Presented at the COMSOL Conference 2010 Paris

On a particle tracking technique to predict disinfection in drinking water treatment systems.

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Van Remmen UV Techniek

wetsus centre for sustainable water technology

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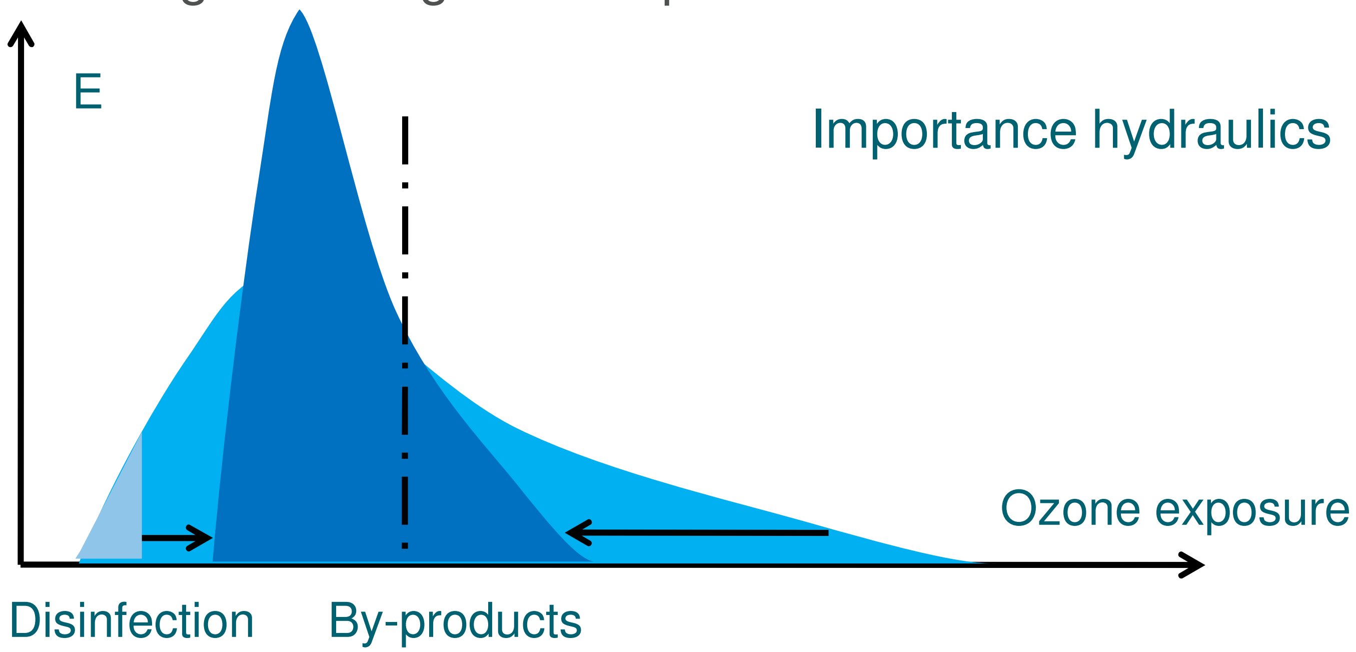
Contents

Introduction – why CFD with particle tracking?

Disinfection of drinking water

- Removing micro-organsims up to 99% to 99.9%



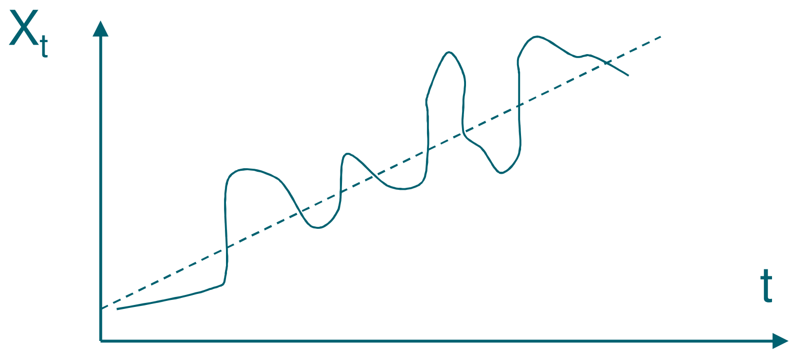
Particle tracking technique

Stochastic differential equation for Brownian motion:

$$dX_t = f(t, X_t)dt + g(t, X_t)dW_t$$

$$X_t(0) = X_0$$

Increments dW_t generated from random number generator



Particle tracking technique

The advection diffusion equation must be obeyed for particles:

$$\frac{\partial C}{\partial t} + u_i \frac{\partial C}{\partial x_i} = \frac{\partial C}{\partial x_i}\left(D_{ij} \frac{\partial C}{\partial x_j} \right)$$

