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Growth Dynamics & Microstructure of Soot Deposits in Diesel Particulate Filters

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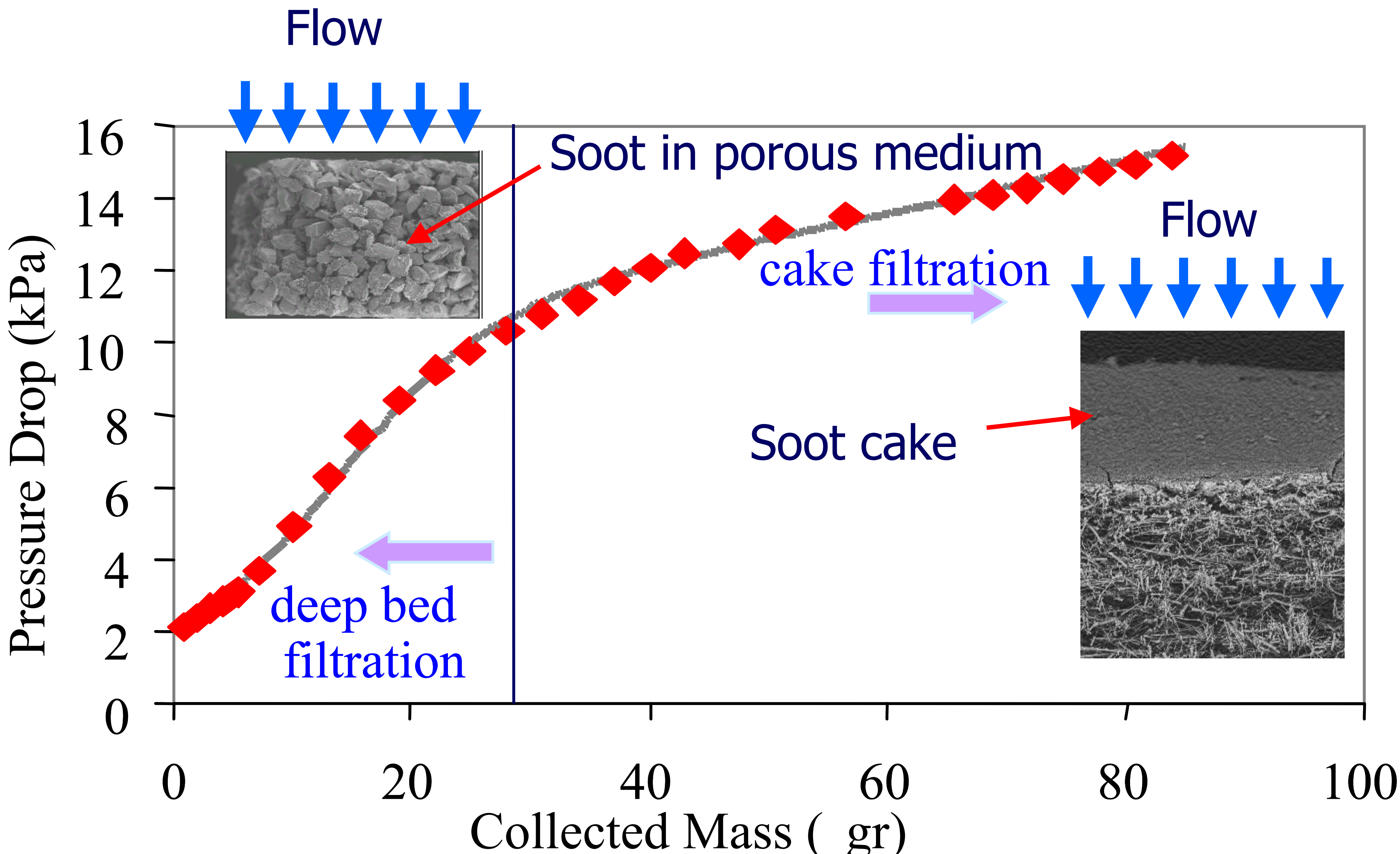
Outline

