Numerical Modeling of Catalytic Particulate Filters in Transient Operation with Multiple Concurrent Reactions

Mohamad Mobin Nurzad Liyasi [1], David Vidal[1], Robert Greiner[2], Martin Votsmeier[2]

[1] URPEI, Department of Mechanical Engineering, Polytechnique Montréal, Montréal, Québec, Canada

[2] UMICORE - Automotive Catalysis Division, Research and Development, Hanau, Germany

GPS Génie par la simulation SBES Simulation - Based Engineering Science

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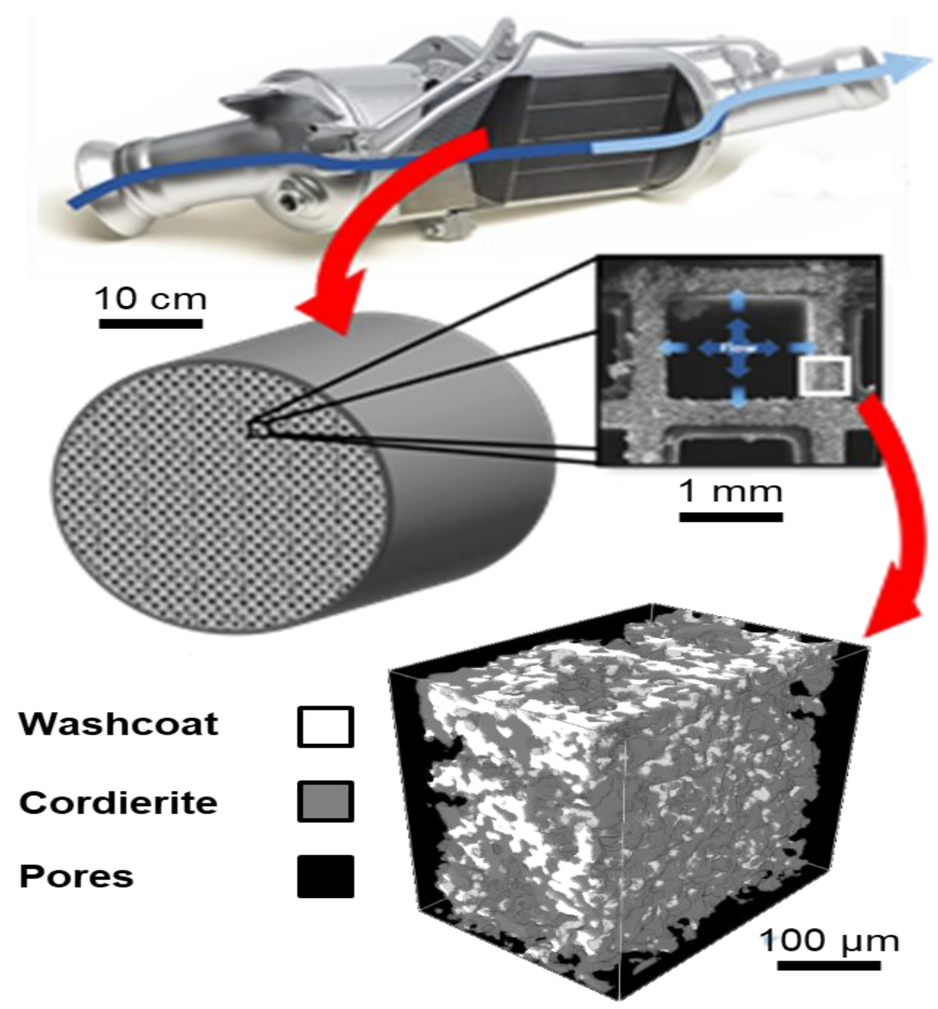
1. CATALYST-COATED PARTICULATE FILTERS



→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**

2. OBJECTIVES

General objective:

✓ **Improving gasoline particulate filters performance through a better catalyst deposition**

Specific objectives:

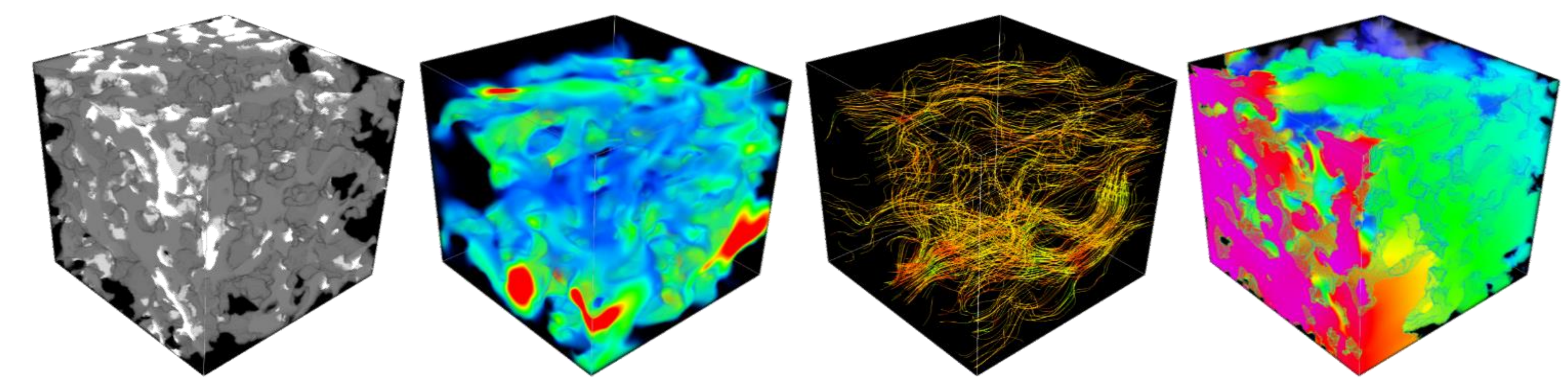
✓ **Develop a numerical model accounting for :**

- ❖ **a complex concurrent reaction scheme**
- ❖ **the transient behavior of exhaust conditions**
- ❖ **various catalyst depositions**

✓ **Study the stability of lattice Boltzmann and finite difference schemes**

✓ **Speed-up computations by porting the numerical scheme onto GPU**

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

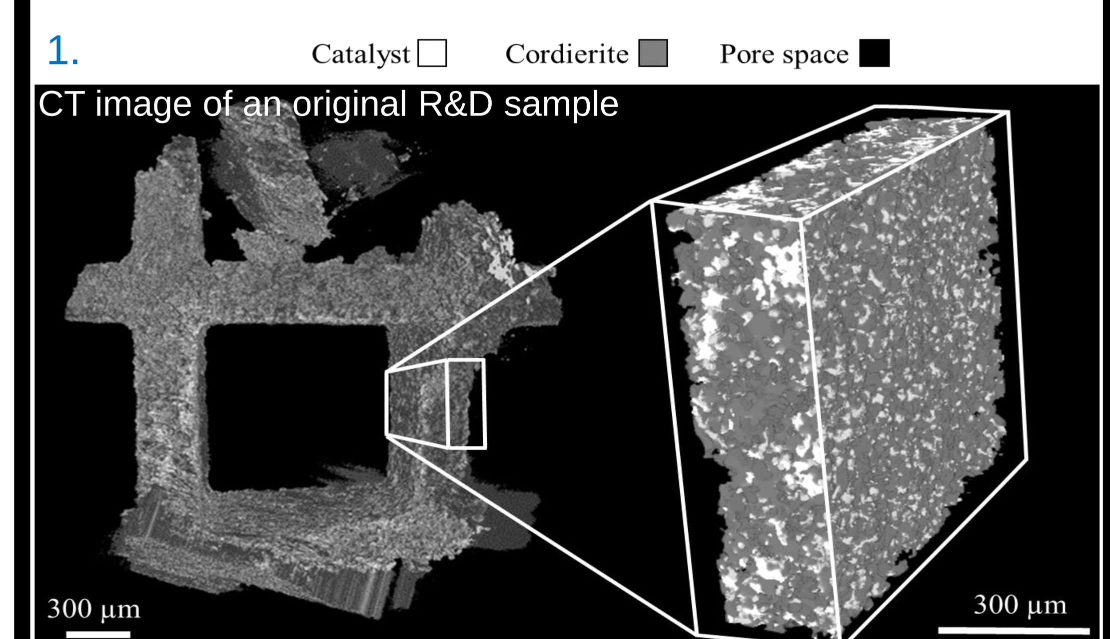
Catalyst coating characterization

Pressure drop | **Capture efficiency** → **Filter quality factor**

Catalyst effectiveness

Best coating deposition profile

1.



