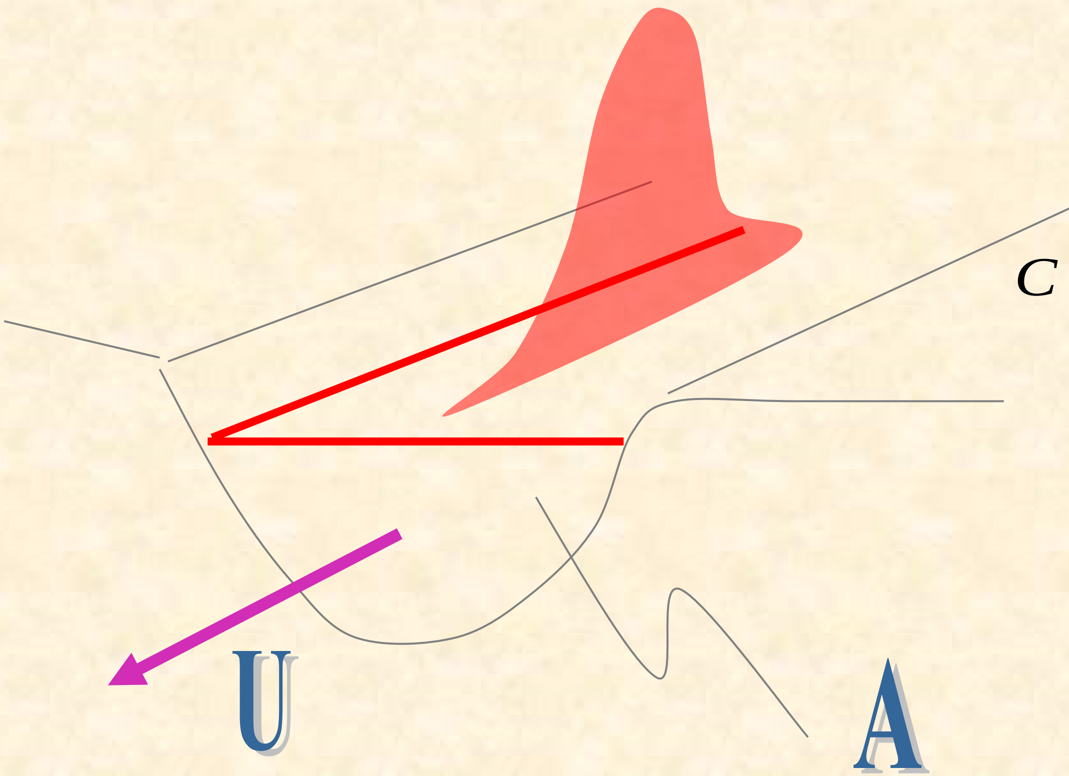


$$(f * g)(t) := \int_{-\infty}^{\infty} f(\tau)g(t-\tau)\,d\tau.$$

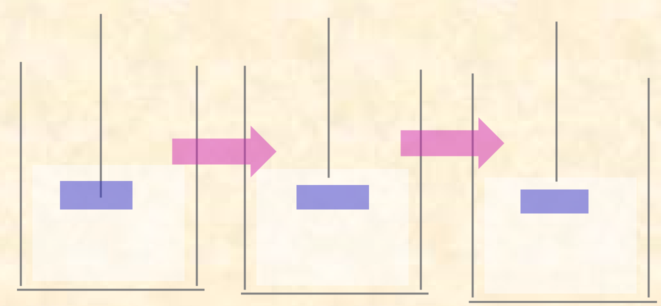


Cross-section integrated 1D model

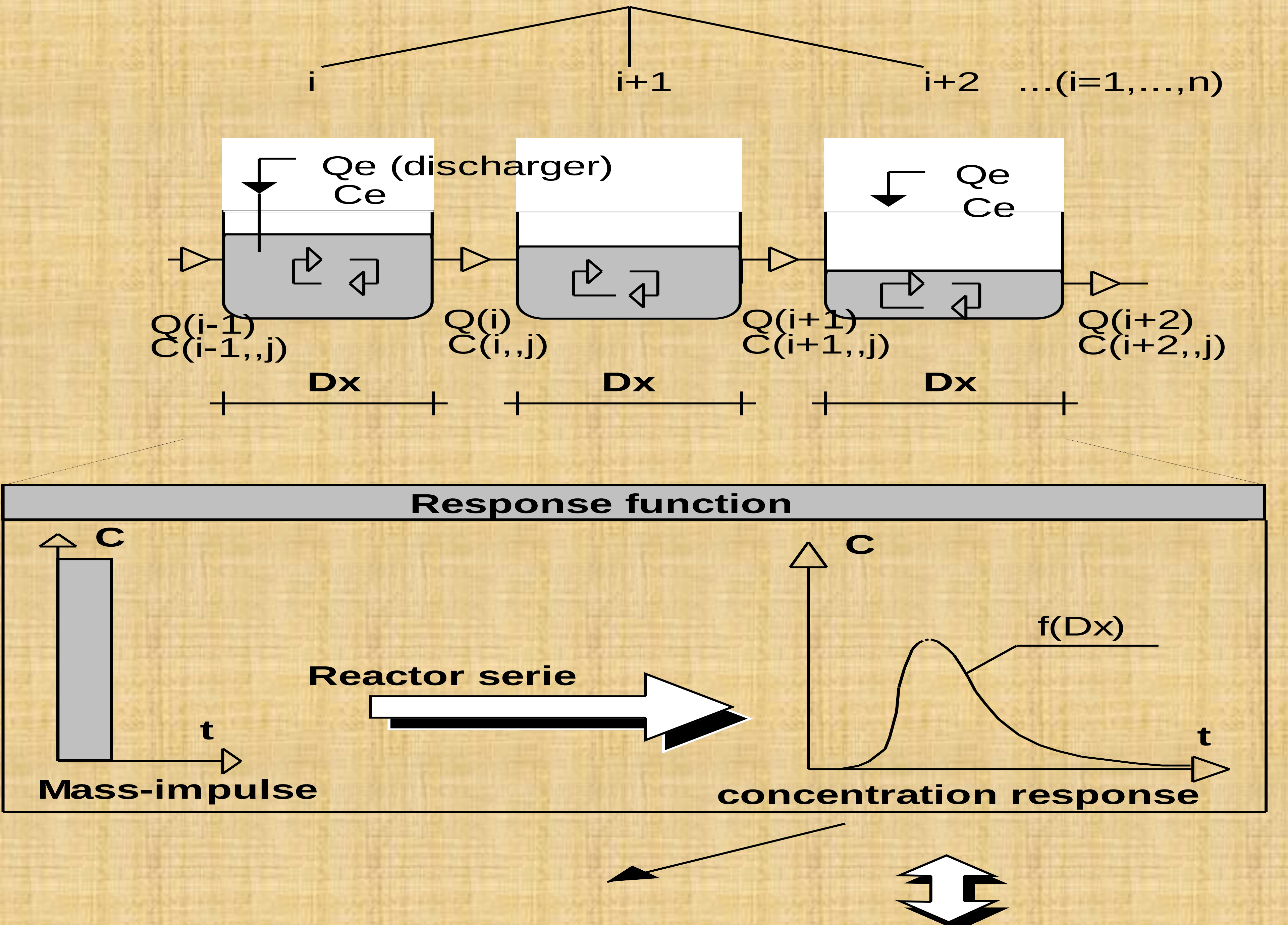
$$\frac{\partial(A\cdot C)}{\partial t}+\frac{\partial}{\partial x}(A\cdot v_x C)=\frac{\partial}{\partial x}(A\cdot D_x\frac{\partial C}{\partial x})$$



$$C=\frac{G}{2A\sqrt{D_x \Pi t}}\exp(\frac{-(x-v_x t)^2}{4D_x t})$$



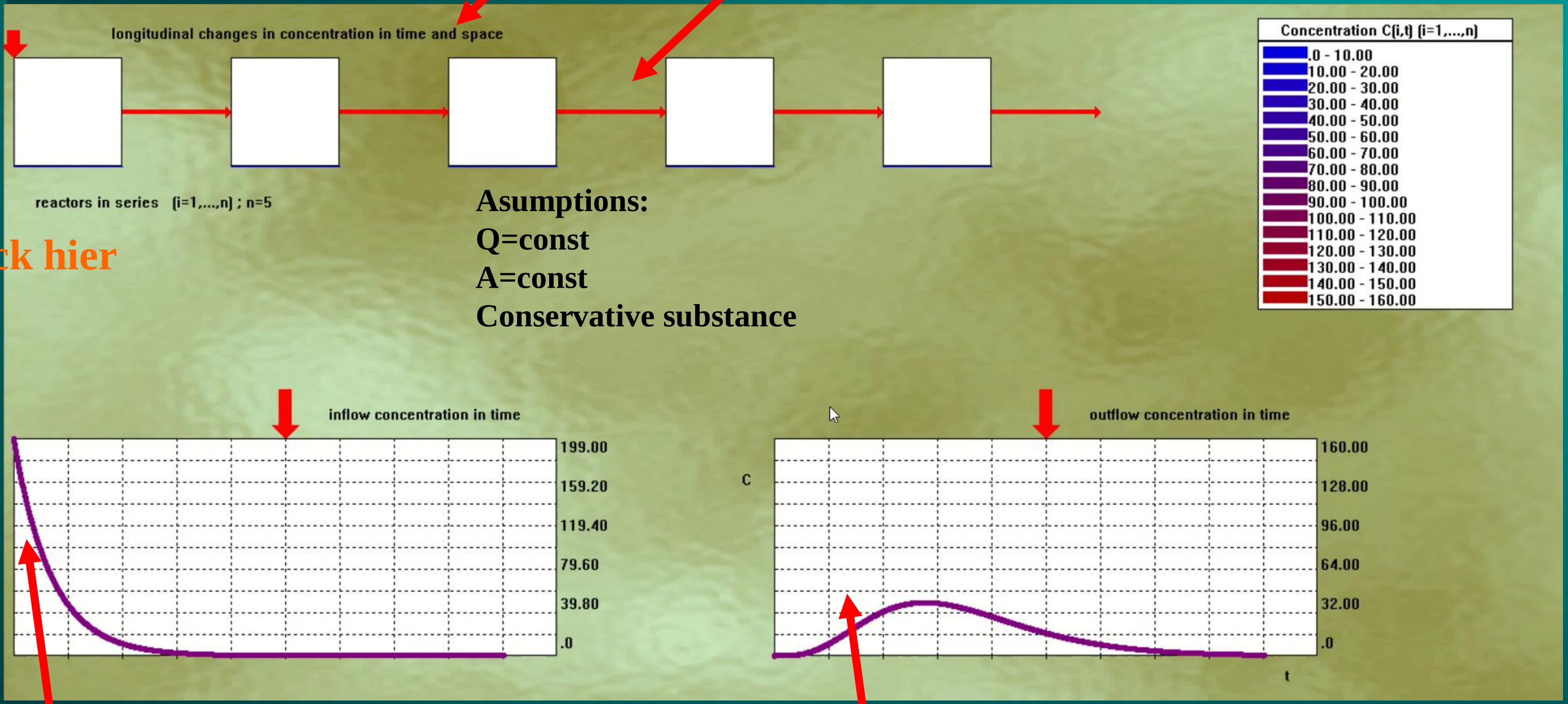
REACTOR SERIE



Reactors in serie (n reactors)

