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

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Contents

Introduction

Particle tracking technique

Test cases

Application of water treatment with ozone
Disinfection of drinking water

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

Introduction – why CFD with particle tracking?

Importance hydraulics

Ozone exposure

Disinfection  By-products
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:

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

\[ Y_{n+1} = Y_n + \frac{dD}{dx} \Delta t + \sqrt{2D} \Delta W_n + \frac{1}{2} \frac{dD}{dx} ((\Delta W_n)^2 - \Delta t) \]
Test case: wall treatment

Diffusion coefficient:

$$Y_{\text{max}}/L$$

$$0.14$$
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: \[ D_L = 5.86 u \cdot h \]
Implementation in COMSOL

COMSOL Multiphysics with $k$-$\varepsilon$ 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

$k$-$\varepsilon$ turbulence model
Application water treatment

Ozone concentration

Advection-diffusion
(+ reaction)
Verschillende configuraties
Filmpje, als het werkt…
Application water treatment – Particle trajectories
Distribution of CT values (ozone exposure)

Log inactivation

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<thead>
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<tbody>
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<td>Plug flow</td>
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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