2.

External force

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}.\nabla\mathbf{u} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{u} + \mathbf{F}$$

$$\nabla.\mathbf{u} = \mathbf{0}$$

3.

Brownian diffusion

$$m\frac{d\mathbf{v}(t)}{dt} = \frac{3\pi\mu d_p}{C_c}(\mathbf{u}(\mathbf{r}) - \mathbf{v}(t)) + \boldsymbol{\Gamma}(t)$$

4.

Reaction rate

$$\frac{\partial c}{\partial t} + \mathbf{u}.\nabla c = \nabla.(D\nabla c) + r$$

4. THE LATTICE BOLTZMANN METHOD (LBM)

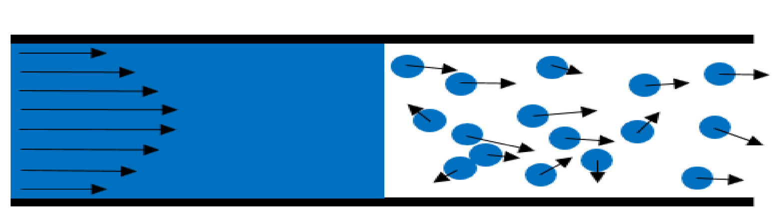
Navier-Stokes Equations
(continuum mechanics)

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = -\frac{1}{\rho}\nabla P + \nu\nabla^2\mathbf{u} + \mathbf{f}$$

$$\nabla\cdot\mathbf{u} = 0$$

Discretization in space & time FEM/FDM/FVM

$$\mathbf{Au} = \mathbf{b} \quad \text{or} \quad \mathbf{u}^{t+\delta_t} = f(\mathbf{u}^t)$$



$\mathbf{u}(\mathbf{x},t)$ $\qquad$ $\mathbf{u} = \frac{1}{\rho}\sum_i f_i\mathbf{e}_i$

Boltzmann Equation
(statistical mechanics)

$$\partial_t f + \mathbf{e}\cdot\nabla f = -\frac{f - f^{eq}}{\tau}$$

Discretization in velocity space ($\mathbf{e}_i$)