Coupling by Fokker-Planck equation results in:

$$dX_{i,t} = \left(u_i + \frac{\partial D}{\partial x_i} \right) dt + \sqrt{2D} dW_{i,t}$$

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Particle tracking technique – numerical solution

The diffusion part, Euler scheme:

$$Y_{n+1} = Y_n + \frac{dD}{dx}\Delta t + \sqrt{2D}\Delta W_n$$

Milstein scheme:

$$Y_{n+1} = Y_n + \frac{dD}{dx}\Delta t + \sqrt{2D}\Delta W_n + \frac{1}{2}\frac{dD}{dx}\left(\left(\Delta W_n\right)^2 - \Delta t\right)$$

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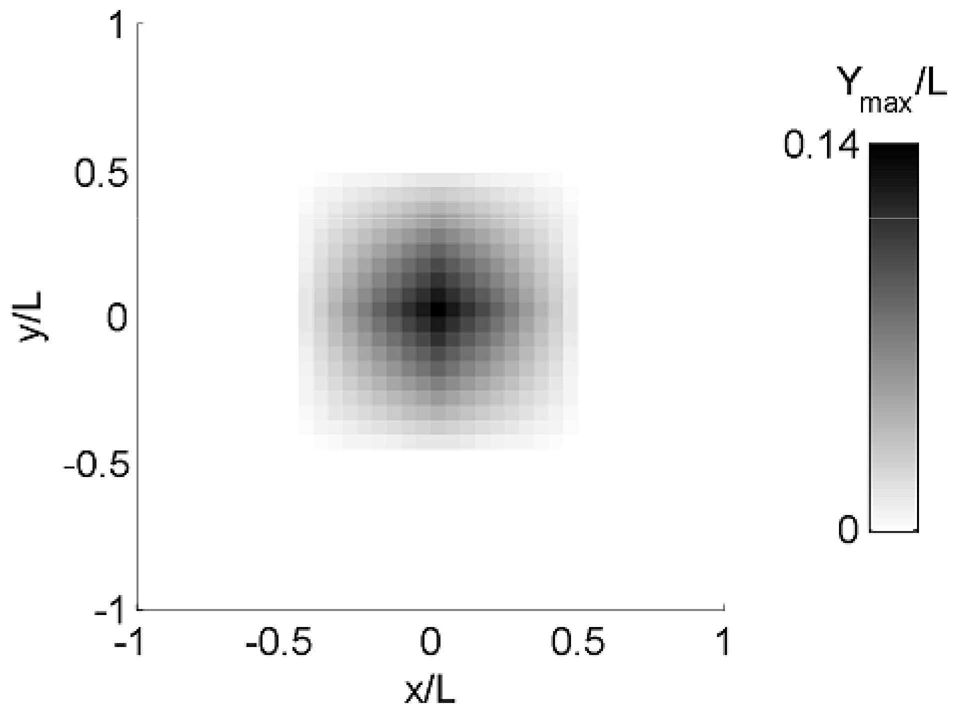
Test case: wall treatment

Diffusion coefficient:



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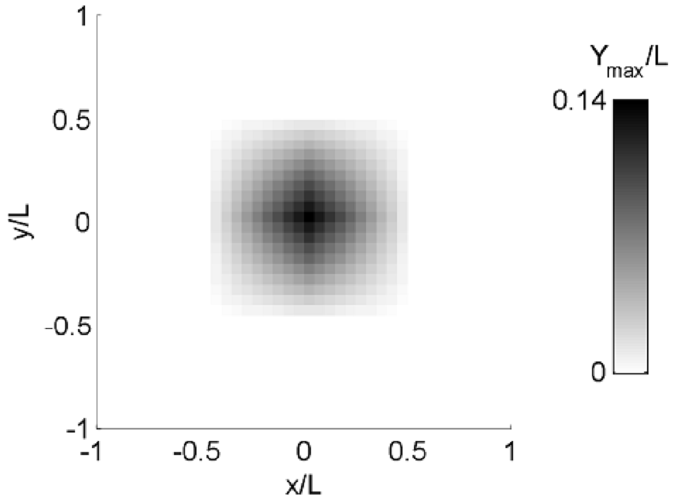
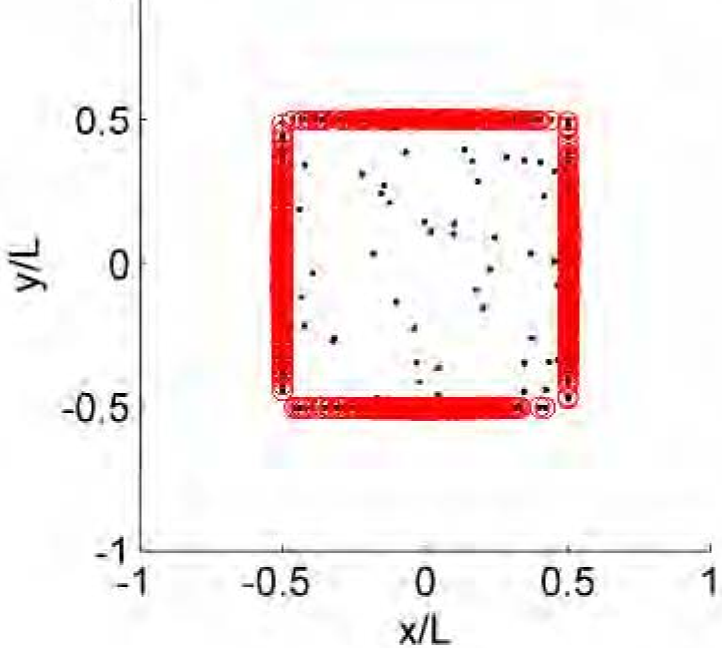
Test case: wall treatment

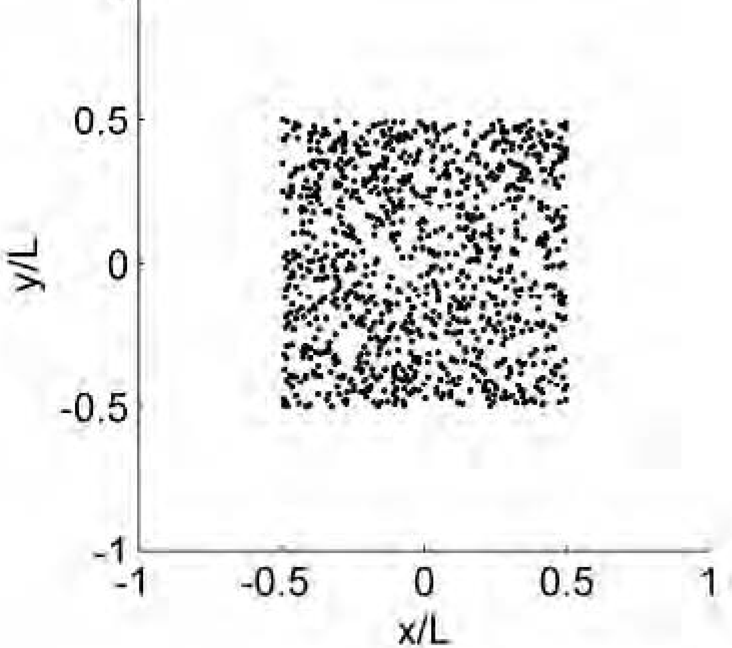


Particle positions after 1000 steps:

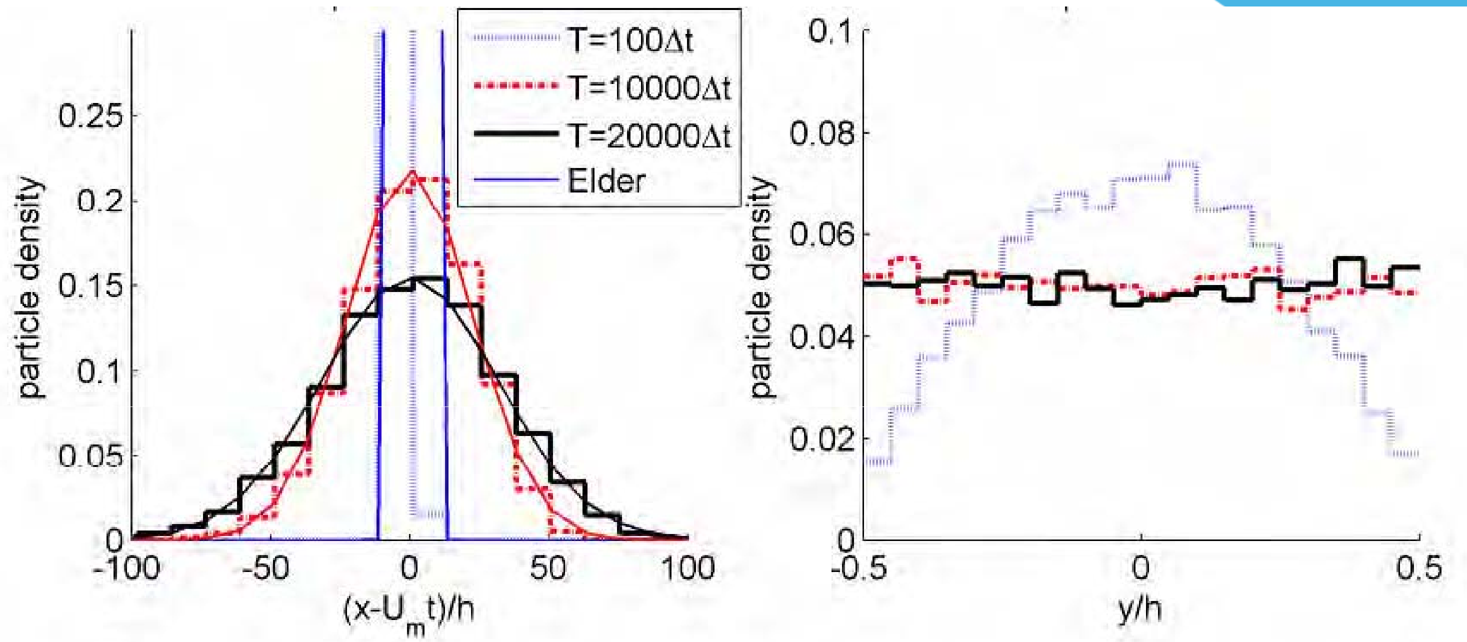
Euler



Milstein



Test case: channel flow Elder



Logarithmic velocity profile

Parabolic diffusion profile

Theoretical dispersion coefficient of: $D_L = 5.86 u_* h$

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Implementation in COMSOL

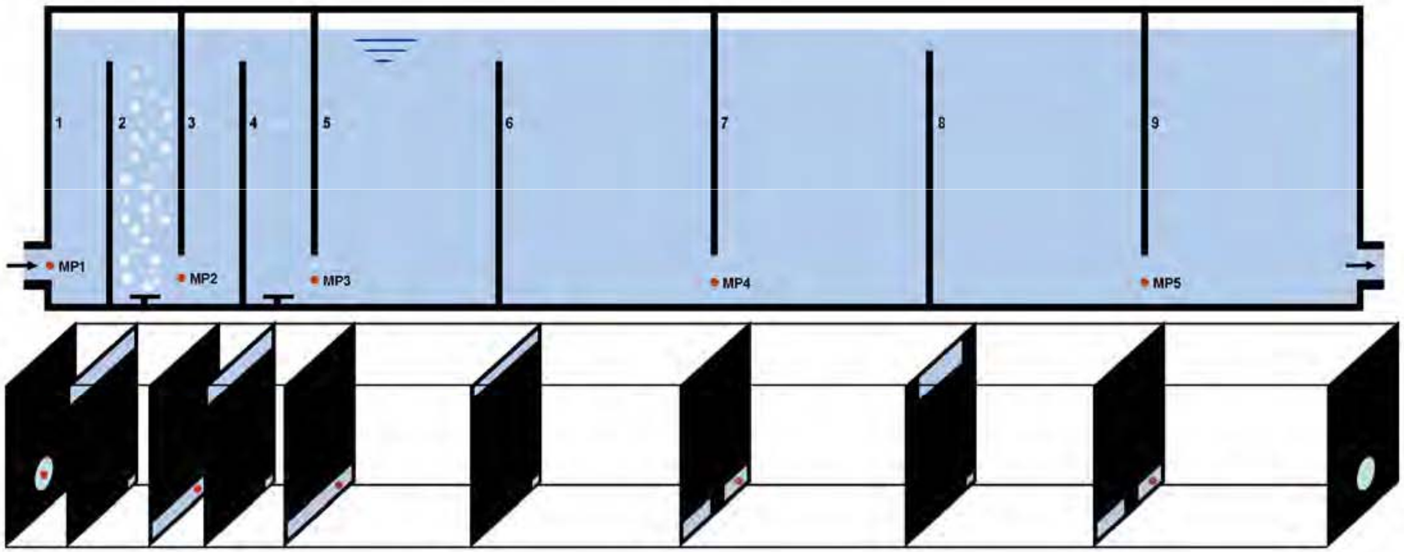
COMSOL Multiphysics with k-ε turbulence model

