

# On Coupled Particle Level and Filter Element Level Simulation for Filtration Processes

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## Motivation

Multiple scales in filtration

## Independent models at different scales

Macroscale model

Microscale model

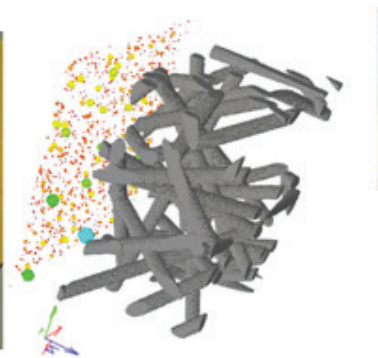
## Micro-macro coupling

Sketch of the algorithm

## Some preliminary results

Results

## Summary

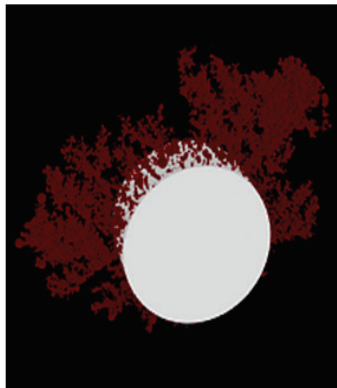


## Multiple scales in filtration

## Particles level

Nano scale

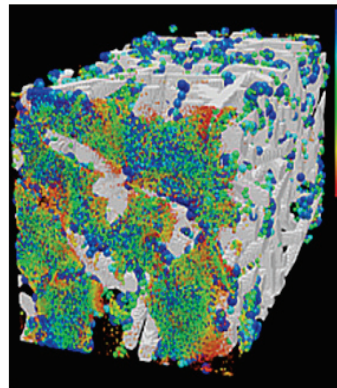
(Navier-)Stokes in pore space  
coupled with stochastic  
ODE for particles, ....



Particles-Fiber  
interaction

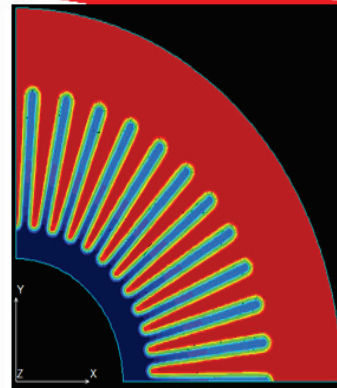
## Filter components

Micro scale



Dirt loading of  
the filtering medium

Millimeter

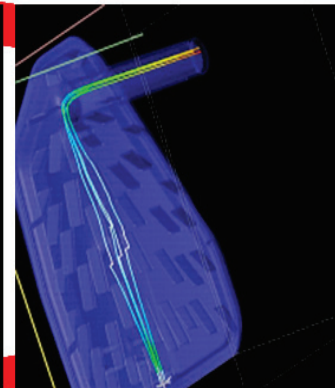


Pleats in cartridge  
filters

## Filter element

Centimeter

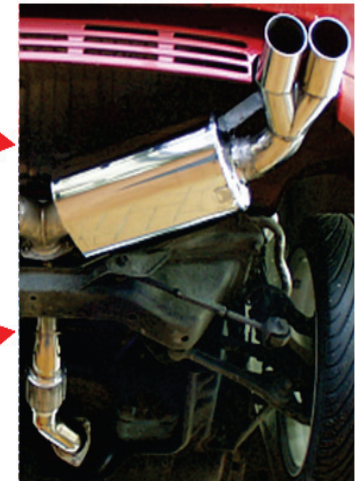
(Navier-)Stokes-Brinkmann in fluid and  
in porous media coupled with  
concentration of particles



