

1 CATALYST-COATED PARTICULATE FILTERS

→ Gasoline Direct Injection (GDI) engines are fuel efficient but release **soot nanoparticles** and **harmful gases**
→ Gasoline Particulate Filters (GPF) coated with Three-Way Catalyst (TWC) have been developed to **capture soot** while **reducing NO_x, CO and HC emissions**
→ Optimizing exhaust gas after-treatment systems is making our **air cleaner** and our **lives longer**

Washcoat □
Cordierite ■
Pores ■

2 OBJECTIVE

Determine the optimal catalyst amount and profile into the GPF porous wall

1. Pressure drop (ΔP)
2. Filter efficiency (E_F)
3. Catalyst coating conversion

To help address the problem of air quality in our cities

3 FOUR-STEP NUMERICAL METHODOLOGY

1. Reconstruct porous wall using Computed Tomography images
2. Compute the flow field using the LBM
3. Calculate aerosol capture by solving a Langevin equation
4. Compute the concentration field using the LBM

Catalyst coating characterization → Pressure drop → Capture efficiency → Catalyst effectiveness

Filter quality factor → Best coating deposition profile

1. CT image of an original R&D sample
2. $\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{F}$ External force
 $\nabla \cdot \mathbf{u} = 0$
3. $m \frac{d\mathbf{v}(t)}{dt} = \frac{3\pi\mu d_p}{C_c} (\mathbf{u}(\mathbf{r}) - \mathbf{v}(t)) + \mathbf{F}(t)$ Brownian diffusion
4. $\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = \nabla \cdot (D \nabla c) + \mathbf{r}$ Reaction rate

4 TWO CATALYST DISTRIBUTIONS INVESTIGATED

From the original R&D sample substrate

Non-uniform profile → 2D representation of 2 of the 10 catalyst amounts

Uniform profile → 2D representation of 2 of the 5 catalyst amounts

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5 THE LATTICE BOLTZMANN METHOD (LBM)

Navier-Stokes Equations (continuum mechanics)
 $\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f}$
 $\nabla \cdot \mathbf{u} = 0$

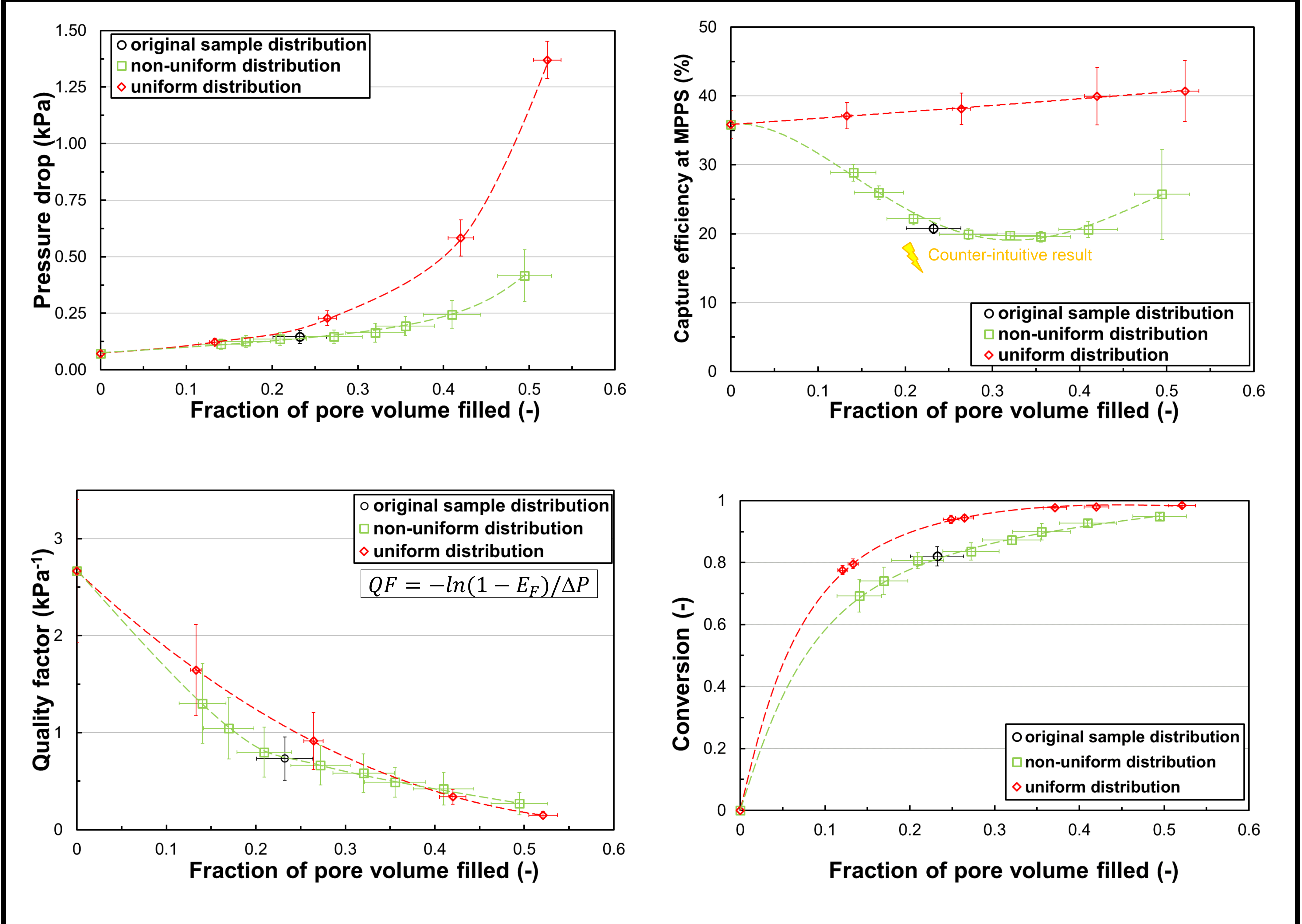
Boltzmann Equation (statistical mechanics)
 $\partial_t f_i + \mathbf{e}_i \cdot \nabla f_i = -\frac{f_i - f_i^{eq}}{\tau}$