- Motivation
- Transient filtration model validation for cordierite, SiC, woven, non-woven & gradient porosity filters
- Deposit microstructure vs. Peclet number
- Application to On-Board trap soot load estimation
- Conclusions
- Future outlook

Motivation

- Soot deposit is major contributor to filter ΔP. Need to study its microstructure vs. growth mechanism
- Need reliable soot deposit (and filter) microstructural properties as input for DPF Simulators
- Develop on-board soot sensing methods in conjunction with filter management and control

Dynamics of Particle Deposition in Filters

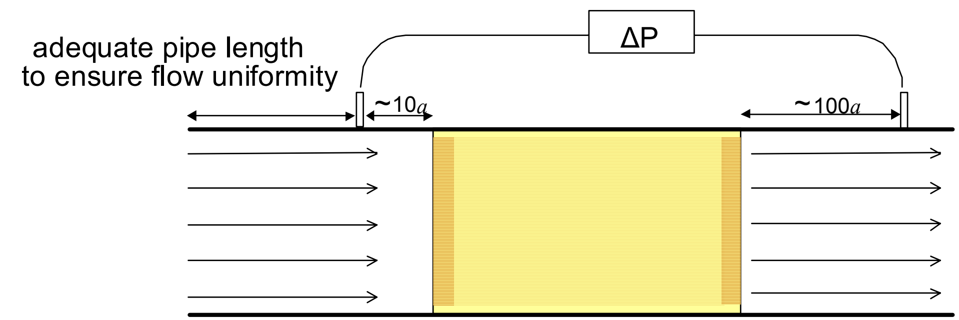


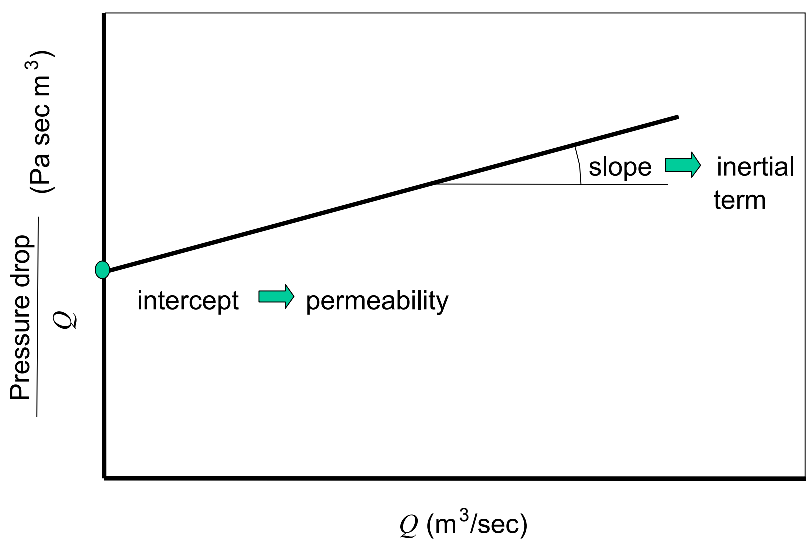
Clean Filter Flow Resistance Desriptors

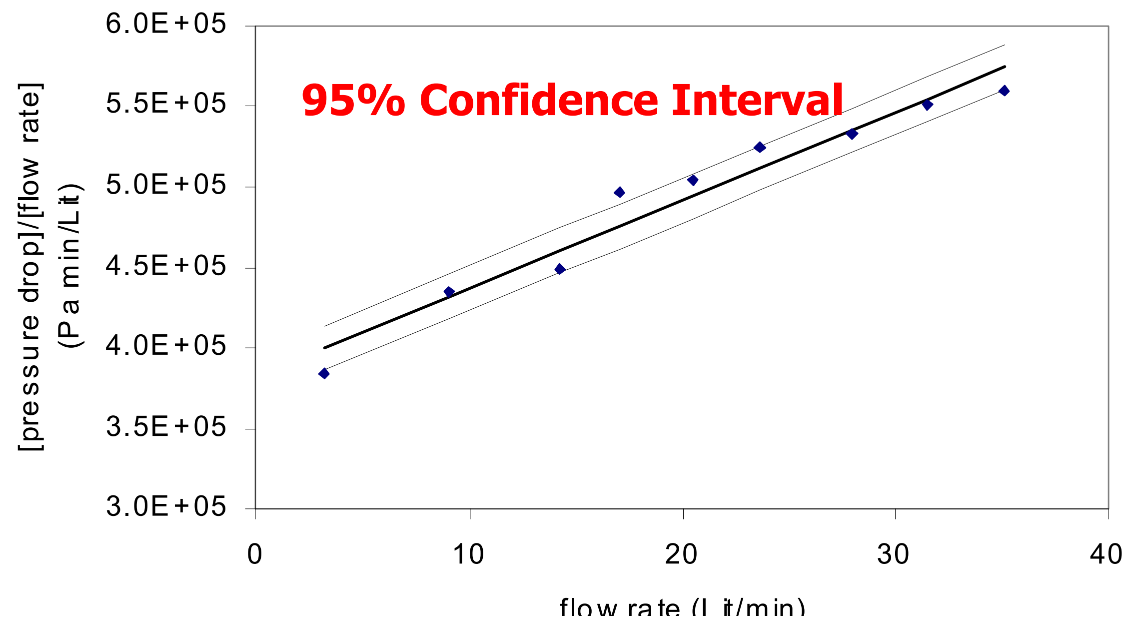
Standardized Measurement Methodology (Konstandopoulos et al. 2002)

$$\Delta P = \frac{\mu Q}{2V_{trap}}(\alpha + w_s)^2\left[\frac{w_s}{k\alpha} + \frac{8FL^2}{3\alpha^4}\right] + \frac{\rho Q^2(\alpha+w_s)^4}{V_{trap}^2\alpha^2}\left[\frac{\beta w_s}{4} + 2\zeta\left(\frac{L}{\alpha}\right)^2\right]$$