Flow within  
Filter element

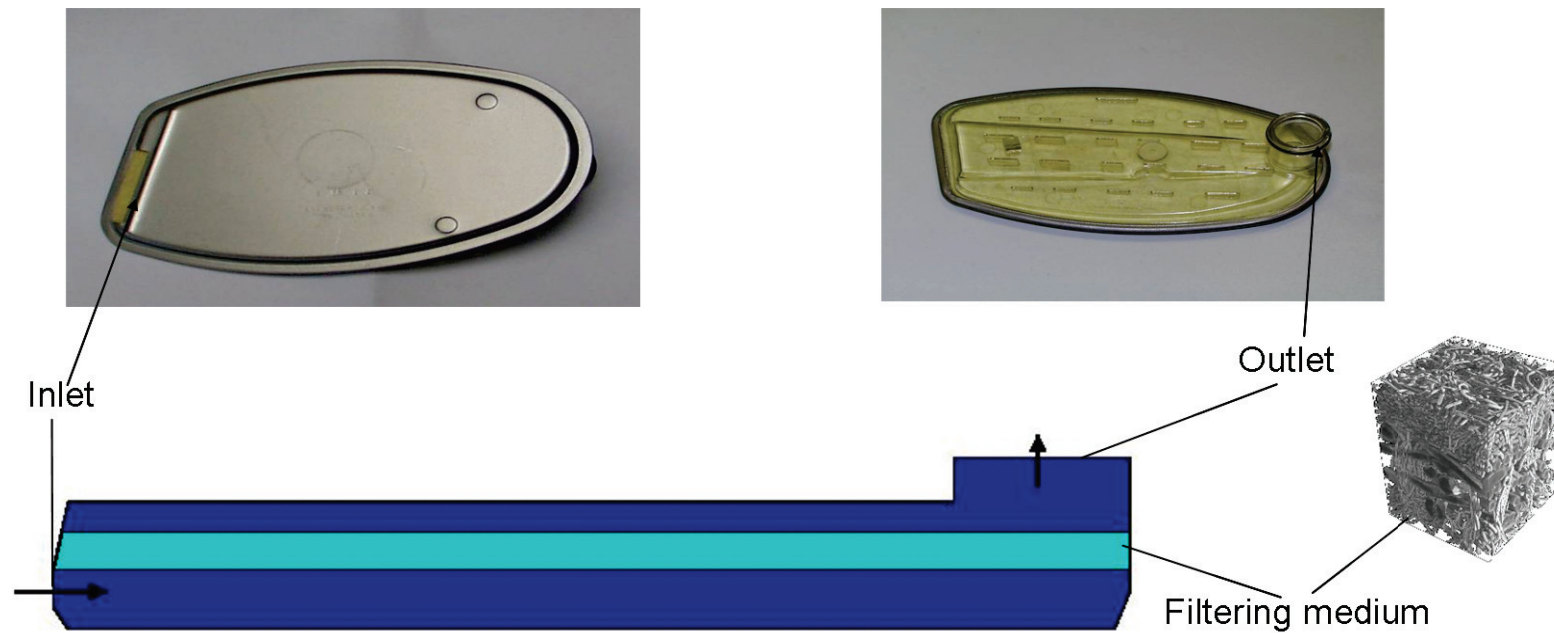
## Complete system

Meter



Filter installation

## Multiple scales in filtration



## Determining performance of a filter

- ▶ Pressure drop - flow rate ratio
- ▶ Dirt Storage capacity
- ▶ Size of penetrating particles

Depend on microscale (e.g. fibrous geometry) and macroscale (e.g. pressure, velocity) quantities.

## Navier-Stokes-Brinkmann System

Incompressible laminar flow through filters

$$\underbrace{\frac{\partial \vec{u}}{\partial t} - \nabla \cdot (\tilde{\mu} \nabla \vec{u}) + (\rho \vec{u}, \nabla) \vec{u}}_{\text{Navier-Stokes}} \underbrace{+ \mu \tilde{K}^{-1} \vec{u} + \nabla p}_{\text{Darcy}} = f$$

$$\nabla \cdot \vec{u} = 0 \quad \text{continuity equation}$$

## Fictitious Region Method

Type continuation of coefficients:

$$\tilde{K}^{-1} = \begin{cases} K^{-1}, & x \in \Omega_p \\ 0, & x \in \Omega_f \end{cases}$$

## Interface conditions

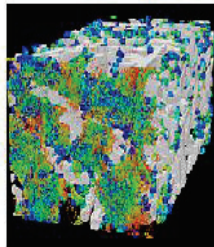
$$[\vec{u}]_{\Gamma} = 0$$

$$[\vec{n} \cdot (\tilde{\mu} \nabla \vec{u} - p \vec{l})]_{\Gamma} = 0$$

Justification in Angot 1998

## Macroscale model

- ▶ Estimate the pressure drop within the filter element
- ▶ Varying permeability (depending on loading)
- ▶ **Missing: Information about the processes at the pore/particle level**



## Extension of macroscale model to account for particles' loading

- ▶ Solve the convection-diffusion-reaction equation at the meso scale.

