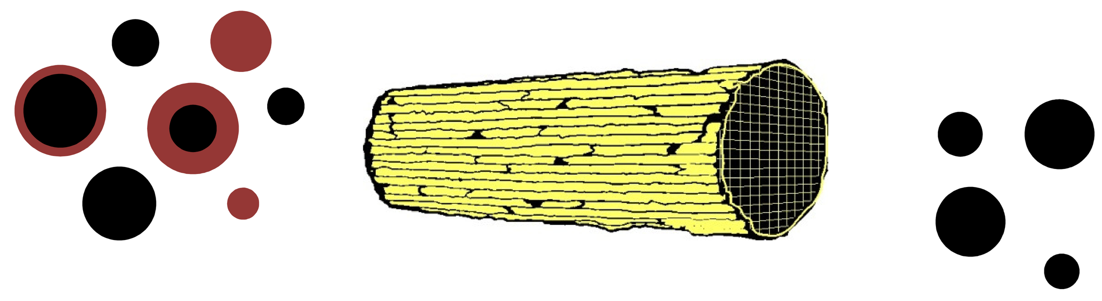
Modeling of Particulate Matter Transformations and Capture Efficiency

Jonas Sjöblom, Ananda Subramani Kannan, Houman Ojagh and Henrik Ström*
Department of Applied Mechanics, Chalmers University of Technology, SE 412 96 Gothenburg, Sweden, *henrik.strom@chalmers.se

Introduction

- Particulate Matter (PM) emission causes problem for human health as well as for the environment
- PN (particle Number) legislation requires wall-flow filters (DPF) and increases fuel consumption
- Detailed understanding of capture related phenomena is necessary to reduce fuel penalty
- The use of open substrates as *in-situ* analyzer for HC content recently presented [1]



$$CE = \frac{PSD_{before} - PSD_{after}}{PSD_{before}}$$

Objectives

- To validate the tanks-in-series model by use of comprehensive simulations
- To assess the HC evaporation process at high flow (real conditions)
- To describe the potential benefits of using open substrates

The Conceptual Model

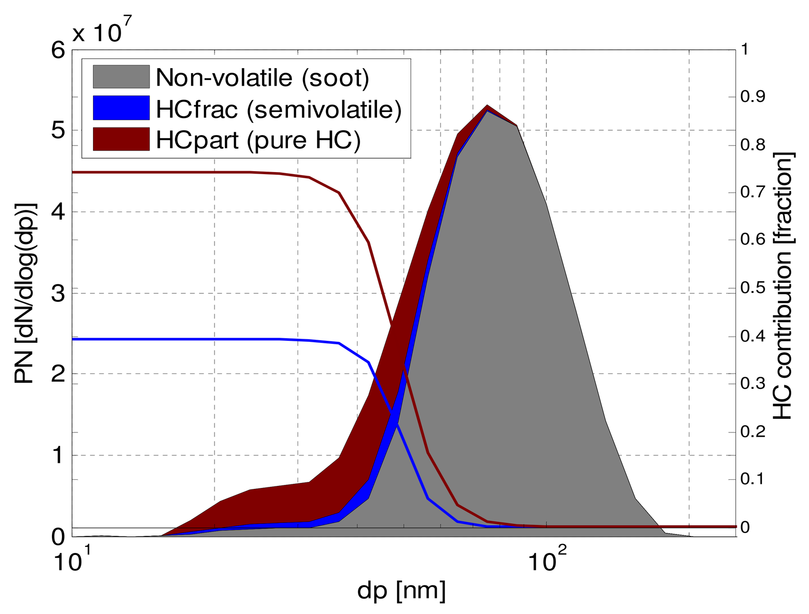
Sigmoid functions to describe HC contents [1]

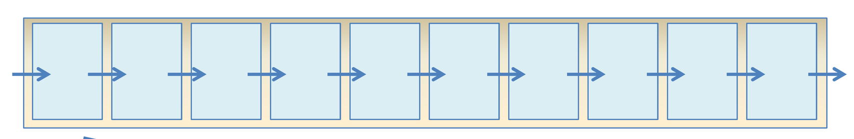
- Pure volatiles and semivolatile HC (solid core)
- Assuming heavy hydrocarbon ($C_{40}H_{82}$)
- 8 adjustable parameters , fitted to experimental data by gradient search method (lsqnonlin)

Simulations at real conditions

- Using same Particle Size Distribution (PSD) as in the validation ("case B4")
- Increasing flow from 0.1 m/s to 10 m/s (Re from 2 to 386)