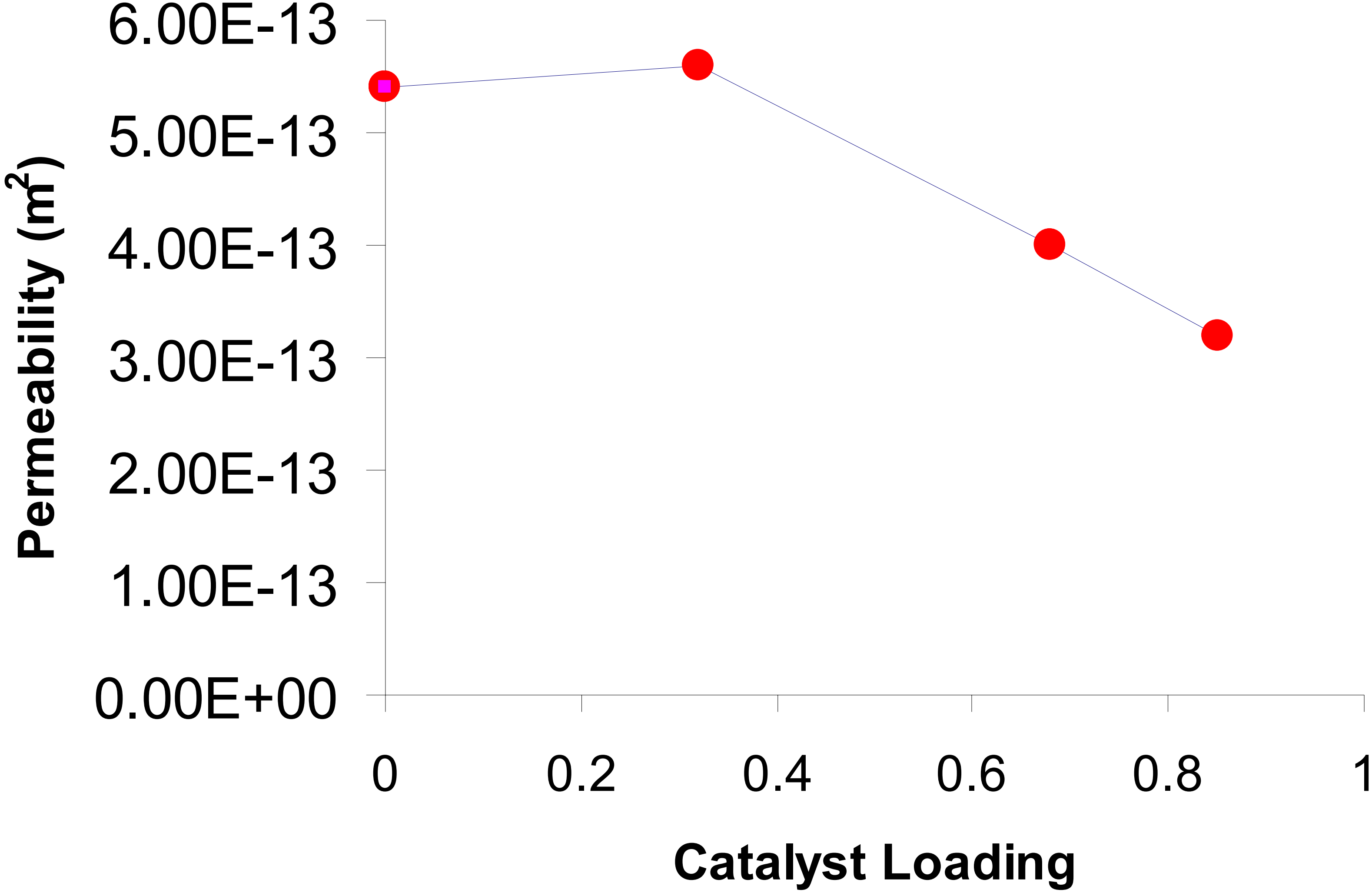
k = ? **ζ = ?**





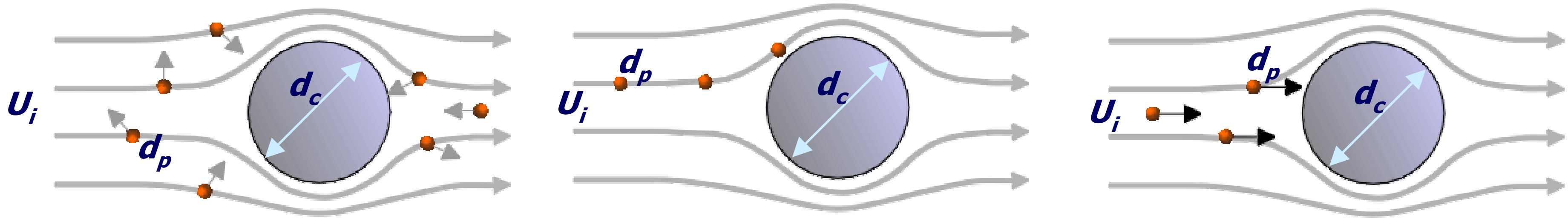


Application to characterize catalyzed DPFs



Filtration mechanisms in extruded DPFs

Brownian diffusion | **interception** | **inertial impaction**



Peclet number

$$Pe = \frac{U_i \cdot d_c}{D_p}$$

Particle diffusion coef.

$$D_p = \frac{k_B \cdot T}{3\pi \cdot \mu \cdot d_p} \cdot SCF$$

"pore" velocity

$$U_i = \frac{u_w}{\varepsilon}$$

Single collector collection efficiency by diffusion

$$\eta_D = 3.5 \cdot g(\varepsilon) \cdot Pe^{-2/3}$$

Interception parameter

$$N_R = \frac{d_p}{d_c}$$

Exponent

$$s = \frac{3 - 2\varepsilon}{3\varepsilon}$$

Single collector collection efficiency by interception

$$\eta_R = 1.5 \cdot N_R^2 \cdot \frac{[g(\varepsilon)]^3}{(1 + N_R)^s}$$

Single grain combined collection efficiency

$$\eta = \eta_D + \eta_R - \eta_D \cdot \eta_R$$

Lee and Gieseke (1978)
Konstandopoulos and Johnson (1989)