Changes of concentration in all reactors

Click hier

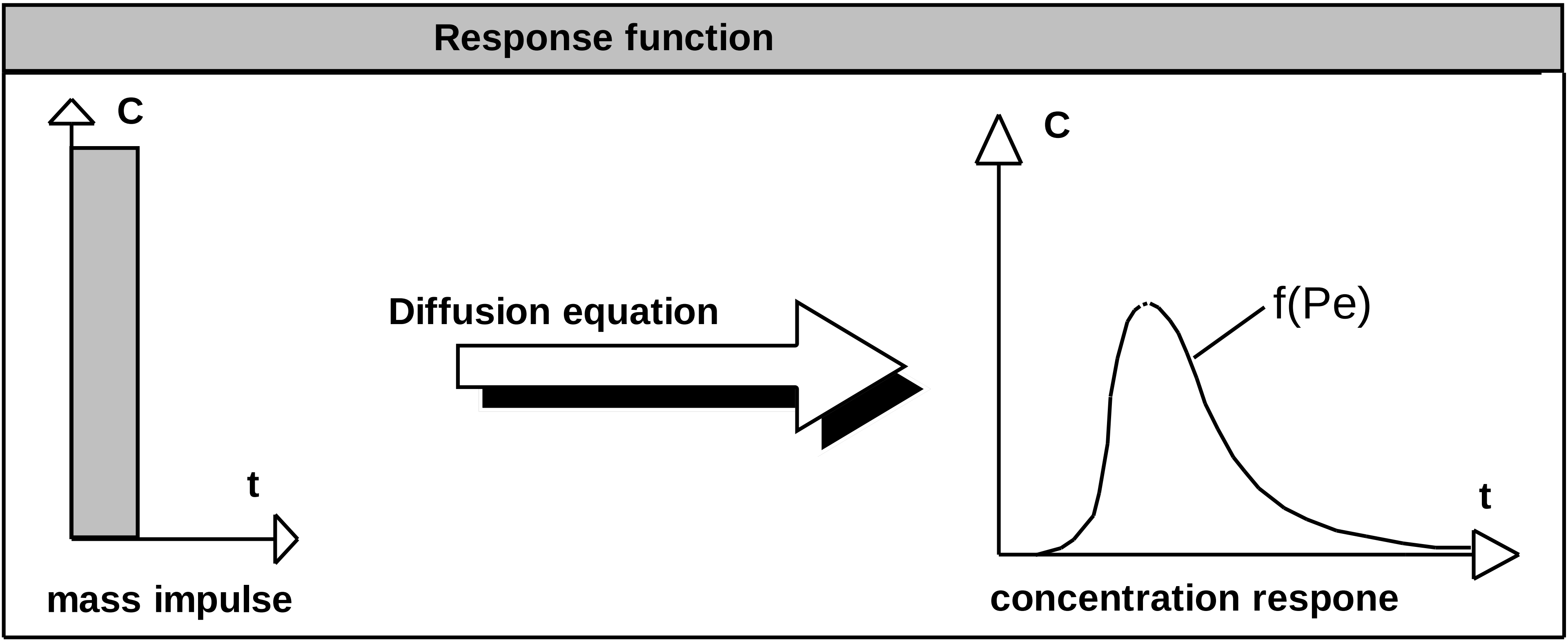


Asumptions:
Q=const
A=const
Conservative substance

Concentration in 1st reactor After unit mass impulse

Response function (C(t)) to unit impulse

The continuous stirred-tank reactor, also known as vat- or backmix reactor, mixed flow reactor, or a continuous-flow stirred-tank reactor, is a common model for a chemical reactor in chemical engineering and environmental engineering.



$$\frac{C}{C_0} = \frac{n}{(n-1)!}\left(\frac{t}{t^*}\right)^{n-1} \exp\left(-\frac{t}{t^*}\right)$$

$$t^* = V / Q$$

Average residence time in reactor

Optimal number of reactors

- **Using the Peclet-number**
  - **dimensionless**
  - **rate of convection and diffusion**

$$Pe = \frac{QL}{AD} \quad \Rightarrow \quad n \cong \frac{Pe}{2}$$

$$h(t) = \frac{C}{C_0} = \frac{n}{(n-1)!}\left(\frac{t}{t^*}\right)^{n-1} \exp\left(-\frac{t}{t^*}\right)$$

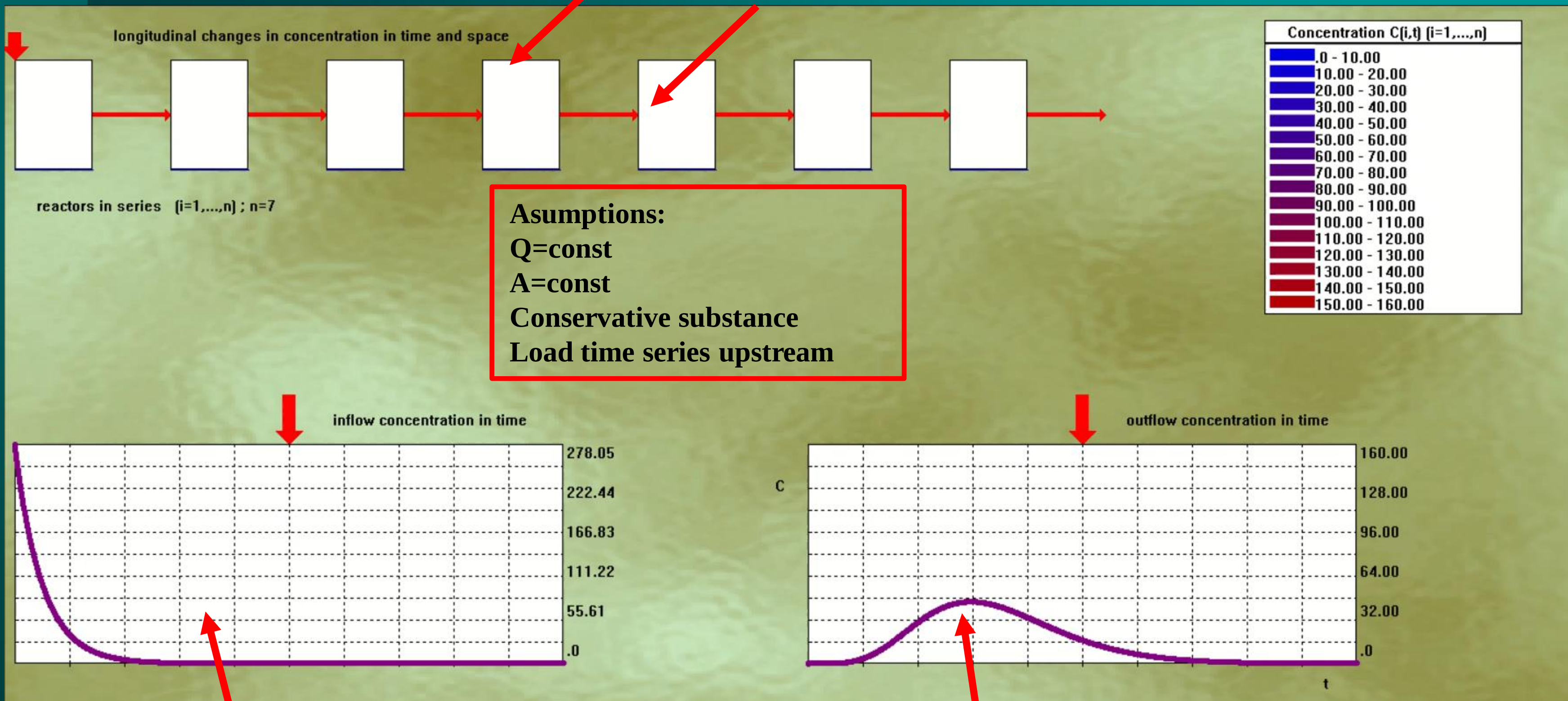
$$C_0 = \frac{M}{nV}$$

Convolution: linear model

$$X(T) = \int_0^T I(T-\tau)h(\tau)d\tau$$

Reactors in serie (n reactors)

Changes of concentration in all reactors



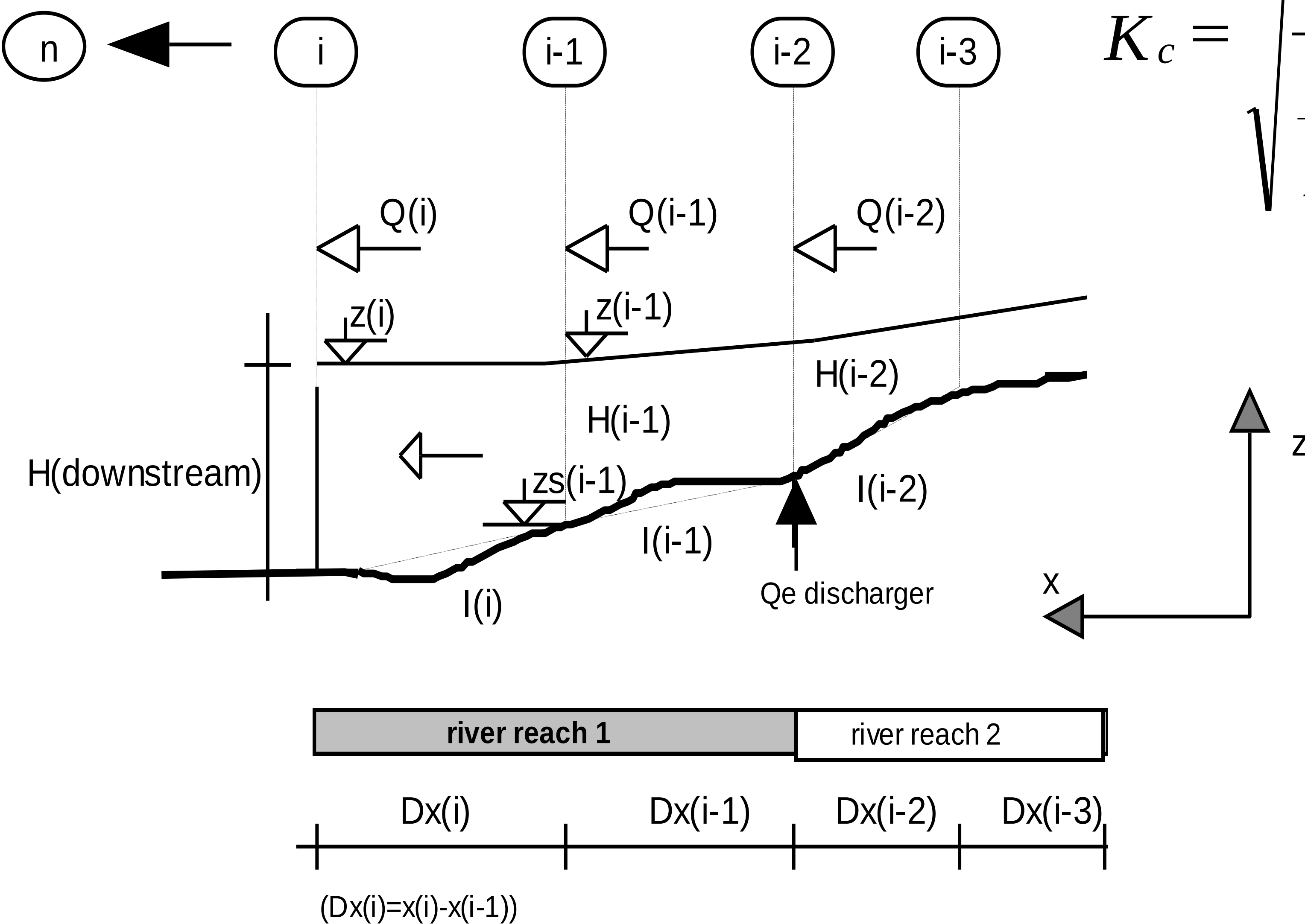
Concentration in 1st reactor: pollutant load time series

Outflow concentration (C(t)) to pollutant load time series

Hydraulics

$$z_i + \frac{Q_{(i)}^2}{A_{(i)}^2 2g} + \overset{\textbf{friction}}{\frac{Q_{(i)}^2}{K_c^2} Dx(i)} = z_{i-1} + \frac{Q_{(i)}^2}{A_{(i-1)}^2 2g}$$

$$K_c = \sqrt{\frac{2}{\frac{1}{K_{(i-1)}^2} + \frac{1}{K_{(i)}^2}}}$$

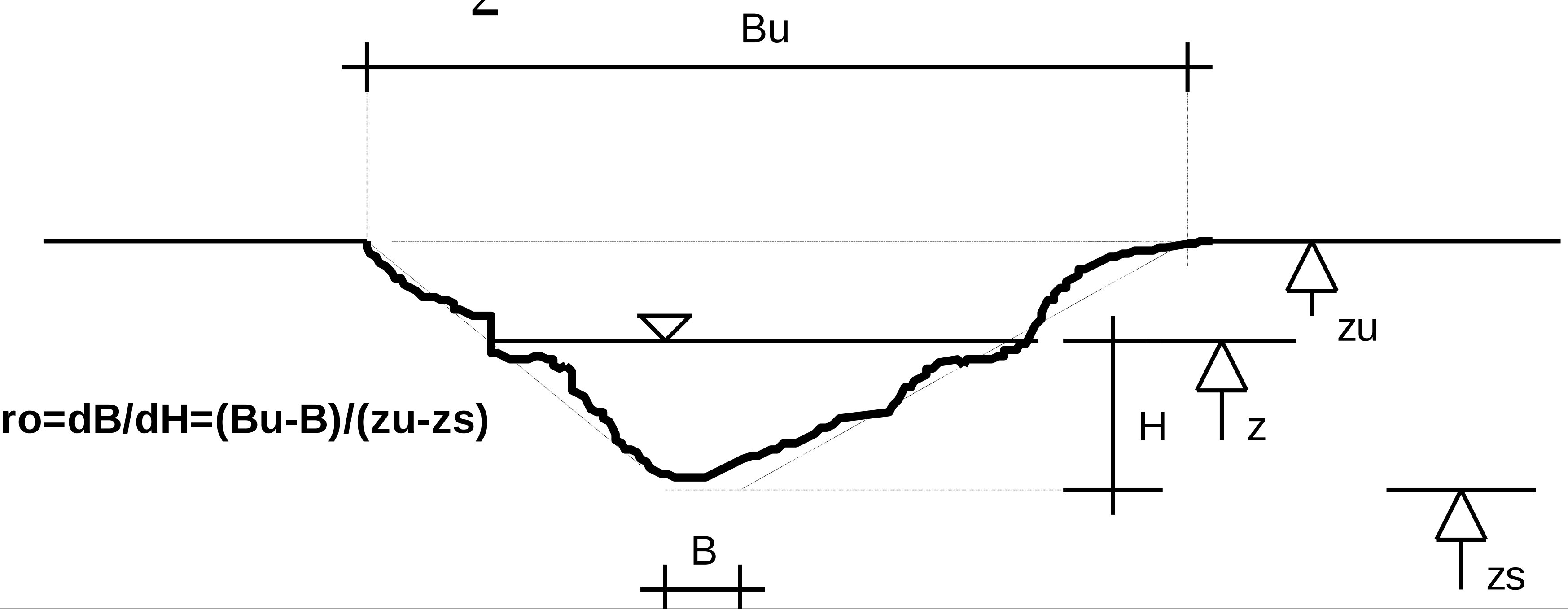


$$z_i + \frac{Q_{(i)}^2}{A_{(i)}^2 2g} + \frac{Q_{(i)}^2}{K_c^2} Dx(i) = z_{i-1} + \frac{Q_{(i)}^2}{A_{(i-1)}^2 2g}$$