Flow fields are captured from fem-structure in Matlab

Particle tracks are resolved in Matlab

Application water treatment

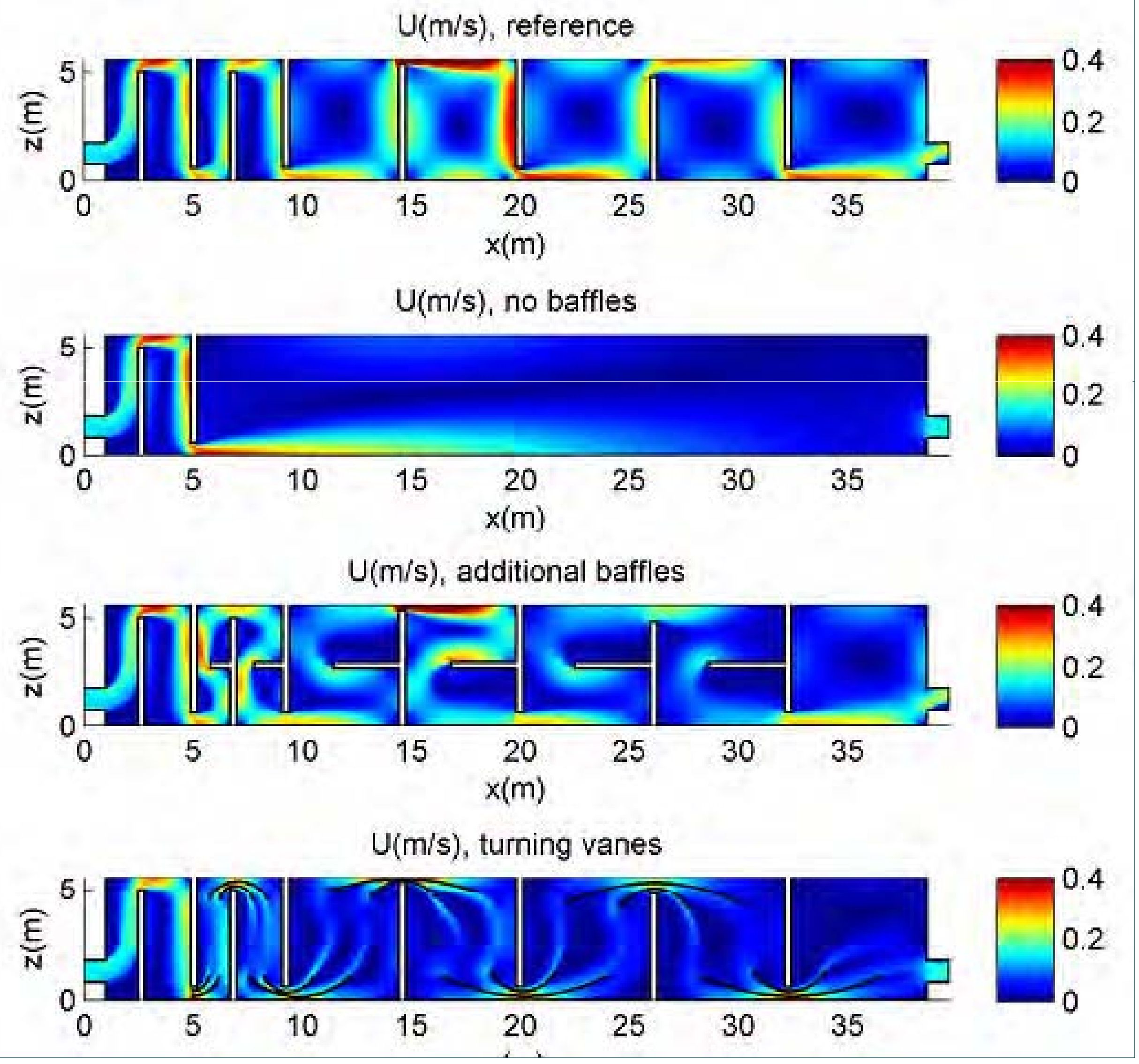
Ozone installation



Application water treatment

Flow fields

k-ε turbulence model