Filtration mechanisms in fibrous DPFs

Single collector collection efficiency by diffusion

$$\eta_D = 2.7 \cdot Pe^{-\frac{2}{3}} \left(1 + 0.39 \cdot h(\varepsilon, Kn)^{-\frac{1}{3}} \cdot Pe^{\frac{1}{3}} \cdot Kn \right) + 0.624 \cdot Pe^{-1}$$

Single collector collection efficiency by interception

$$\eta_R = \frac{1}{2h(\varepsilon, Kn)} \left[\frac{1}{(1+N_R)} - (1+N_R) + 2(1+N_R)\ln(1+N_R) + 2.86 \cdot Kn \frac{(2+N_R)N_R}{(1+N_R)} \right]$$

Single collector collection efficiency by inertial impaction

$$\eta_I = 0.16 \left[N_R + \left(\tfrac{1}{2} + \tfrac{4}{5} N_R \right) Stk - 0.105 \cdot N_R \cdot Stk^2 \right]$$

$$Stk = \rho_p \cdot d_p^2 \cdot U_i / (18 \mu \cdot d_f) \cdot SCF$$

$$SCF = 1 + Kn \cdot (1.257 + 0.4 e^{\frac{-1.1}{Kn}})$$

Interaction term Diffusion and Interception

$$\eta_{DR} = \frac{1.24 \cdot N_R^{\frac{2}{3}}}{\sqrt{h(\varepsilon, Kn) \cdot Pe}}$$

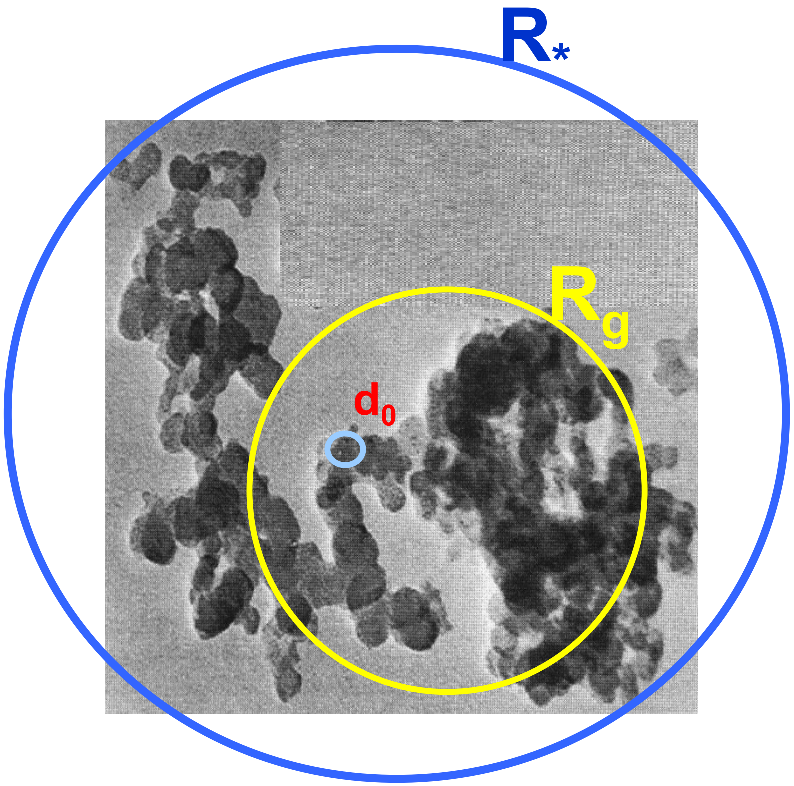
Single fiber combined collection efficiency

$$\eta = \eta_D + \eta_R + \eta_I + \eta_{DR}$$

Kirsch and Stechina(1978)
Vlachos et al (2002)