Discretization in space & time FEM/FDM/FVM → $\mathbf{u}(\mathbf{x}, t)$

Discretization in velocity space (\mathbf{e}_i) → $\mathbf{u} = \frac{1}{\rho} \sum_i f_i \mathbf{e}_i$

Integration in the velocity space (\mathbf{e}_i) → $f_i(\mathbf{x} + \mathbf{e}_i \delta t, t + \delta t) - f_i(\mathbf{x}, t) = -\frac{f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)}{\tau}$

6 PREDICTED FILTRATION AND CONVERSION PERFORMANCE



7 LBM: A LARGELY PARALELIZABLE METHOD

280 millions voxels, 2 hours on 100 cores, 160 hours on 48 cores

8 UNDERSTANDING COUNTER-INTUITIVE RESULT

1/16 sections of the original domain

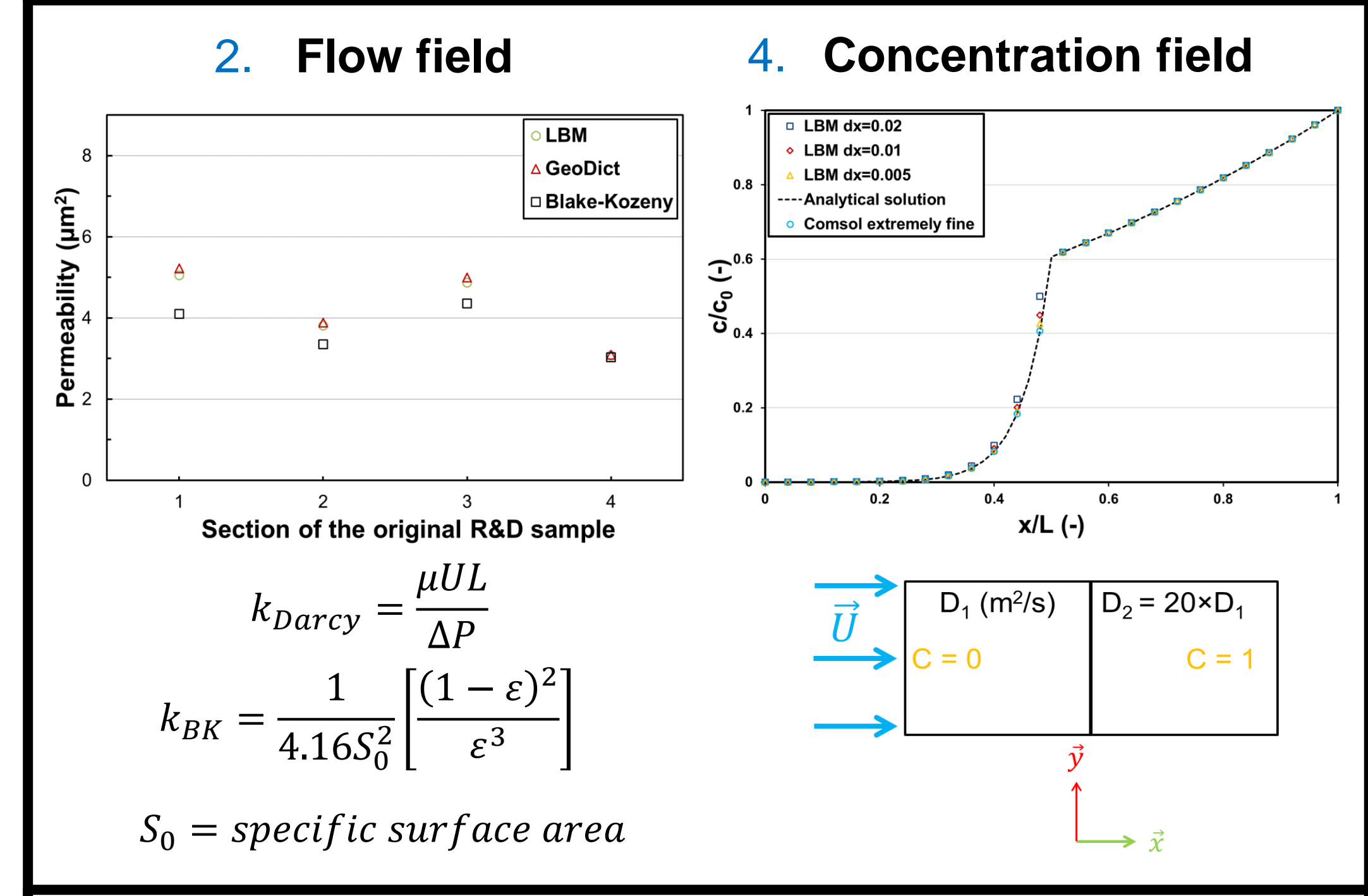
Low coat weight vs. High coat weight

uniform vs. non-uniform

The fluid pathways remain the same from a low to a high coat weight but channel cross-sections are reduced leading to a better capture efficiency

Enhanced channeling results from an increase of coat weight, but largest channels are less efficient at capturing aerosols

9 LBM VERIFICATION



10 CONCLUSIONS

- A uniform catalyst distribution profile provides up to 30% better filtration and 10% better conversion
- Detailed flow field analysis provides good insights in the physical phenomena impacting GPF performance
- The proposed model provides guidelines to GPF manufacturers in search of a simple and controllable way of optimizing the integration of TWC and GPF