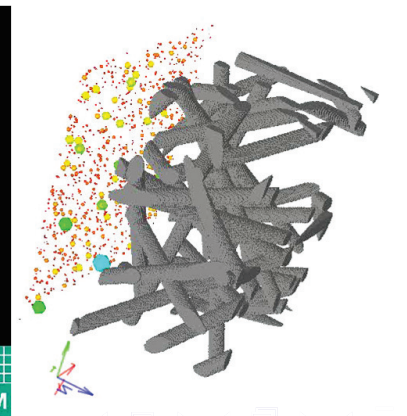
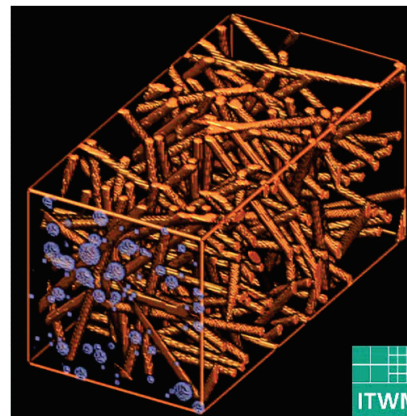
## Convection Diffusion Reaction equation

$$\frac{\partial C^J}{\partial t} + (\vec{u}, \nabla C^J) - D \Delta C^J = \frac{\partial M}{\partial t}$$

$$\frac{\partial M}{\partial t} = -\alpha^J C^J$$

 $J$  - particle size $t$  - time $u$  - velocity $C$  - concentration $D$  - diffusion coefficient $\alpha(t, u, C)$  - Absorption Rate $\alpha$  derived from measurements or directly from microscale simulations

$t$	$\beta$
1	51.9
3	39.0
5	33.2
7	25.3
9	10.9





## Stokes system

$$\begin{aligned}\mu\Delta\vec{u} + \vec{f} &= \nabla p \\ \nabla \cdot \vec{u} &= 0\end{aligned}$$

$t$  - time

$\vec{u}$  - fluid velocity

$p$  - pressure

$\mu$  - fluid viscosity

## Stochastic ODE

$$\frac{\partial \vec{u}_0}{\partial t} = -\gamma \times (\vec{u}_0(\vec{x}) - \vec{u}(\vec{x})) + \frac{Q\vec{E}(\vec{x})}{m} + \sigma \times \frac{d\vec{W}(t)}{dt}$$

$$\frac{\partial \vec{x}}{\partial t} = \vec{u}_0$$

$$\sigma^2 = \frac{2k_B T \gamma}{m}$$

$$\gamma = 6\pi\rho\mu\frac{R}{m}$$

$$\langle d\vec{W}_i(t), d\vec{W}_i(t) \rangle = \delta_{ij} dt$$

$\vec{x}$  - particle position

$\vec{u}_0$  - particle velocity

$m$  - particle mass

$Q$  - particle charge

$E$  - electric field

$d\vec{W}(t)$  - 3D probability measure

$\rho$  - fluid density

$R$  - particle radius



## Macroscopic scale

- ▶ Used for simulating filtration processes at filter element level
- ▶ Needs measurements at element level to calculate deposition rate and change in permeability
- ▶ Does not provide info about particles at pore/particle level

## Microscopic scale

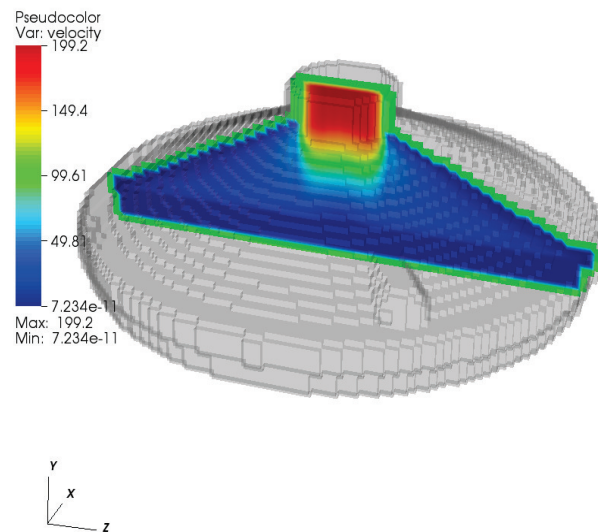
- ▶ Limited computer power
- ▶ Good for local simulations
- ▶ Unable to solve at level of filter element due to computer power limitations.