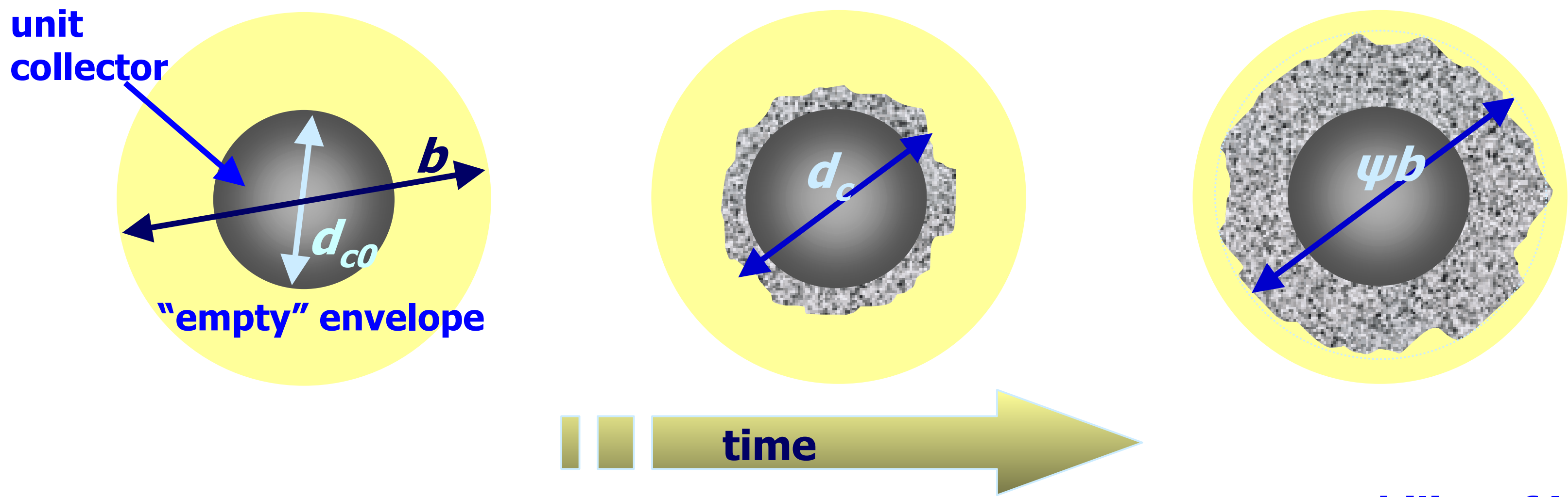
Interception diameter of fractal aggregates

- Mobility diameter correlates with radius of gyration R_g
- For modelling particle capture by interception, a larger particle size is needed
- Better to consider sphere that is inscribed by the fractal aggregate
- Interception N_R parameter modified to account for this.



Transient filtration model : Unit cell/collector concept

Clean unit cell | **Partially loaded unit cell** | **Completely loaded unit cell**



Clean collector diameter

$$d_{c_0} = \frac{3}{2} \cdot \frac{(1-\varepsilon_0)}{\varepsilon_0} \cdot d_{pore}$$

Loaded collector diameter

$$d_c(t) = 2 \cdot \left[\frac{3}{4\pi} \cdot \frac{m_c(t)}{\rho_{soot,w}} + \left(\frac{d_{c_0}}{2} \right)^3 \right]^{1/3}$$

Permeability of loaded medium

$$\frac{k(t)}{k_0} = \left(\frac{d_c(t)}{d_{c_0}} \right)^2 \cdot \frac{f(\varepsilon(t))}{f(\varepsilon_0)}$$