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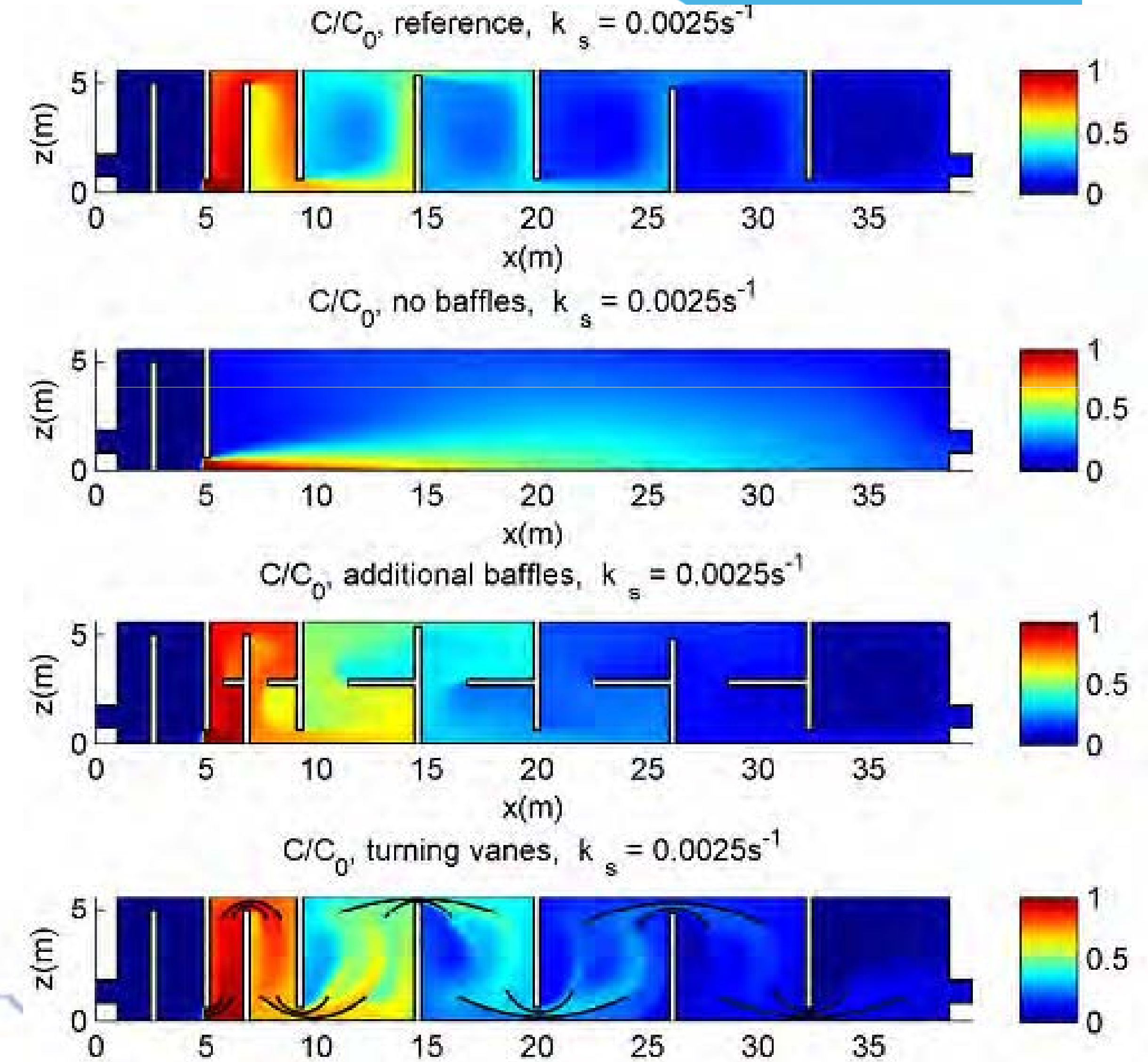
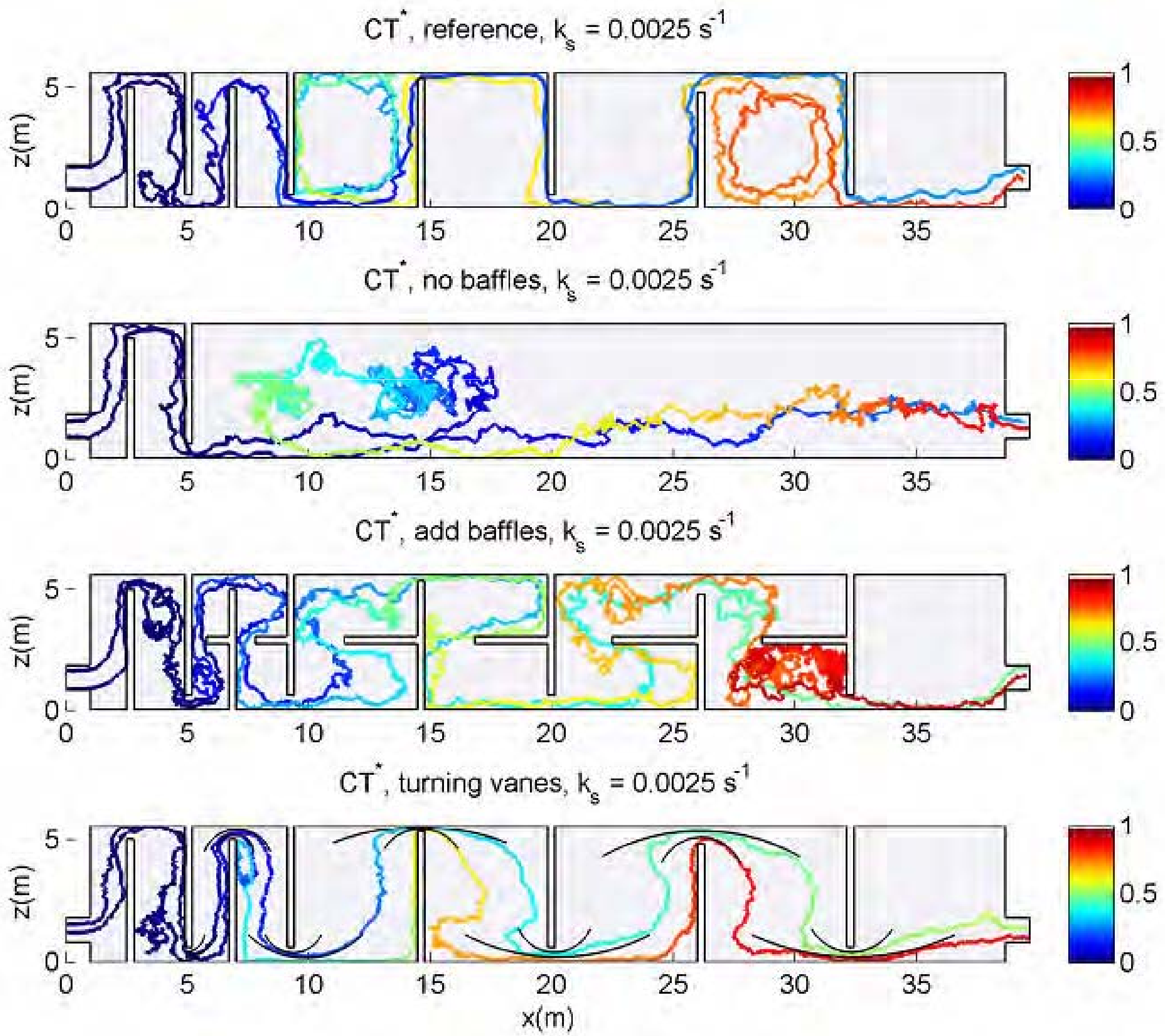
Application water treatment