## Sketch of the algorithm

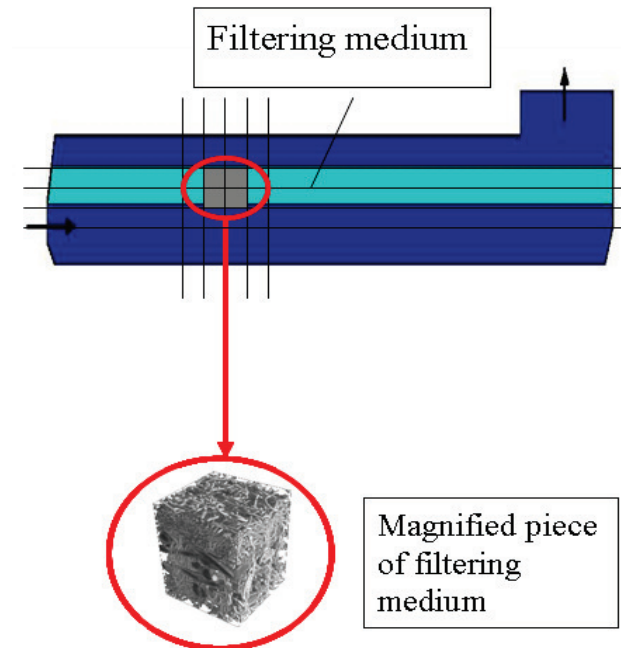
## Step 1

$\Delta p$ ,  $\vec{u}$  and  $C^J$  computed on the macro scale



## Step 2

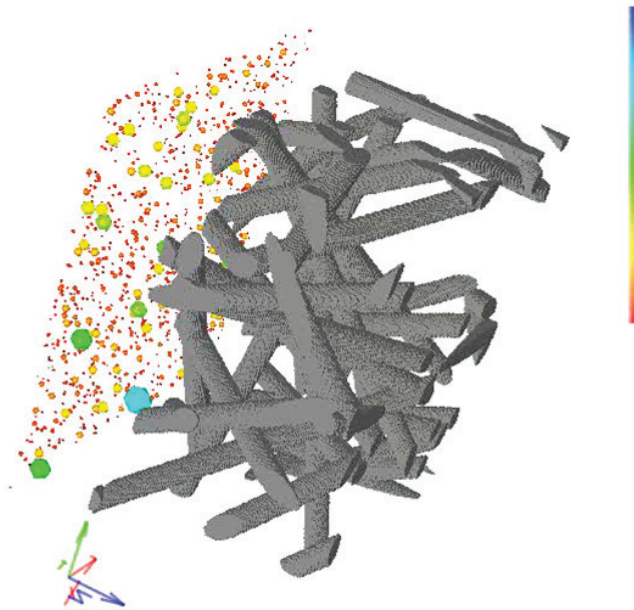
Downscaling of local velocity and particle concentrations on selected voxels