Manning

$$\frac{Q^2}{K^2} Dx = \frac{v^2}{C^2 R} Dx = \frac{Q^2}{A^2 C^2 R} Dx \Rightarrow K = AC\sqrt{R} = AkR^{1/6}\sqrt{R} = AkR^{2/3}$$

$$A_{(i-1)} = B_{(i-1)} H_{(i-1)} + \frac{1}{2} ro_{(i-1)} H_{(i-1)}^2 \qquad H_{(i-1)} = z_{(i-1)} - zs_{(i-1)}$$



$$z_i + \frac{Q_{(i)}^2}{A_{(i)}^2 2g} + \frac{Q_{(i)}^2}{K_c^2} Dx(i) - \frac{Q_{(i)}^2}{A_{(i-1)}^2 2g} = z_{i-1}$$

Iterativ method starting of from downstream:
upstream=downstream as initial conditions

During iteration (starting from upstream):

A_{i-1} **and**

$$K_{i-1} = A_{i-1} k R_{i-1}{}^{2/3}$$

Parameters are being updated (R is hydraulic radius)

$$n \cong \frac{Pe}{2}$$

$$Pe = \frac{QL}{AD}$$

$$D_x = d_x \cdot u_* \cdot R$$

$$\frac{F}{K}$$

parameter

$$\sqrt{gRI}$$

$$d_x \cong 6$$

$$D_x = d_x \cdot u_* \cdot R = d_x \sqrt{gRI} \cdot R$$

$$D_x = d_x \sqrt{gR \frac{U^2}{C^2 R}} \cdot R = d_x \sqrt{g \frac{U^2}{C^2}} \cdot R$$

$$D_x = d_x \frac{U}{C} \sqrt{g} \cdot R = d_x \sqrt{g} \cdot U \frac{R}{k_{st} R^{1/6}}$$

$$D = \frac{K}{k_{st}} U h^{5/6} \Rightarrow Dx = \frac{2K h^{5/6}}{k_{st}}$$

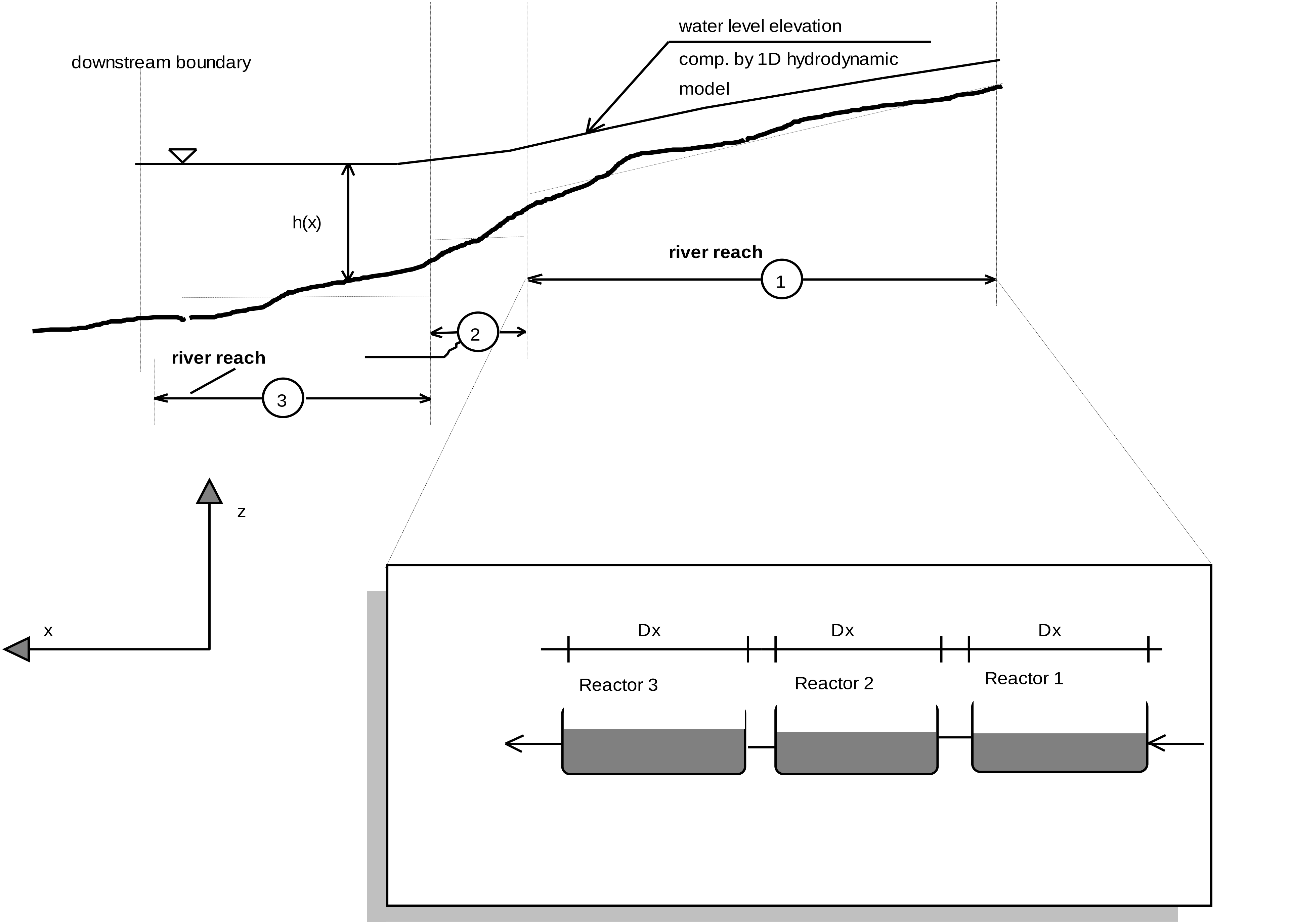
$$(R \cong h)$$

$$n \cong \frac{Pe}{2}$$

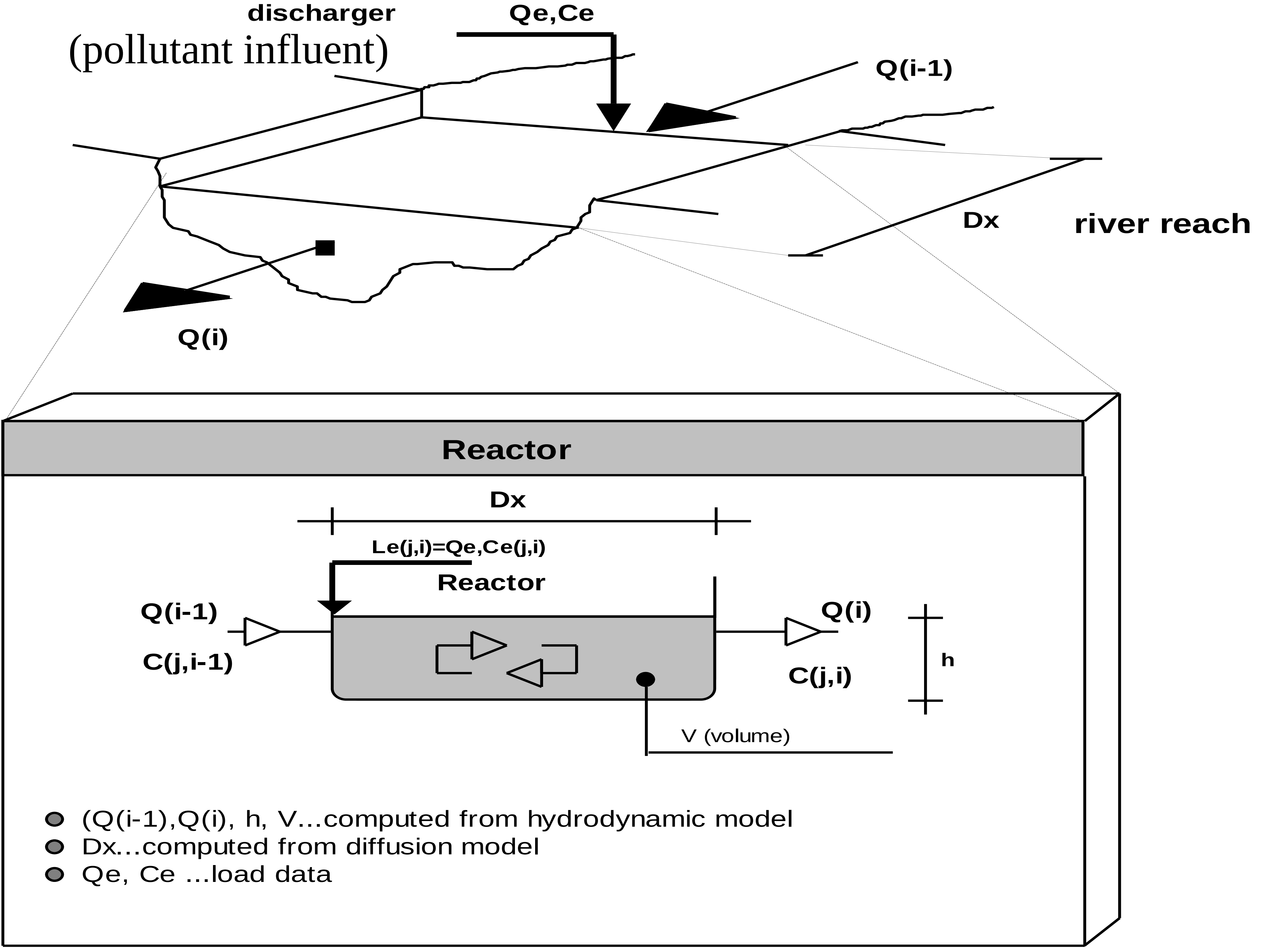
$$Pe = \frac{QL}{AD}$$

$$n = \frac{QL}{2AD} \Rightarrow \frac{L}{n} = Dx = \frac{2AD}{Q} = \frac{2D}{U}$$

River	D(m^2/ s)	H(m)	B(m)	**K(-)**
Sabine River	311	2	103	3100
Powel River	9,3	0.83	33.6	200
Clinch River	53,4	2,1	59	245
Coachella River	9.2	1.53	23.7	140
Nooksack River	34,6	0,74	63	170
John Day River	64,4	2,46	34	146
Yadkin River	108	2.31	69	470



water level elevation
comp. by 1D hydrodynamic
model
downstream boundary
h(x)
river reach
1
2
river reach
3
z
x
Dx
Dx
Dx
Reactor 3
Reactor 2
Reactor 1


discharger
Qe,Ce
(pollutant influent)
Q(i-1)
Dx
river reach
Q(i)
Reactor
Dx
Le(j,i)=Qe,Ce(j,i)
Reactor
Q(i-1)
C(j,i-1)
Q(i)
C(j,i)
h
V (volume)
(Q(i-1),Q(i), h, V...computed from hydrodynamic model
Dx...computed from diffusion model
Qe, Ce ...load data

$$\frac{d}{dt}\left(V_{(i)}C_{(j,i)}\right)=C_{(j,i)}\frac{dV_{(i)}}{dt}+V_{(i)}\frac{dC_{(j,i)}}{dt}=L_{(j,i)}-Q_{(i)}C_{(j,i)}+V_{(i)}S_{(j,i)}$$

(j=1,…,m ; i=1,…,n)