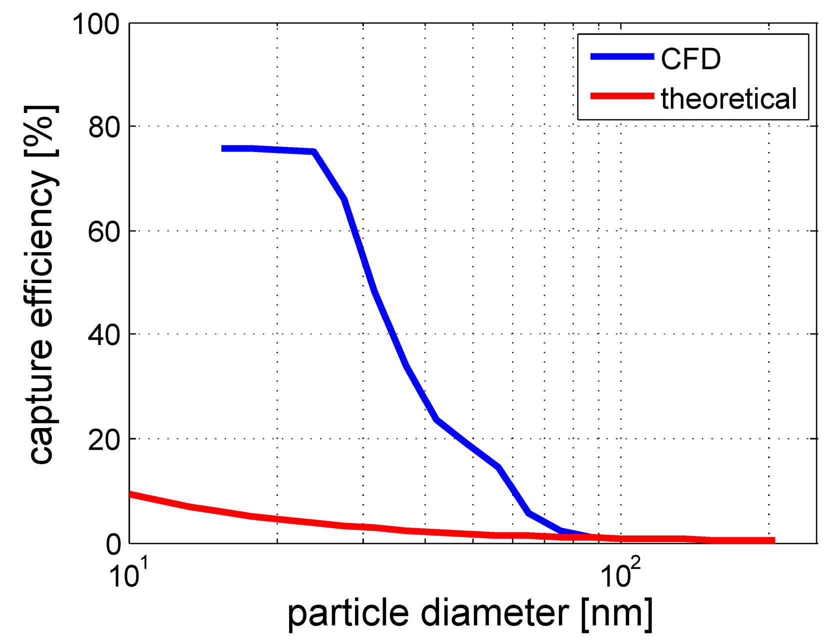
Resulting fitted Particle Size Distribution (PSD)





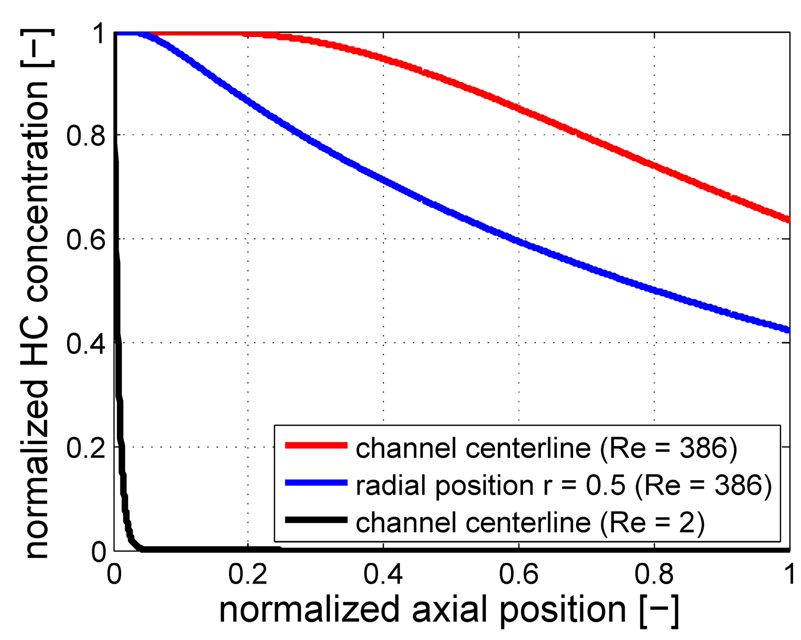
$$CE_{channel} = 1 - PE_{channel} = 1 - e^{-\frac{h_m A_s}{Q}} \Leftarrow h_m = \frac{D_p Sh(D_p)}{d_{ch}}$$

$$\frac{d(d_p)}{dt} = \frac{2M\alpha_c(p_\infty - p_d)}{\rho_p N_A \sqrt{2\pi m k_B T}} \Rightarrow D_p = \frac{k_B T c_C(d_p)}{3\pi\mu d_p}$$



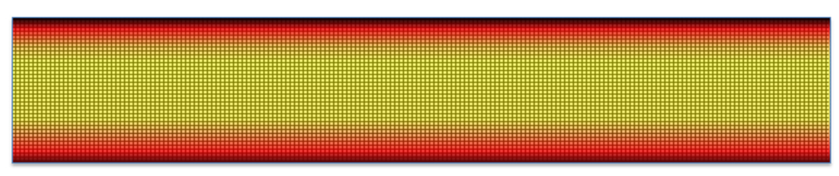
Tanks-in-series model (Matlab)