## Sketch of the algorithm

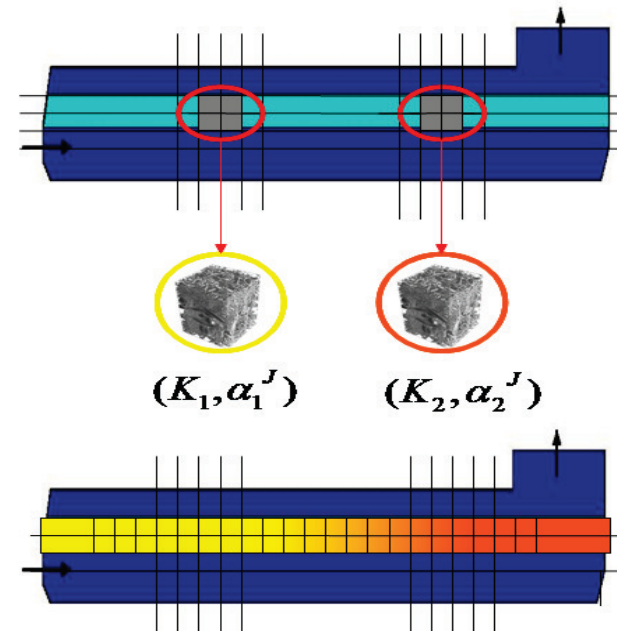
## Step 3

Solve micro problem locally and compute new values for  $K$  and  $\alpha$

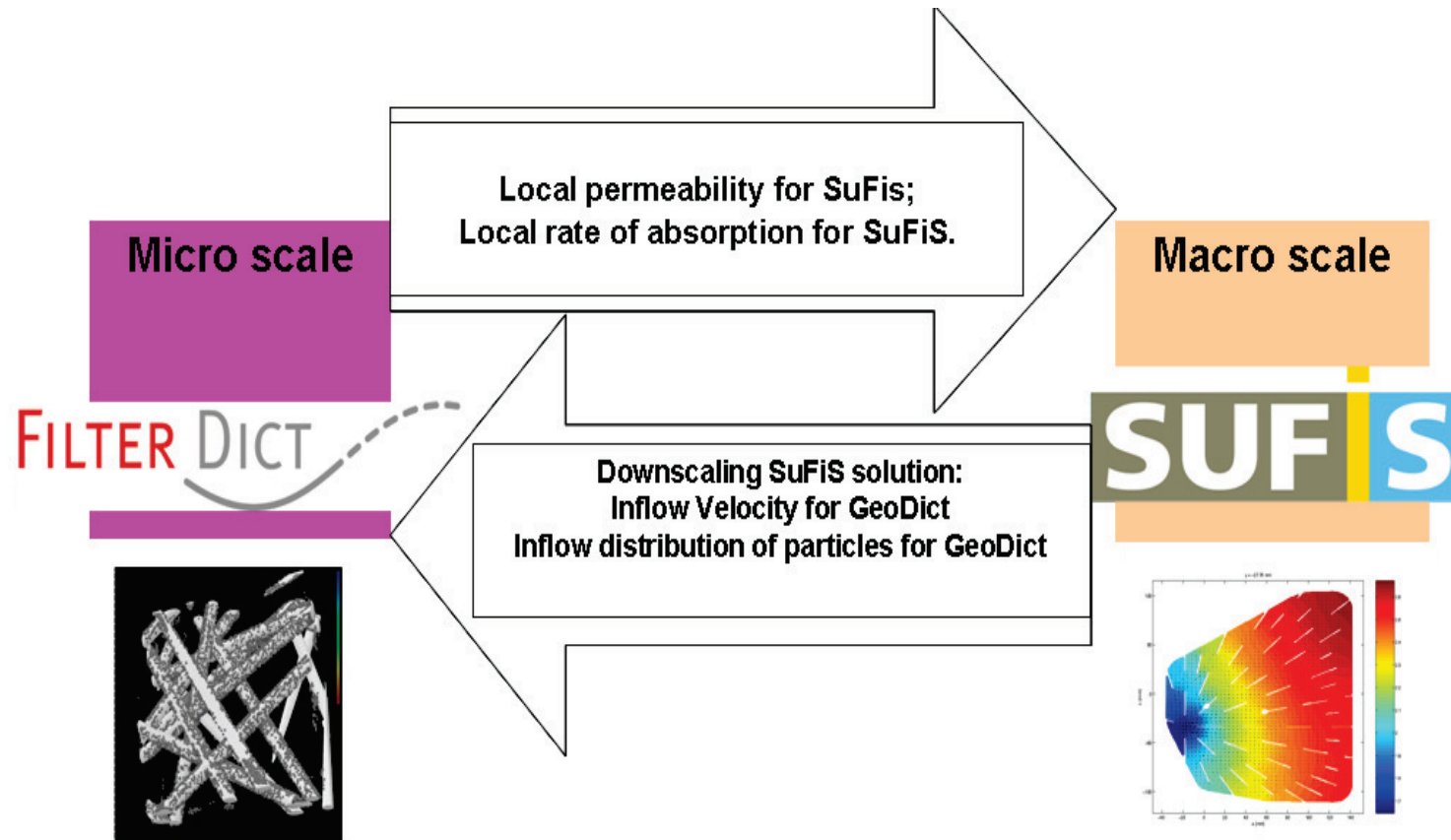