L(j,i)=Q(i-1)*C(j,i-1)+Le(i,j)

$$\frac{dV_{(i)}}{dt}=Q_{(i-1)}-Q_{(i)}+Q_{e(i)}$$

Simplified:

$$\frac{dV(i)}{dt} = 0 \qquad \frac{dC(j,i)}{dt} = 0$$

$$\frac{L(j,i)}{V(i)} - \frac{Q(i)}{V(i)} C(j,i) + S_{(j,i)} = 0$$

$$C(j,i) = \frac{L(j,i)}{Q_{(i)}} + \frac{S(j,i)}{Q_{(i)}} V(i)$$

$$C(j,i)=\frac{L(j,i)}{Q_{(i)}}+\frac{S(j,i)}{Q_{(i)}}V(i)$$

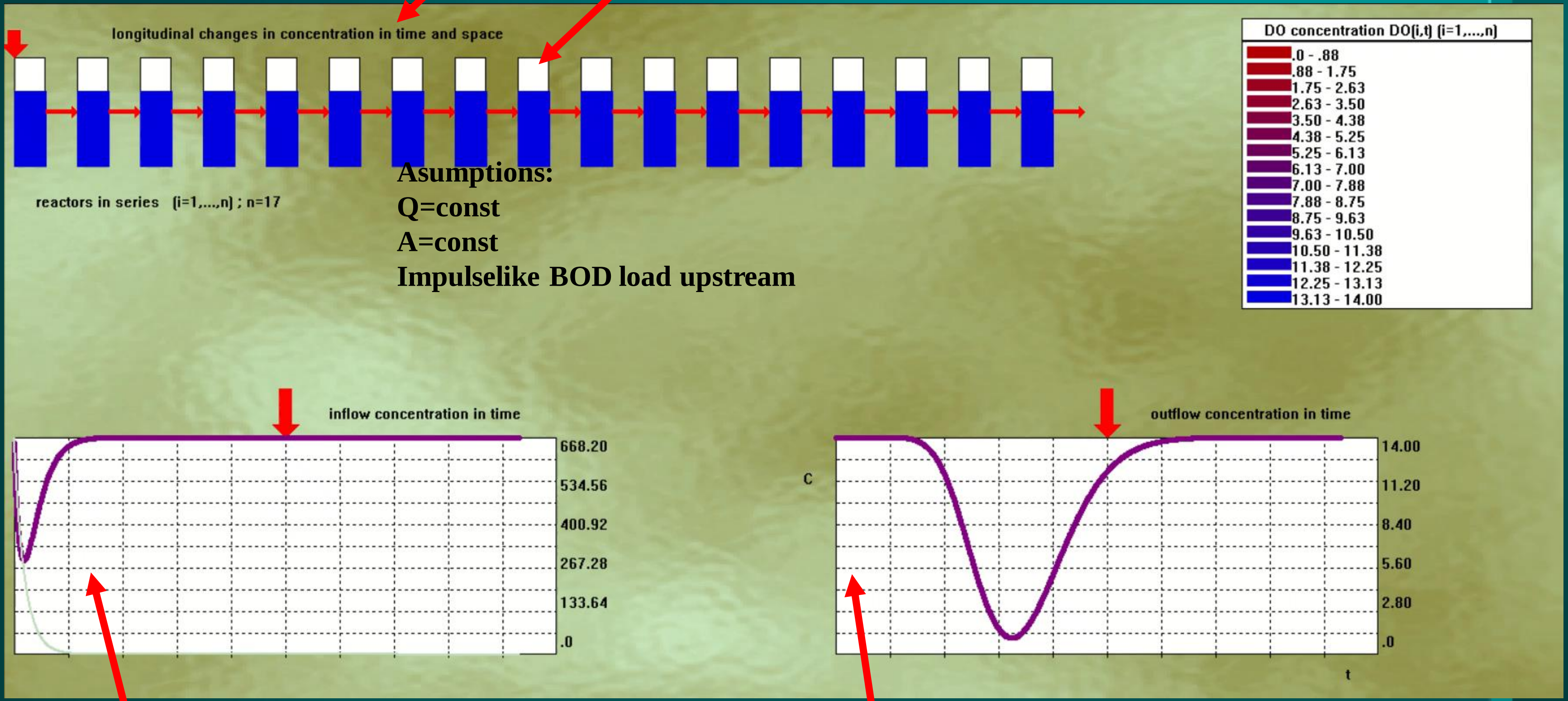
$$\frac{V(i)}{Q_{(i)}}=t_{a}(i)$$

$$C(j,i)=\frac{L(j,i)}{Q_{(i)}}+S(j,i)t_{a}(i)$$

Modelling of dissolved oxygen (DO)- unit impulse

Reactors in serie (n reactors)

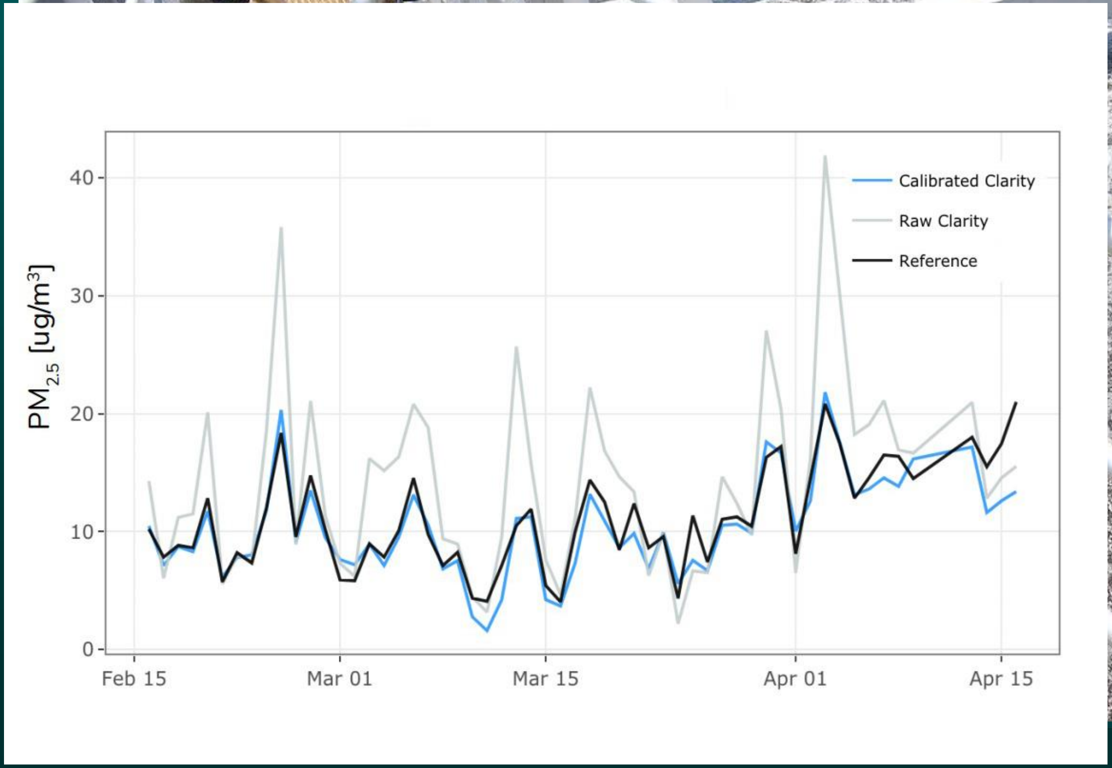
Changes of concentration in all reactors



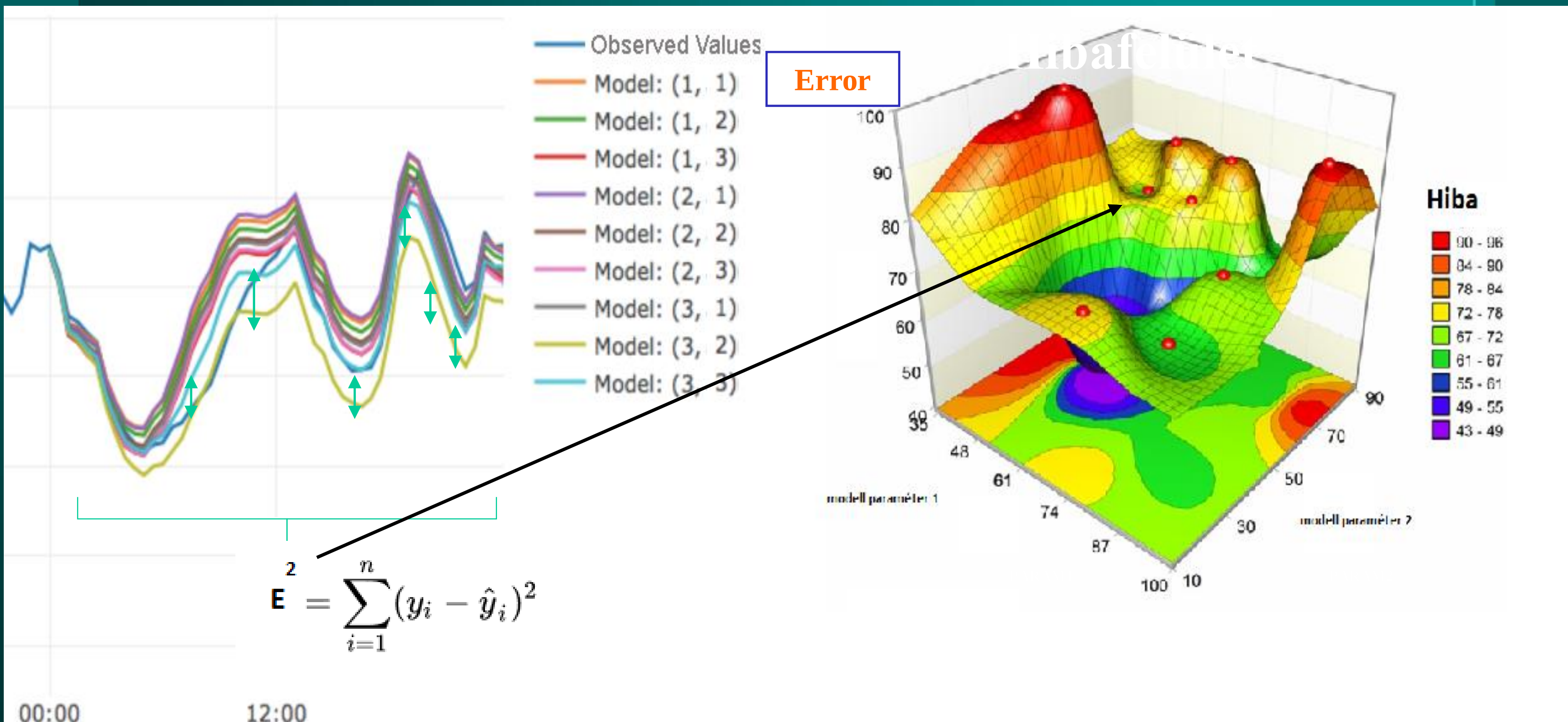
Concentration in 1st reactor as a result of unit impulse of organic pollutant