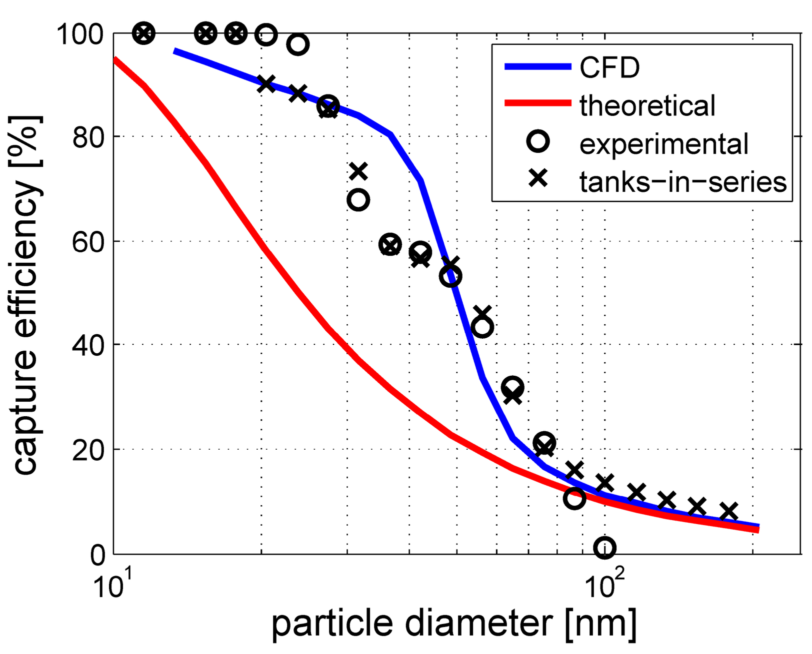
- Evaporation and Shrinkage of PM (residence time divided into 100 time steps), [2]
  assuming $p_\infty = 0$
- Brownian diffusivity [3]
- Using local Sh, $y_{wall} = 0$ [4]
- Penetration efficiency [5]



Validation at low flow (Re = 2)

- CFD simulations show close fit to previous work that HC has time to evaporate
- Almost instantaneous evaporation (not shown)
- Complete HC evaporation enables PM characterization at low flow conditions





CFD modeling validation

- Eulerian-Lagrangian approach (gas-solids)
- Assumptions: Developing flow and concentration fields
- Particle motion: Drag and Brownian motion
- Boundary conditions: HC saturation vapor pressure at inlet, zero at walls
- Implemented in Ansys Fluent 13.0

Results at real conditions

- Capture efficiency high due to high HC content
- Residence time long enough for HC evaporation

Usefulness of methodology

By using a low Re-setup (e.g. case B4) upstream gas phase analyzer, HC characteristics can be obtained. This improves the understanding and assists in the modeling of

- DPF loading and regeneration
- PM-HC effects on DOC performance
- Cold-start phenomena

Experimental

- EATS (Exhaust Aftertreatment System), for details see [6]
- Insulated, inert substrate
- Different temperatures and flows
- This Validation case B4, see [1] :
  - Engine: 5 cyl (2.4 dm^3), diesel fuel (MK1), 1800 rpm, 80 Nm
  - 6 %w/w Alumina coated (5.66" x 6", 400/6 cpsi)
  - PM instrument: DMS 500, $T_{sample\ line}$=75 °C, $P_{instr.}$=0.25 bar, 1dil=4, 2dil=16
  - Substrate: T = 154°C, Flow = 39 slpm, $Re_{channel}$ = 2.0

Conclusions

- Methodology for HC characterization using open substrates is valid
- Useful tool as an *in-situ* analyzer of PM characteristics

References

[1] Sjöblom and Ström, *Ind. Eng. Chem. Res.*, **2013**, 52 (25), 8373-8385
[2] Giechaskiel and Drossinos, SAE Int. J. Engines **2010**, 3 (1), 1140-1151
[3] Einstein, Ann. Phys.-Berlin, **1905**, 17 (8), 549-560
[4] Tronconi and Forzatti, AIChE J., **1992**, 38 (2), 201-210
[5] Johnson and Kittelson, Appl. Catal. B, **1996**, 10 (1-3), 117-137
[6] Sjöblom, Top.Catal., **2013**, 56 (1-8), 287-292