## Step 4

Use interpolation techniques to compute  $\alpha$  and  $K$  everywhere



## Sketch of the algorithm

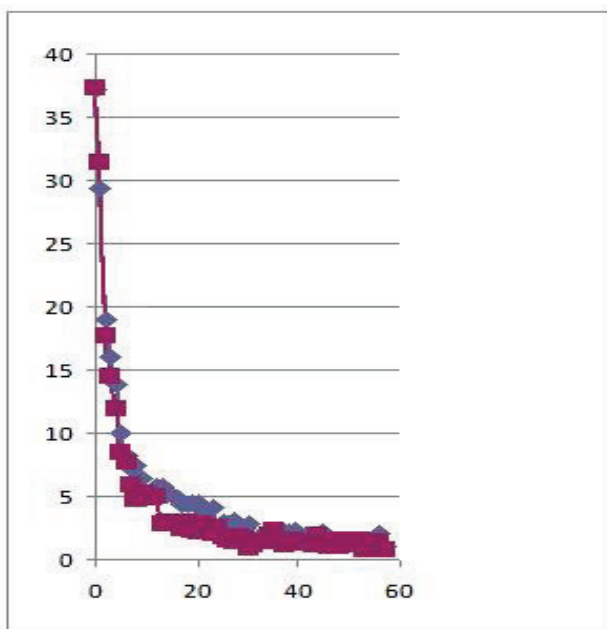
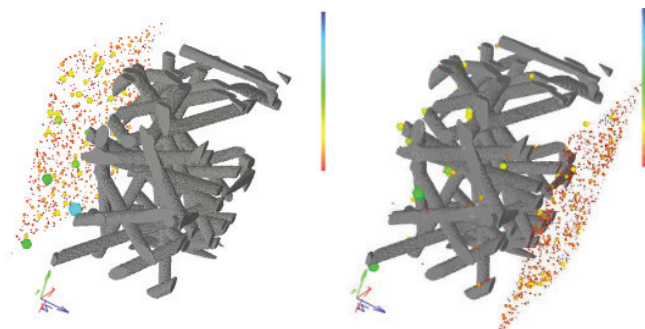