Response function (DO(t)) to unit impulse

Optimization/calibration



Optimization/calibration



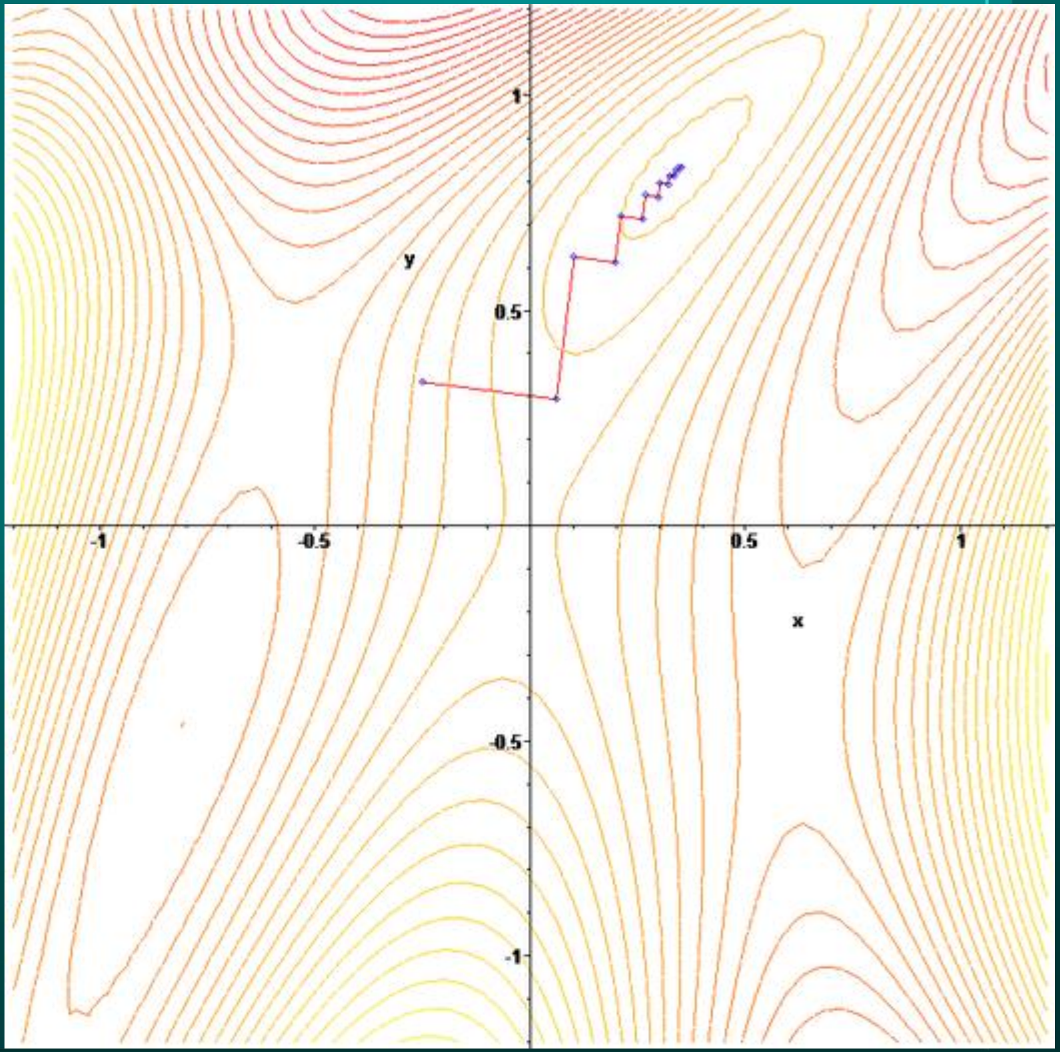
Local minima/maxima

Can be characterized by:
- **space**
- **time complexity**

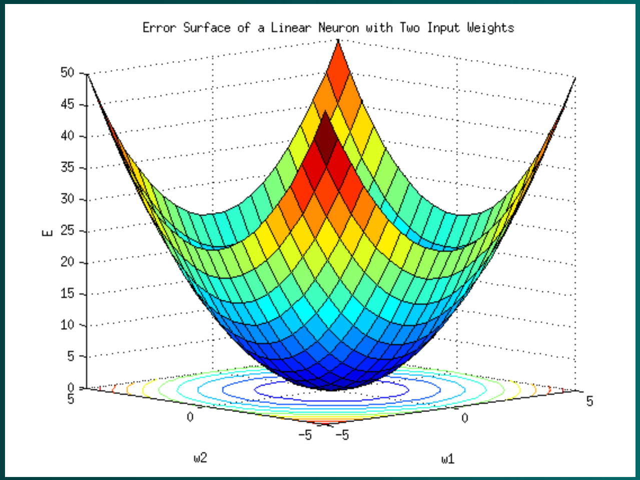
Search types:
- **global**
- **local**

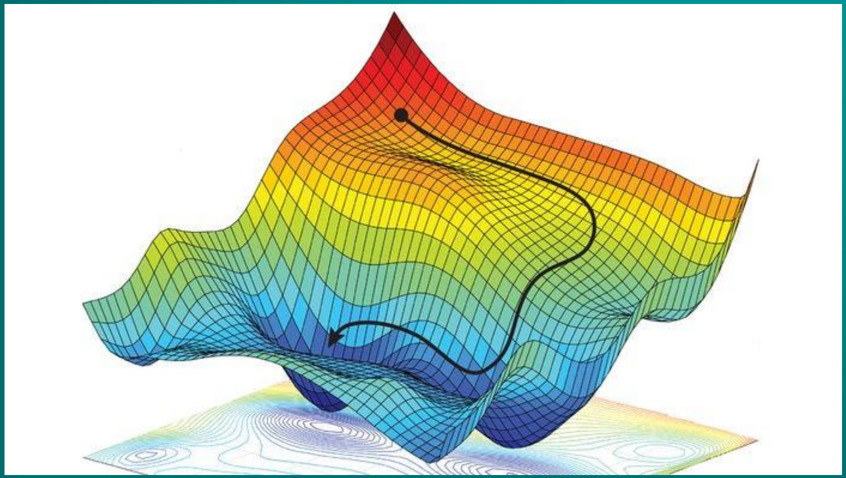
Iterative methods

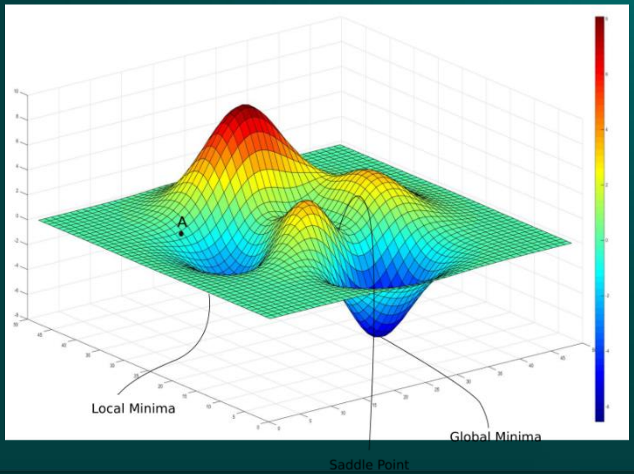
Eg:
- **Gradients descent**
- **stochasztic method (Monte-Carlo)**
- **Evolutionary algorithm**

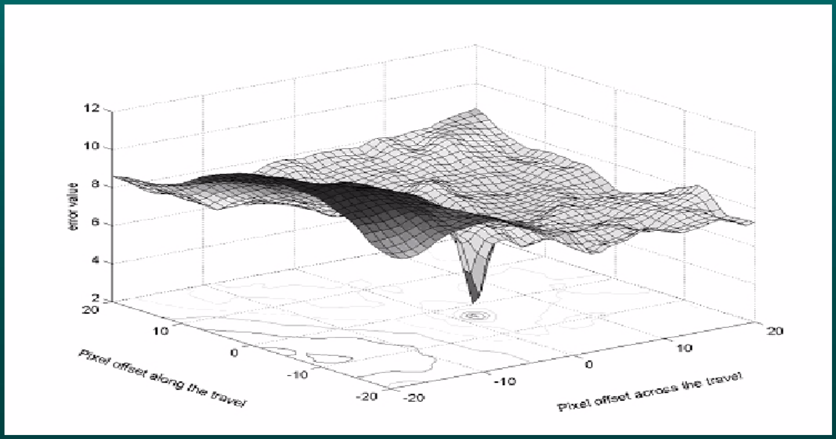


Best algorithm?