Ozone concentration

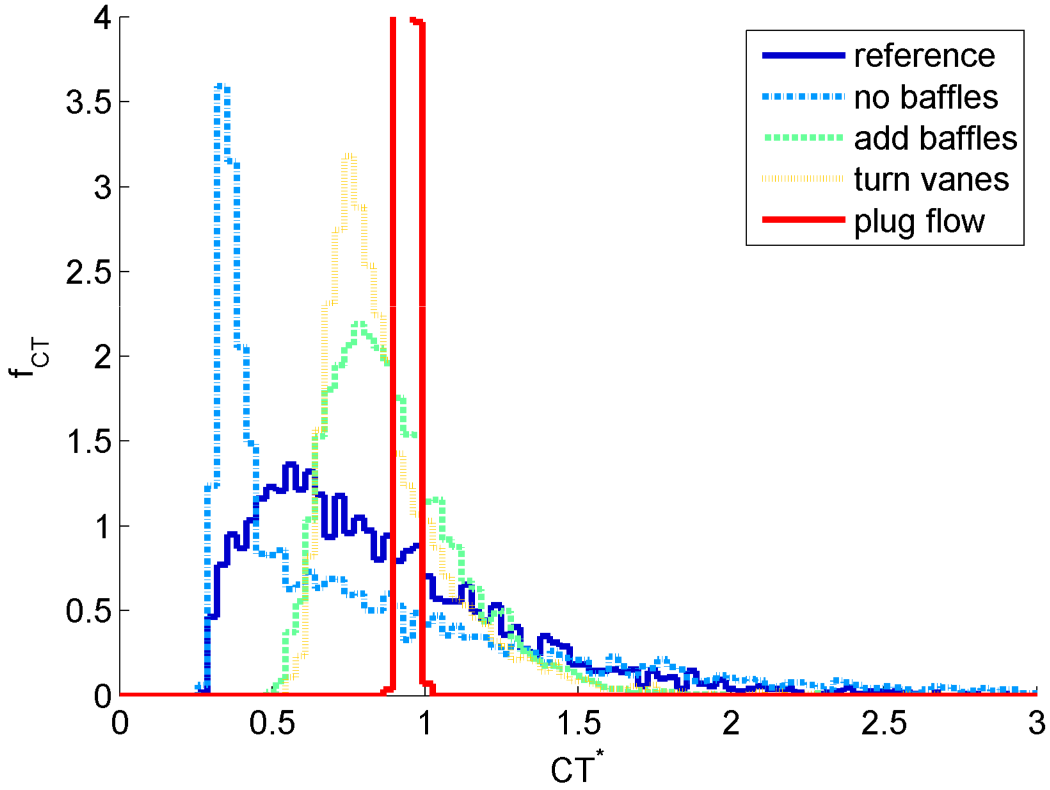
Advection-diffusion
(+ reaction)



Application water treatment – Particle trajectories



Distribution of CT values (ozone exposure)



Log inactivation	
Reference	1.43
No baffles	1.18
Add baffles	**1.88**
Turn vanes	1.86
Plug flow	2.18

Conclusions

Development of particle tracking routine

- Using COMSOL multiphysics with a k-ε turbulence model
- That obeys diffusion and advection
- No problems at the walls

Optimization of drinking water treatment installations established