## Details to be noted

- ▶ different range of velocities
- ▶ change of particle concentration over time

Incorporate info in the form of correlation tables

## Correlation tables from micro simulations

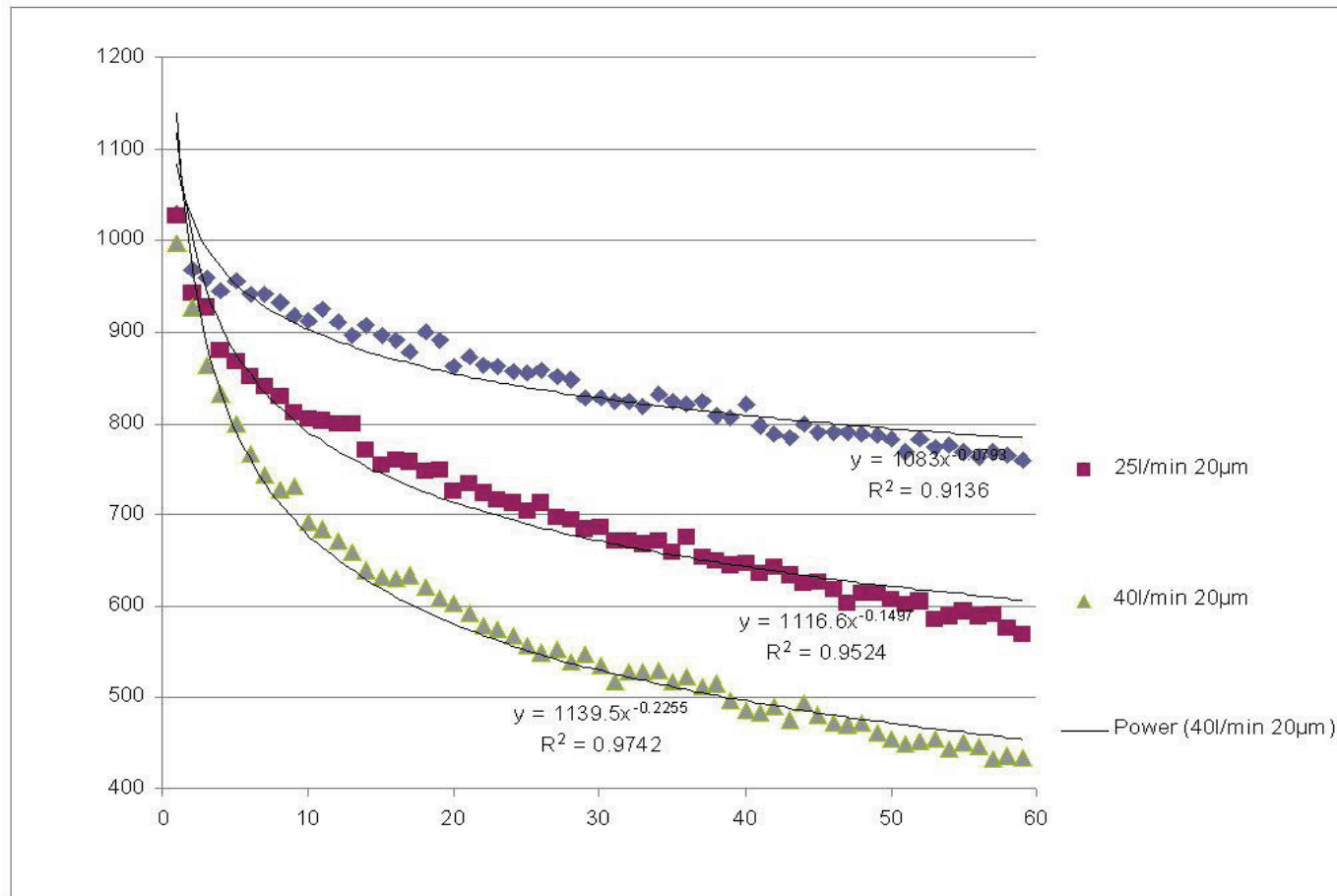


- ▶ different particle sizes
- ▶ different velocities
- ▶ different filter media
- ▶ different concentrations