$$\partial_t f_i + \mathbf{e_i}\partial_i f_i = -\frac{f_i - f_i^{eq}}{\tau}$$

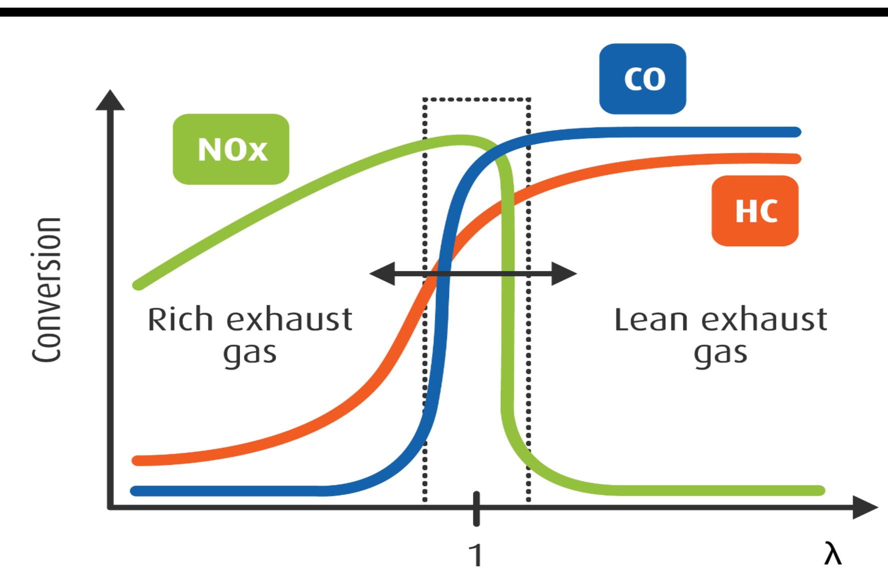
Discretization in time & space by FDM

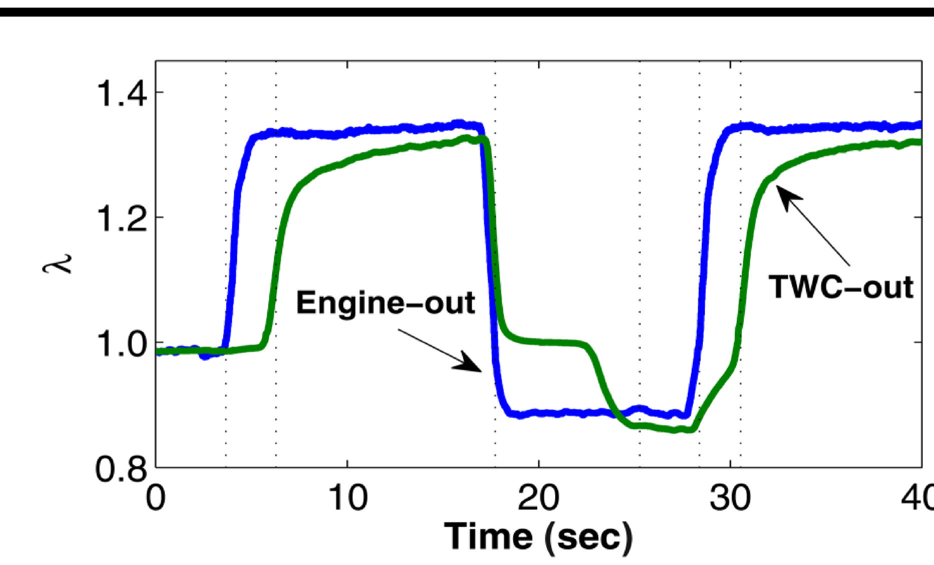
$$f_i(\mathbf{x} + \mathbf{e}_i\delta_t, t + \delta_t) - f_i(\mathbf{x}, t) = -\frac{f_i(\mathbf{x},t) - f_i^{eq}(\mathbf{x},t)}{\tau^*}$$

Integration in the velocity space ($\mathbf{e}_i$)

$$\mathbf{u}(\mathbf{x},t) \leftarrow \mathbf{u} = \frac{1}{\rho}\sum_i f_i\mathbf{e}_i$$

5. PREDICTING THE AIR-FUEL MIXTURE RATIO VARIATION





6. CONCURRENT CATALYST REACTIONS

Oxidation reactions:

- ➢ $C_mH_n + O_2 \rightarrow CO_2(CO) + H_2O$
- ➢ $CO + O_2 \rightarrow CO_2$
- ➢ $O_2 + H_2 \rightarrow H_2O$

H_2 production reactions:

- ➢ $CO + H_2O \rightarrow CO_2 + H2$
- ➢ $C_mH_n + H_2O \rightarrow CO_2 + H_2$

NO_x reduction reactions:

- ➢ $C_mH_n + NO \rightarrow N_2(N_2O, NH_3) + CO_2 + H_2O$
- ➢ $CO + NO \rightarrow CO_2 + N_2(N_2O)$
- ➢ $H_2 + NO \rightarrow N_2(N_2O, NH_3) + H_2O$
- ➢ $NO_x \rightarrow N_2 + O_2$

O_2 storage reaction:

- ➢ $Ce_2O_4 \rightleftharpoons Ce_2O_3 + O_2$

7. UPCOMING STEPS

❖ **Study of the stability of different LBM and FDM schemes for multiple simultaneous reactions**

❖ **Verification and validation of the proposed numerical scheme**

❖ **Implementation of high-performance computing on GPU**

I'm extremely grateful to Igor Belot for his brilliant articles for the part 1,3 pictures.

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d_p : Particle diameter		U : Superficial flow velocity	
D : Diffusion coefficient		C_c : Cunningham correction factor	
v : Particle velocity		c : Concentration	
p : Pressure		ν,μ : Fluid cinematic/dynamic viscosity	
		ρ : Fluid density	

λ : Actual air fuel ratio vs Stoichiometric (ideal) air fuel ratio