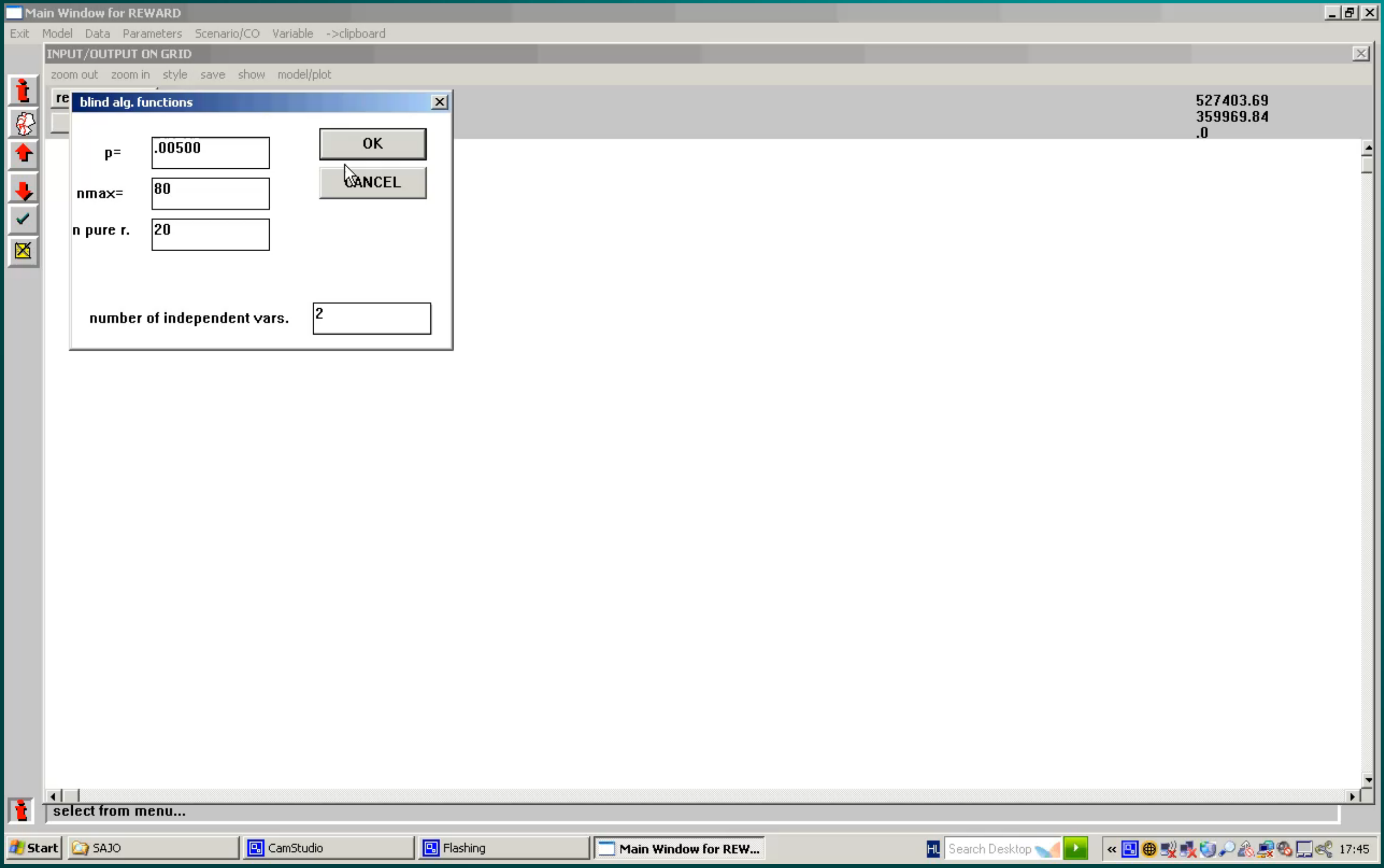






Blind algorithm

- Stochastic interval narrowing

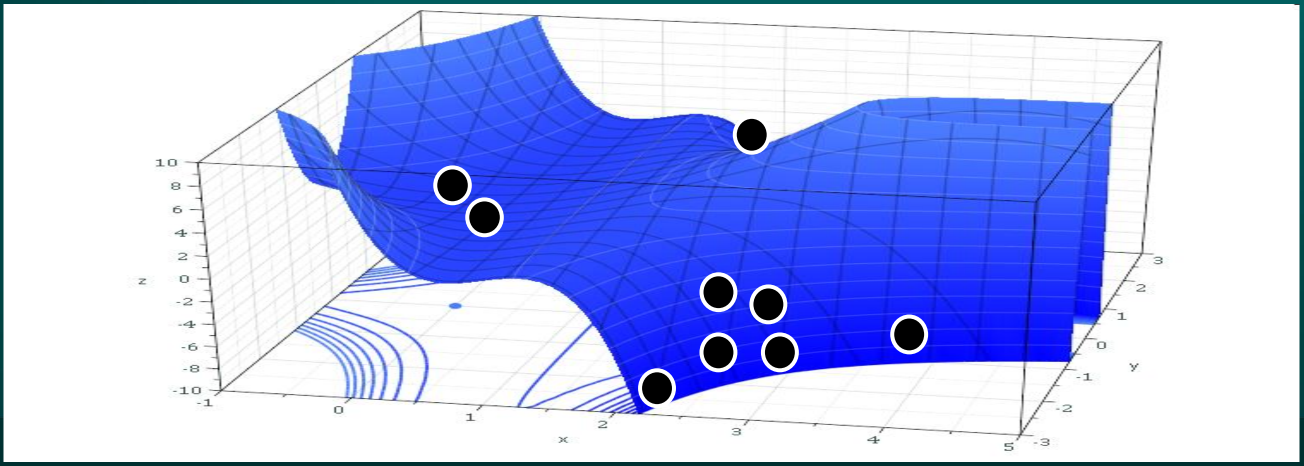


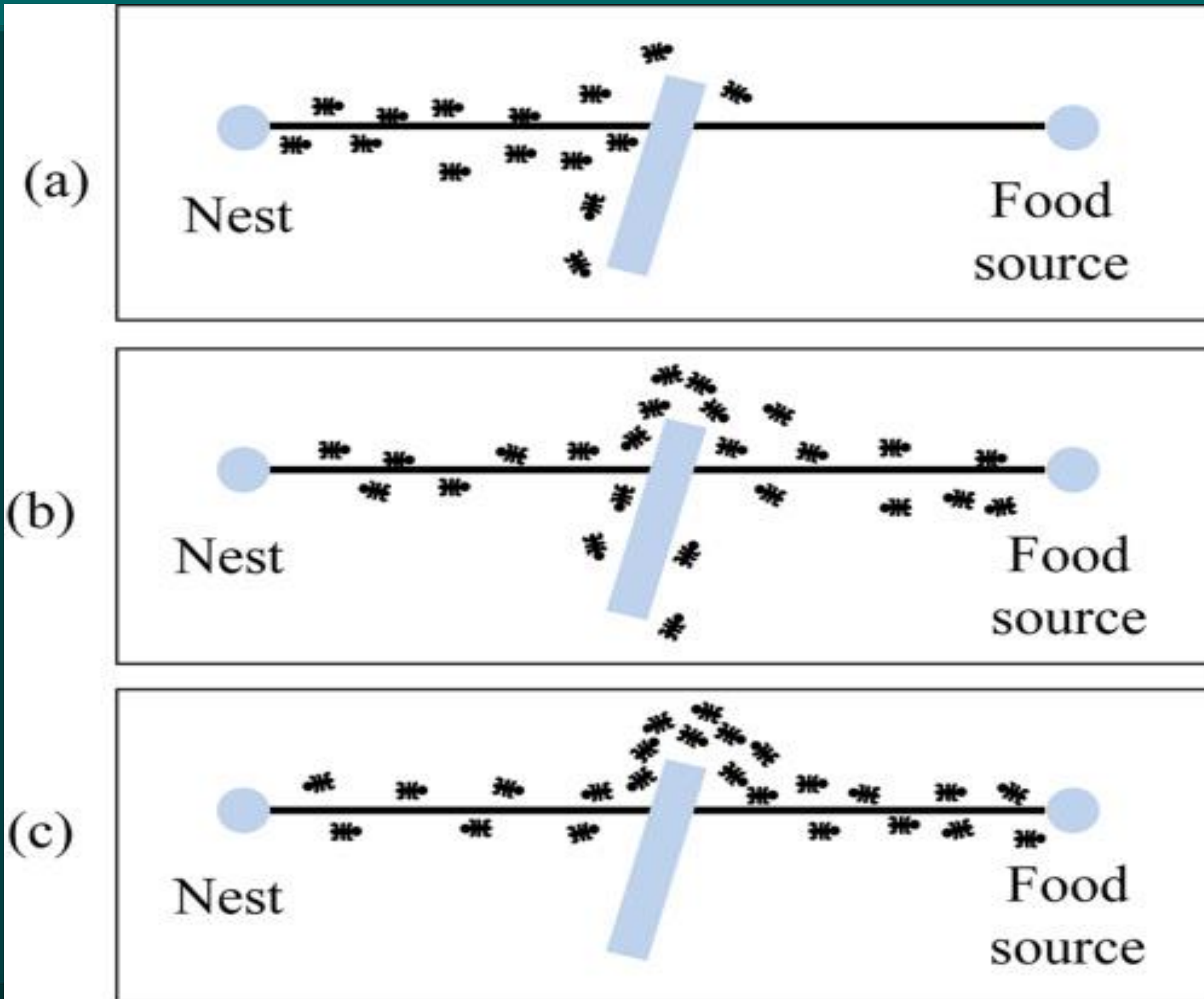
Genetic algorithm

What is genetic algorithm?

- **global search method**

- starting from many points(individuals) who are progressing (cross breeding) into many directions, according to the location probability distribution of the best species.





(a)
Nest
Food source
(b)
Nest
Food source
(c)
Nest
Food source

Genetic algorithm

Thinking abstract:

Dimension of the search space defines the individuals (parameter coordinates= DNA)

Start:

-We make a binary code according to the appended decimal numbers

- Random initialization

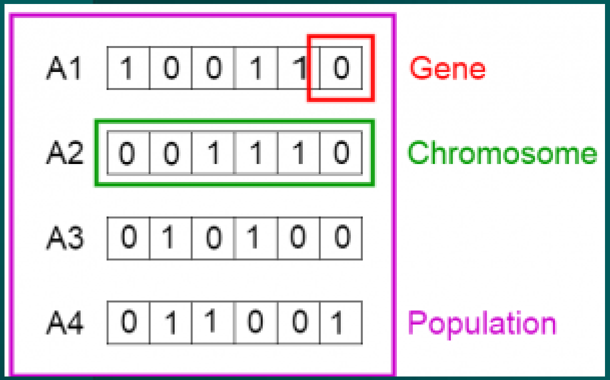
The genetic algorithm uses three main types of rules at each step to create the next generation from the current population:

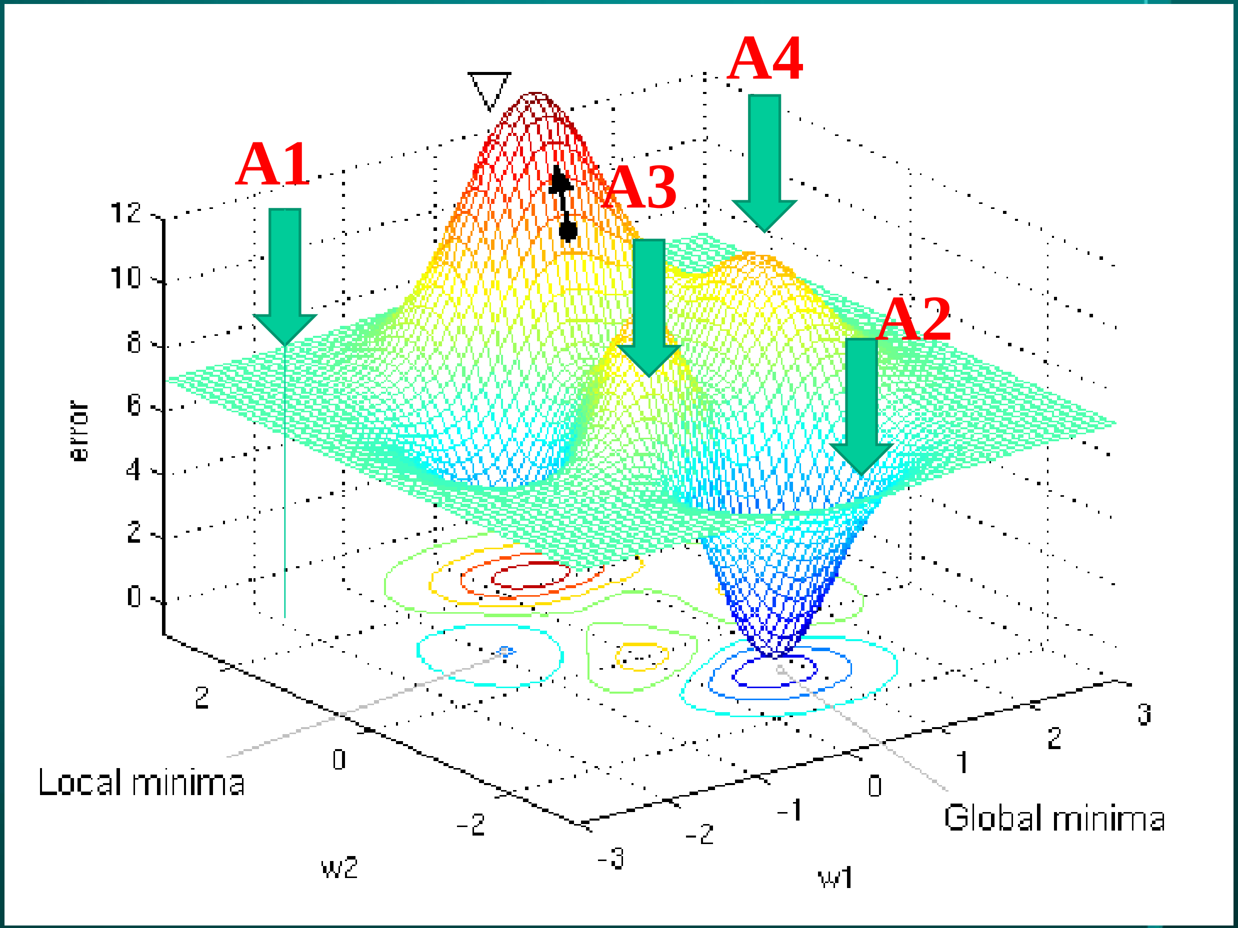
•*Selection rules* select the individuals, called *parents*, that contribute to the population at the next generation. The selection is generally stochastic, and can depend on the individuals' scores.

•*Crossover rules* combine two parents to form children for the next generation.

•*Mutation rules* apply random changes to individual parents to form children.