Simplified to be a pre processing step for macro simulations

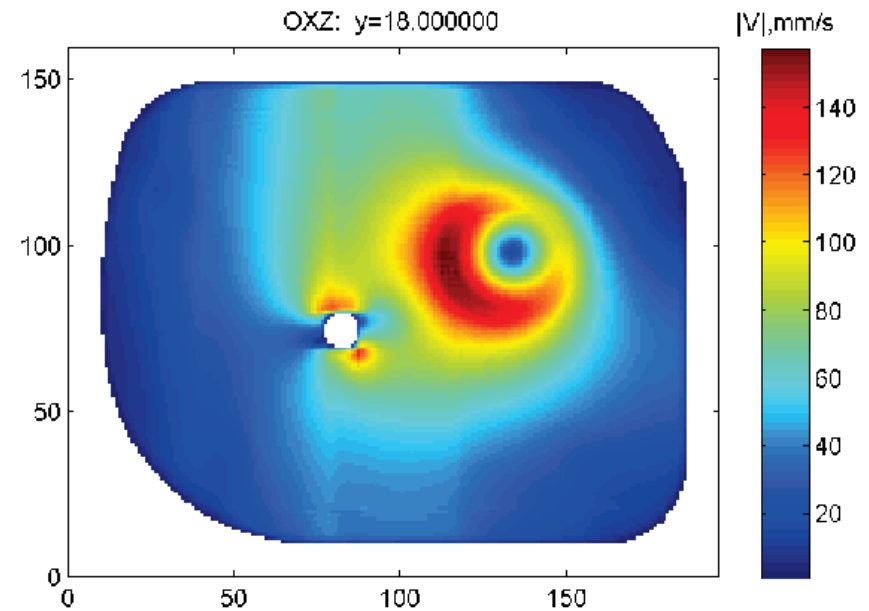
## Results

## Correlation tables from measurements



## Results

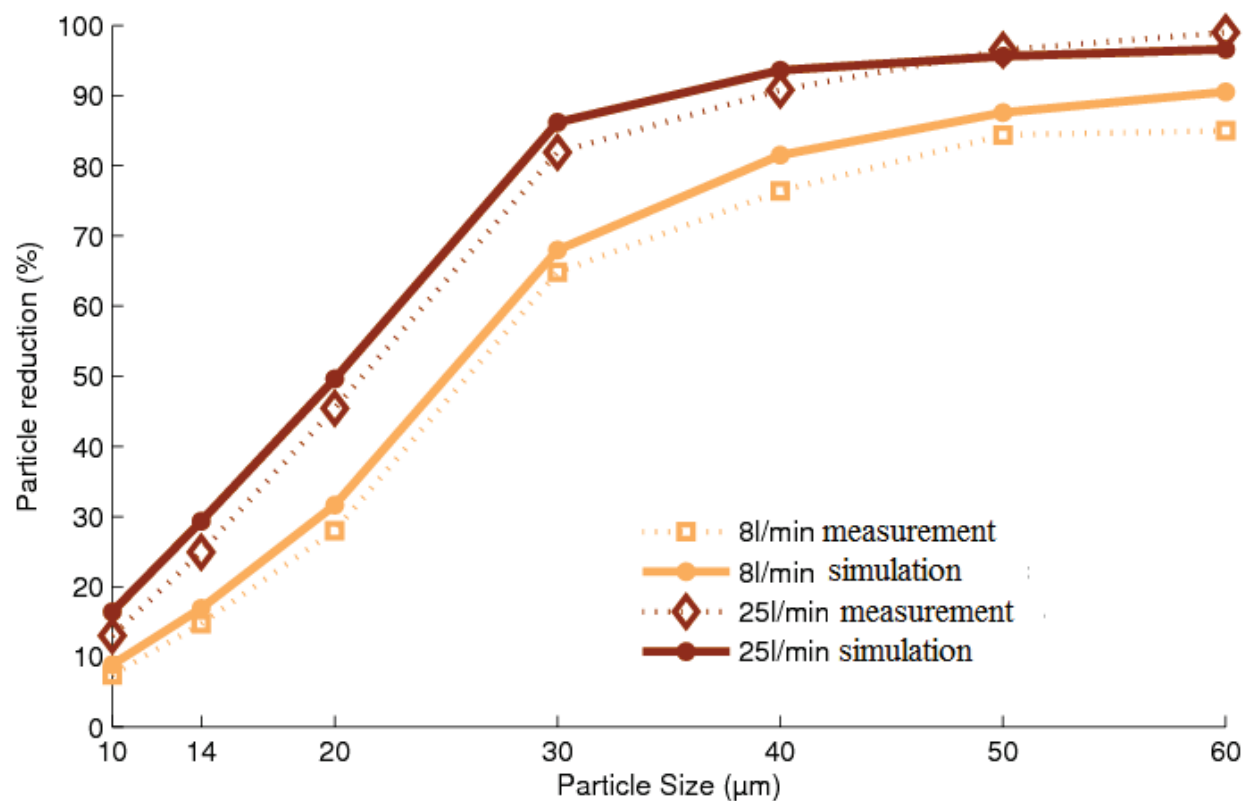
## Macro simulation performed on filter element level



$$\alpha^J(y, z) = \frac{(h + \Delta t u(y, z))(n^J(t) - n^J(t + \Delta t))}{h \Delta t n^J(t)}$$



## Efficiency profile for different particle sizes



## Conclusions

- ▶ Filtration processes vary at different scales
  - ▶ Macroscale: Navier Stokes Brinkmann system
  - ▶ Mesoscale: Particle Concentration Equation
  - ▶ Microscale: Stokes and particle deposition model
- ▶ Micro-meso-macro coupling
  - ▶ Filter element level simulation
  - ▶ Downscaling of local velocities and particle concentrations
  - ▶ Correlation tables - from microscale simulations/measurements
  - ▶ Deriving  $\alpha$  from correlation tables

**THANK YOU FOR YOUR ATTENTION!**