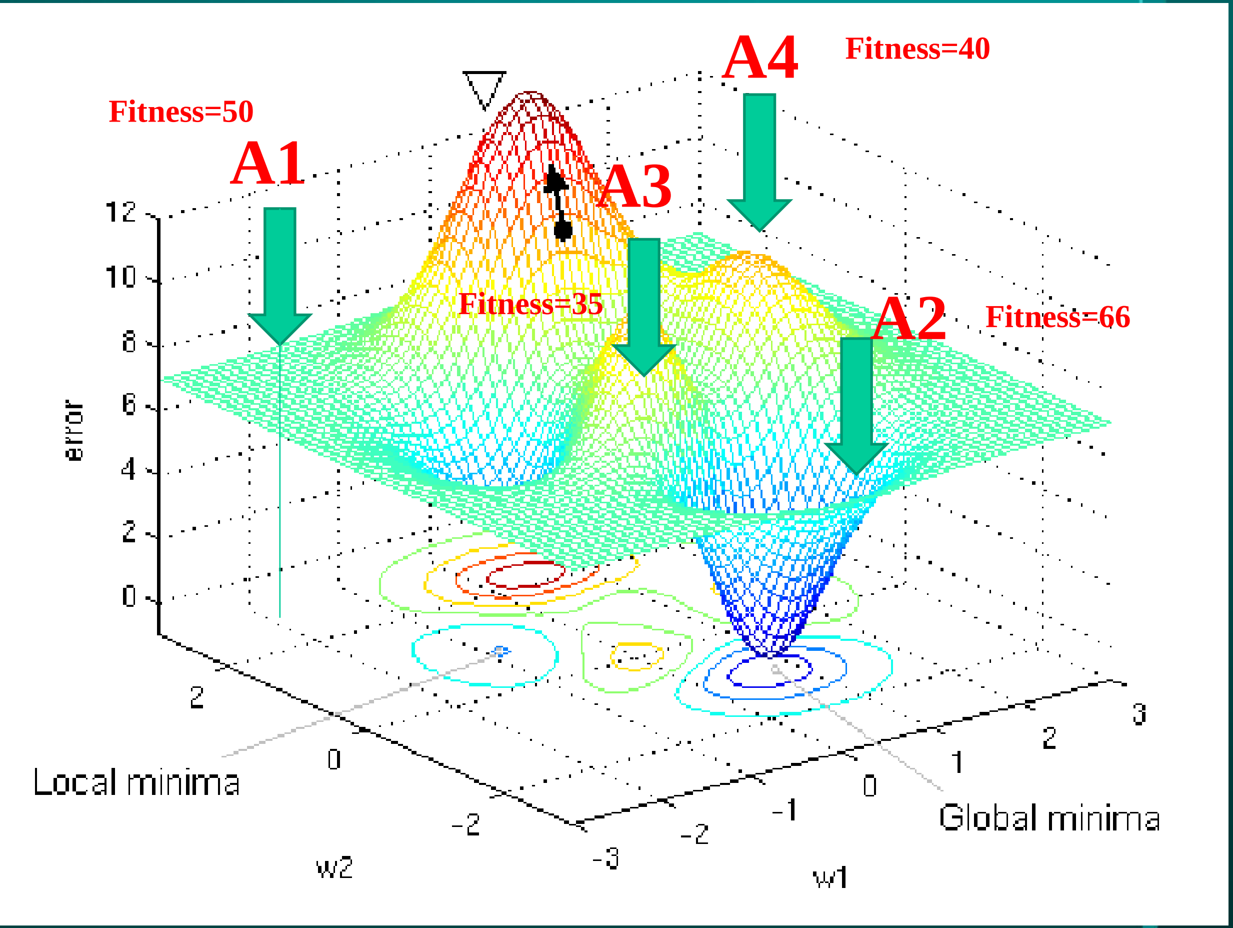
Genetic algorithm





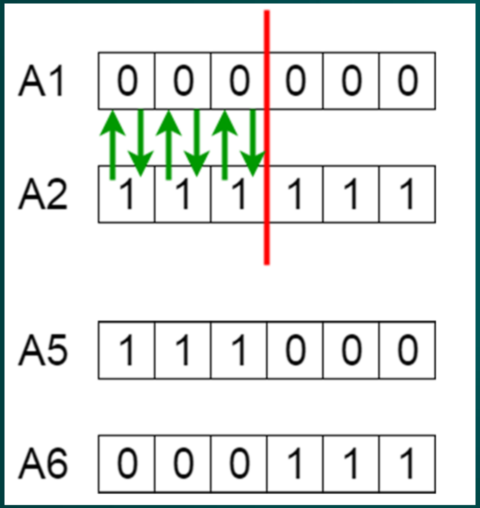
Genetic algorithm

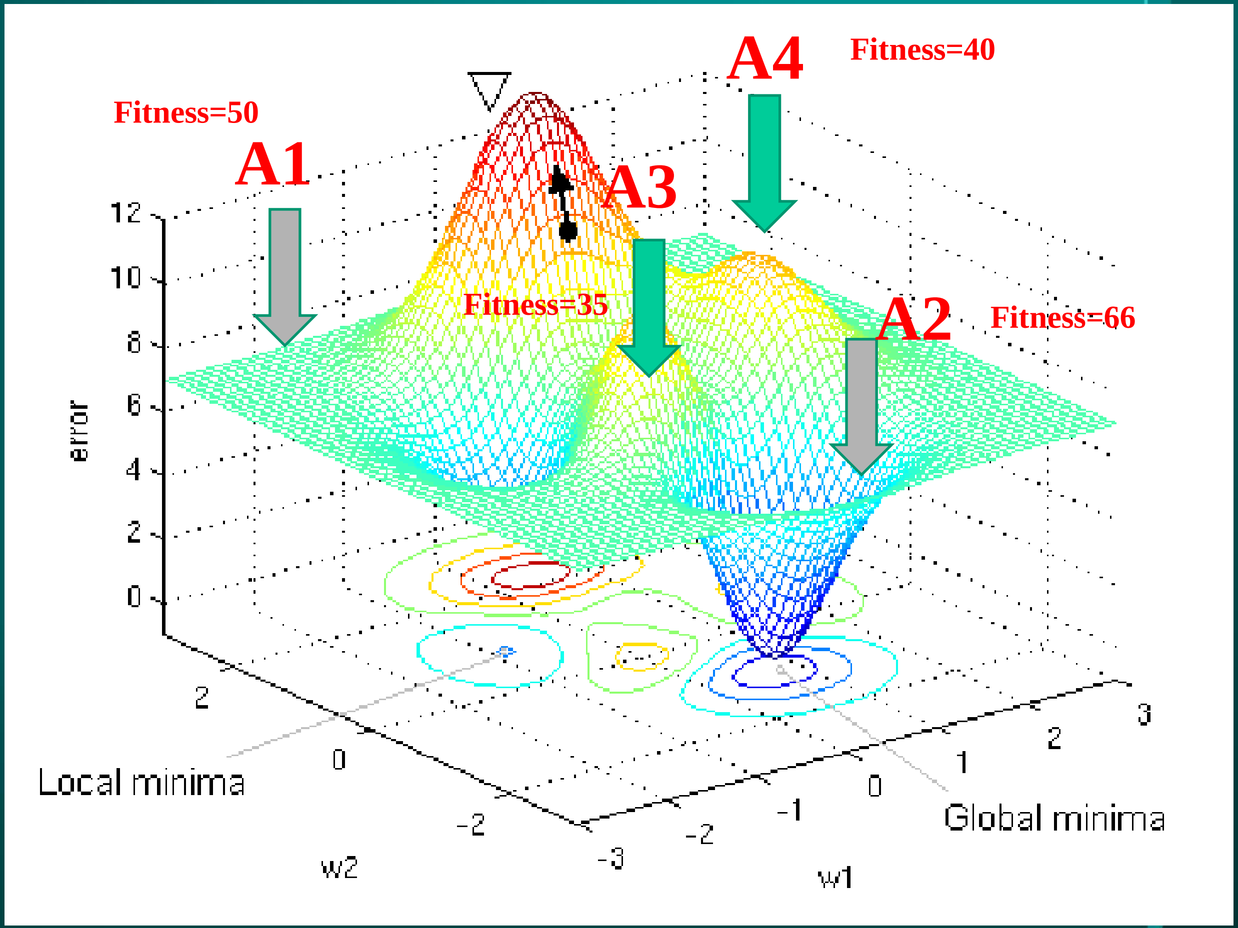
- **Every individual has a fitness value**
- **Fitness= 1/Error**



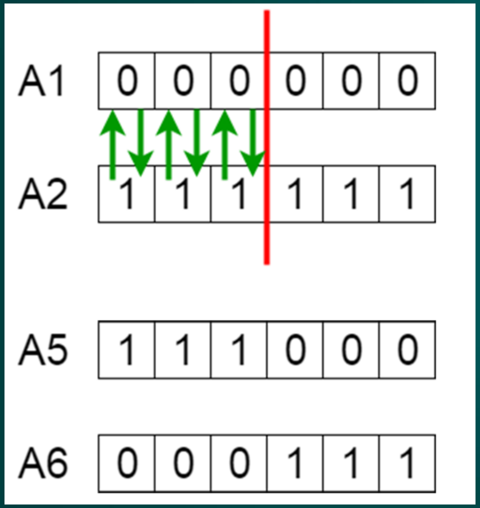
Genetic algorithm

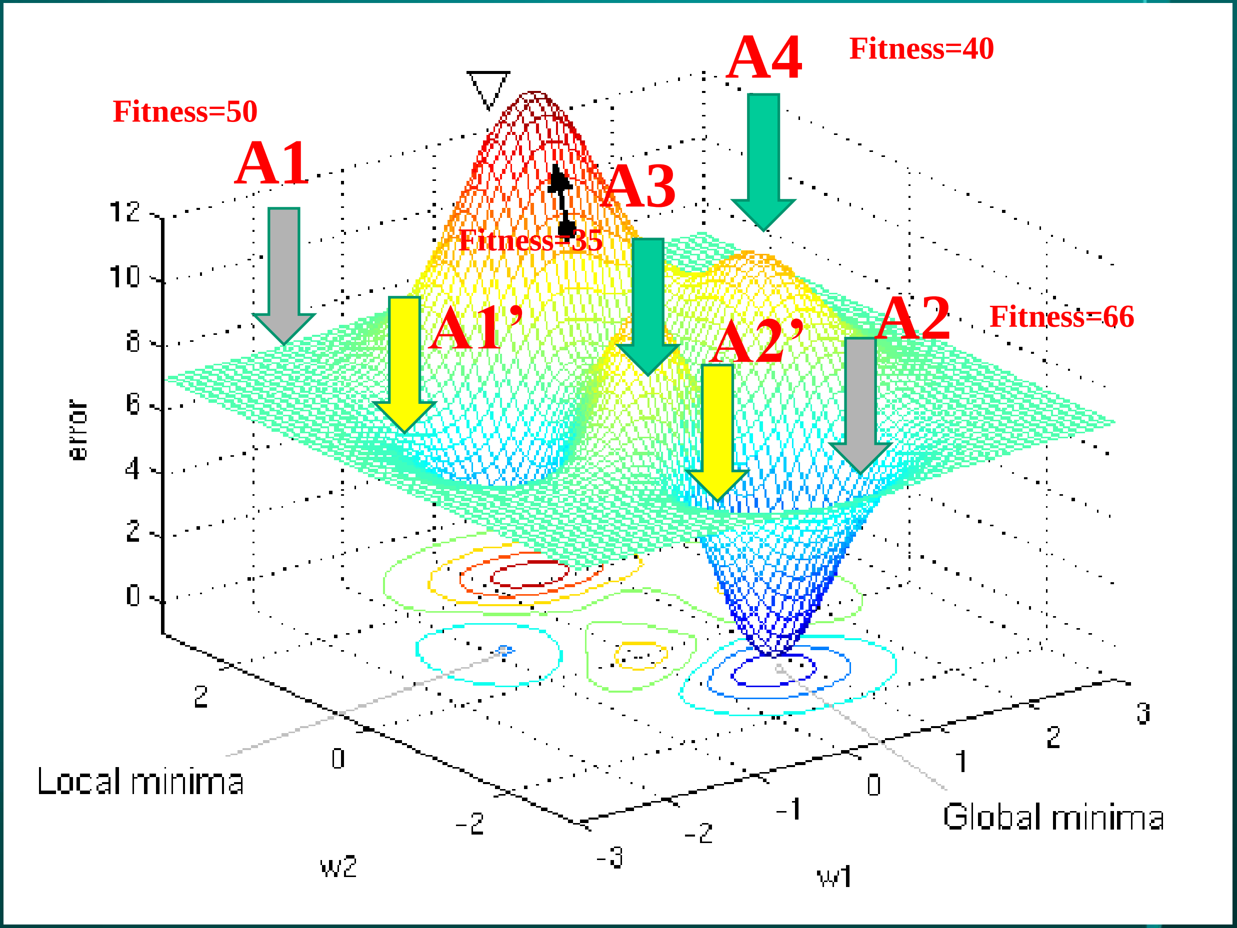
- **Recombination of the best**





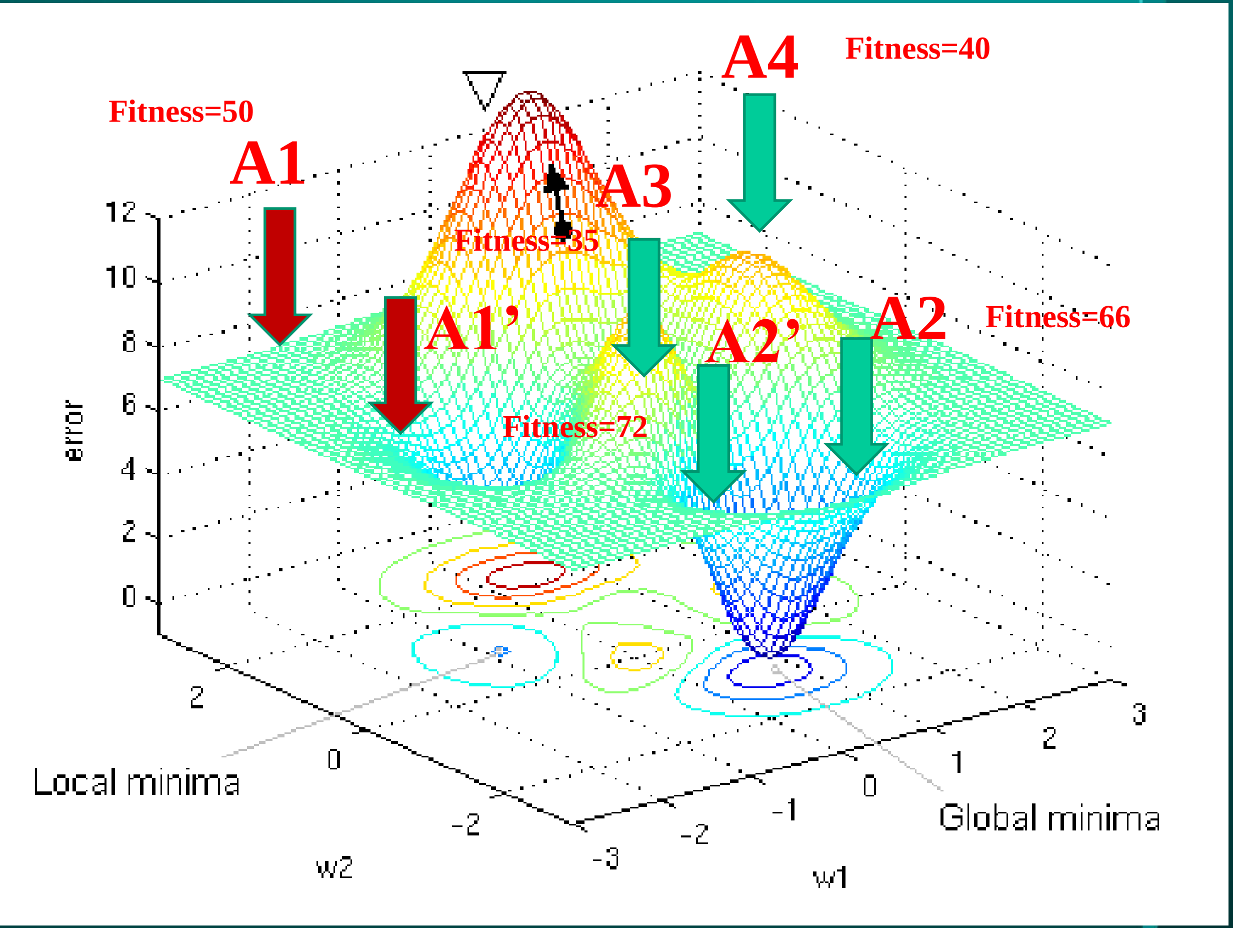
Genetic algorithm



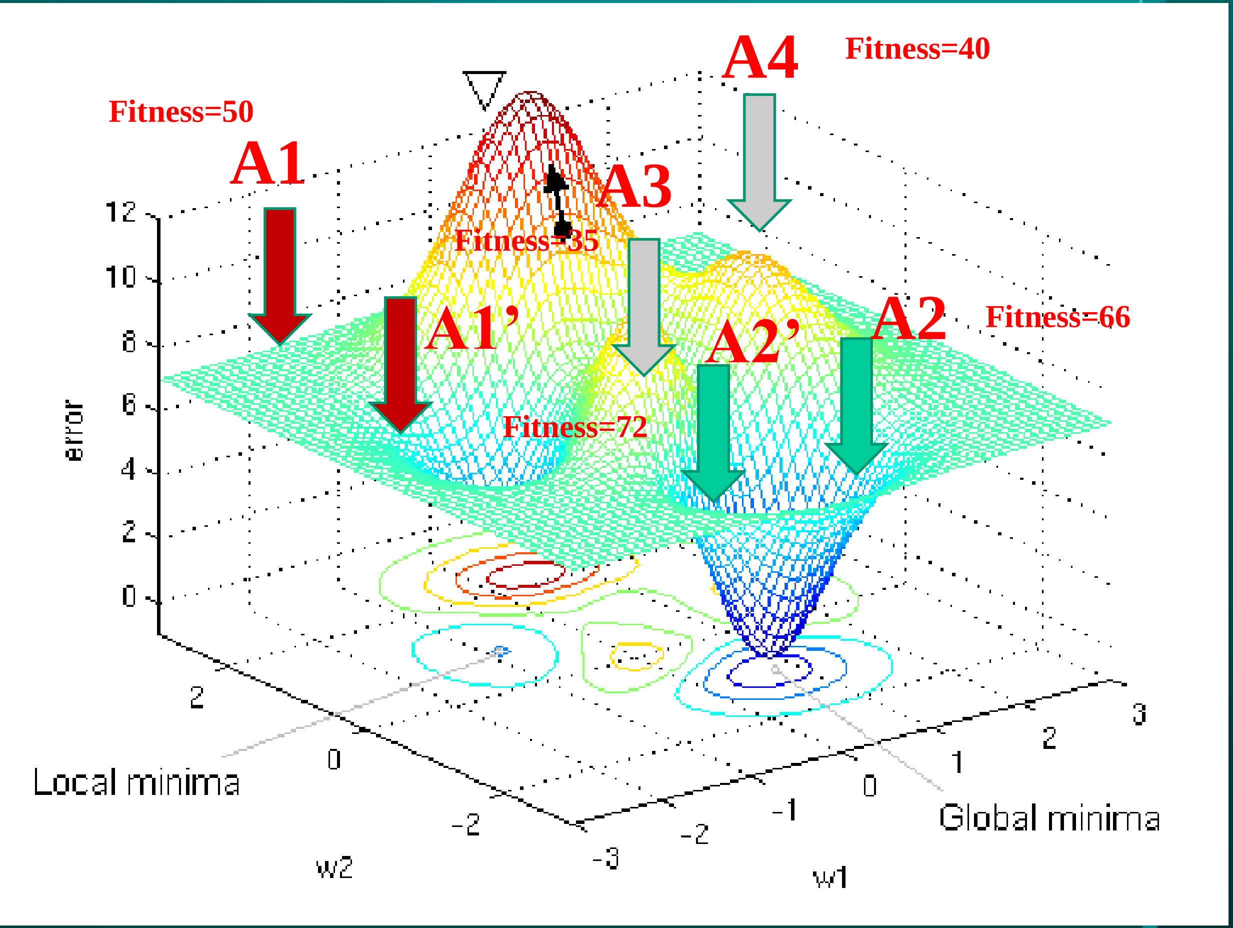


Genetic algorithm

- **Population size remains the same, by removing the worst individual(s)**

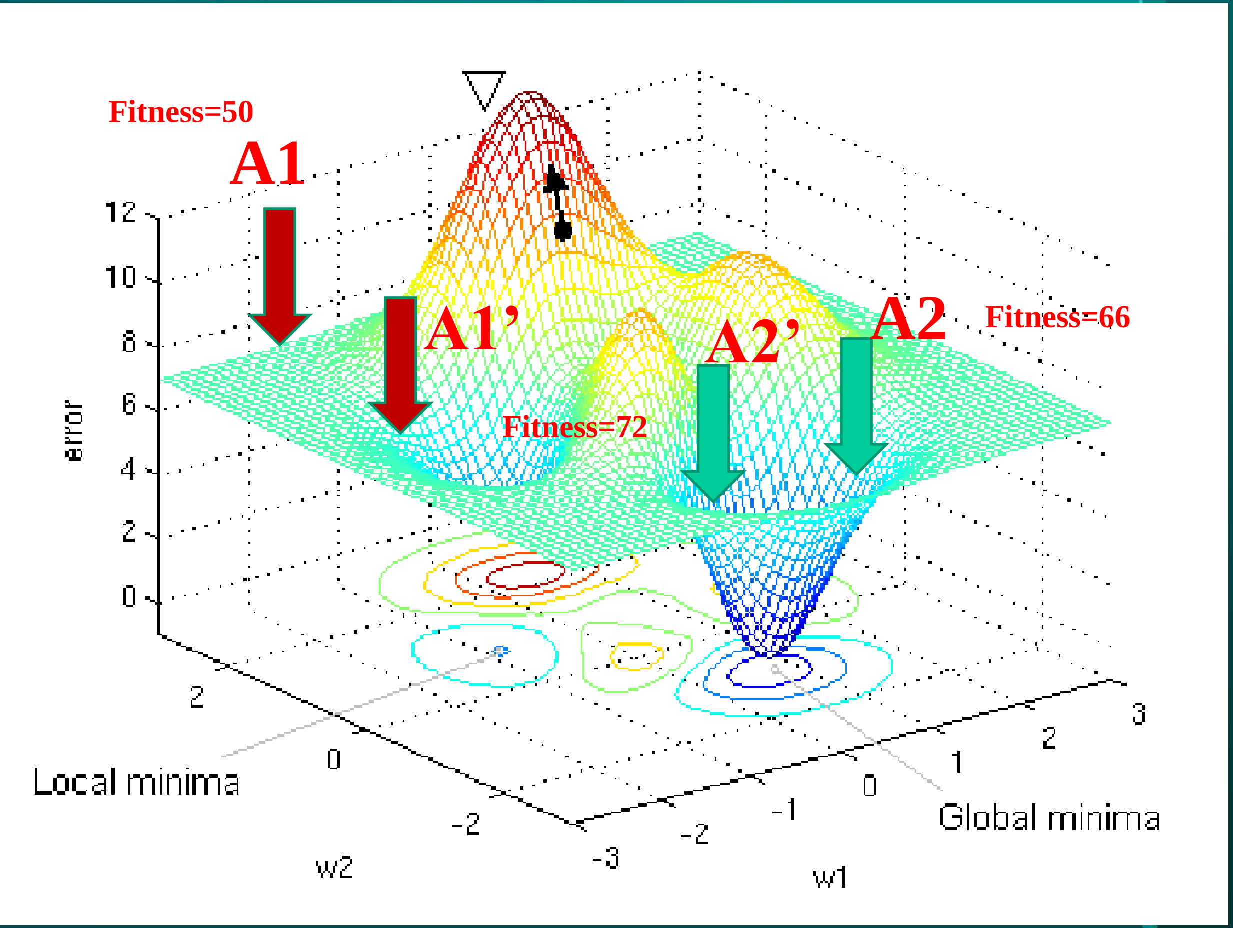


Genetic algorithm

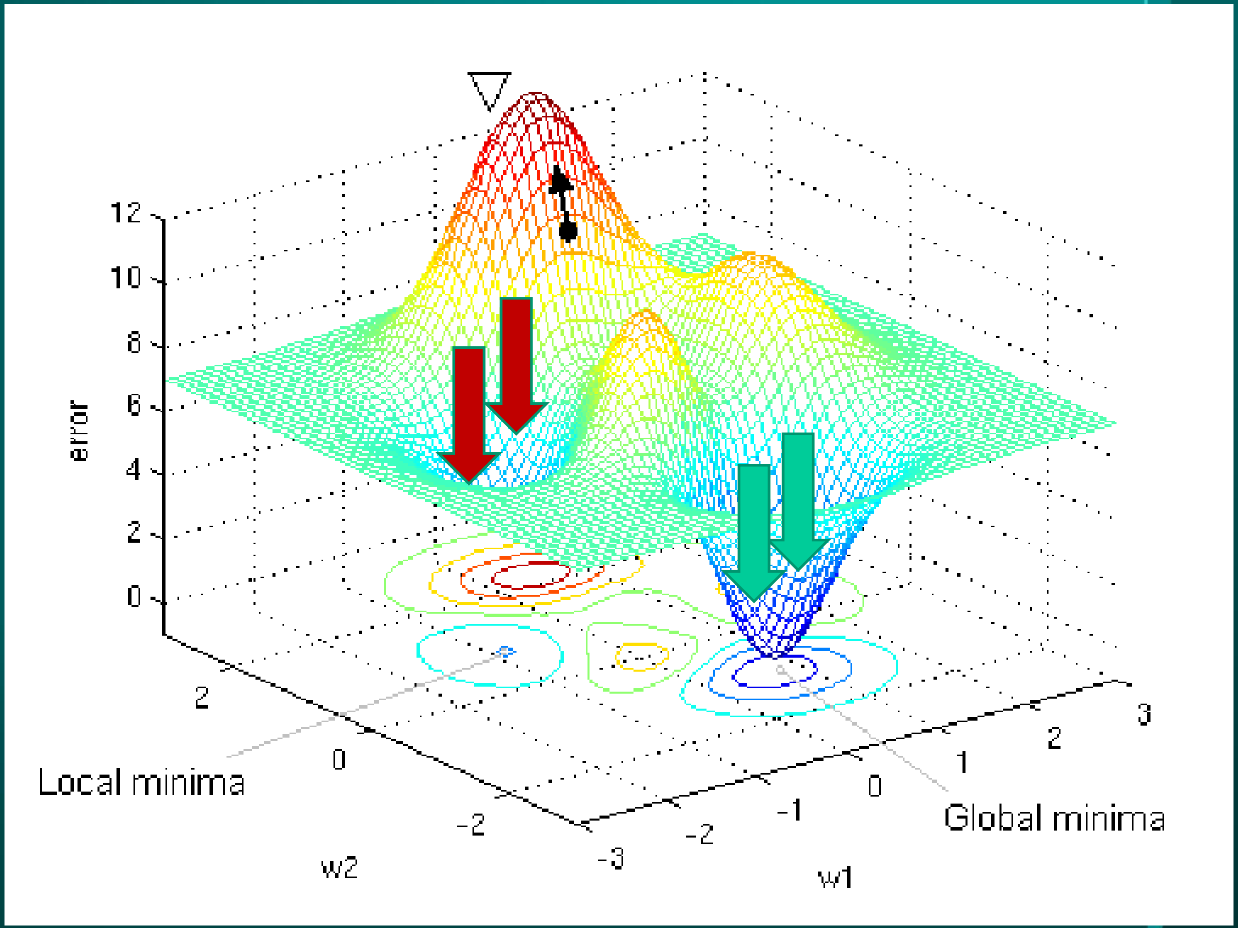


Genetic algorithm

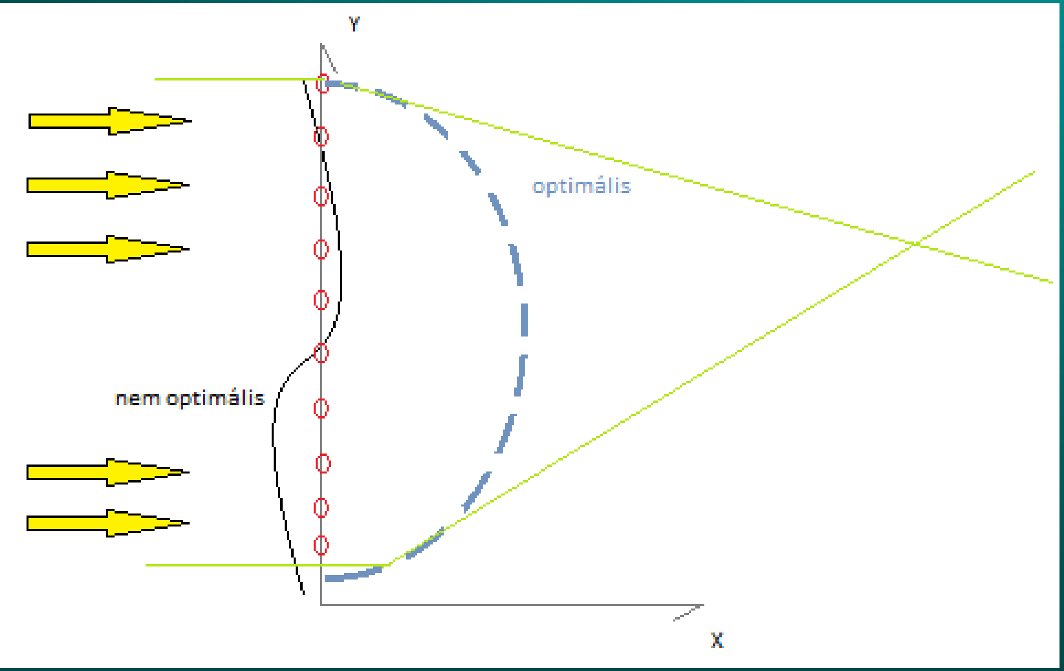
- After certain generations we can observe many individuals at best locations
- To avoid stucking at local minima we introduce random mutation



Genetic algorithm



Lens problem



Lens problem

-Is it fully random?

- Crossbreeding is random.

- Mutation is random.

- Selection <u>non random.</u>

Not a Monte Carlo algorithm

Flexible Muscle-Based Locomotion for Bipedal Creatures

SIGGRAPH ASIA 2013

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