Clean unit cell diameter

$$\frac{d_{c_0}^3}{b^3} = (1-\varepsilon_0)$$

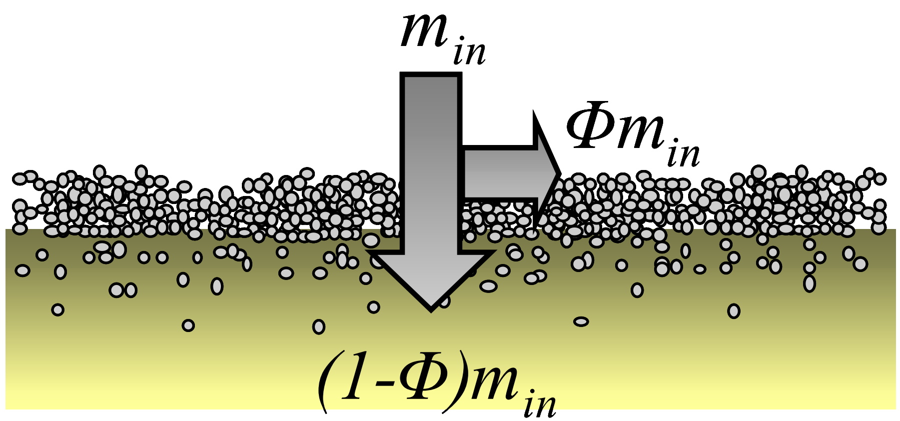
Loaded porosity

$$\varepsilon(t) = 1 - \left(\frac{d_c(t)}{d_{c_0}} \right)^3 \cdot (1-\varepsilon_0)$$

Konstandopoulos et al (2000)

Deep Bed filtration to cake filtration transition

Distribution of particulate mass deposited in the filter



d_{c0}	diameter of clean unit collector
d_c :	diameter of loaded unit collector
b :	diameter of unit cell
ε_0 :	clean filter wall porosity
ε:	loaded filter wall porosity
m_c	particulate mass deposited on unit collector
ψ:	dimensionless percolation constant
Φ :	particulate mass partition coefficient
$\rho_{soot,w}$:	particulate density inside filter wall

Partition coefficient

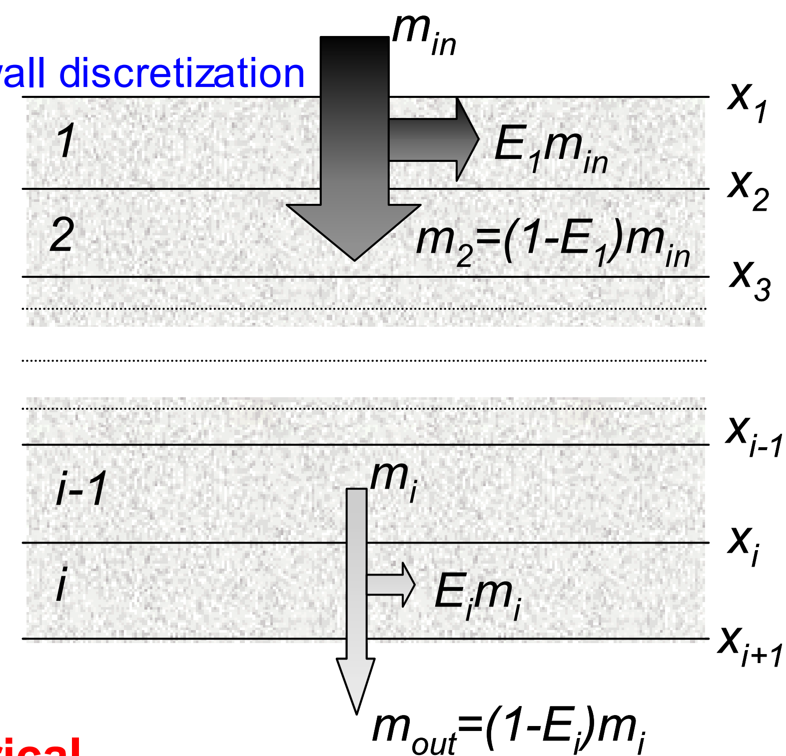
$$\Phi(t) = \left(\frac{(d_c(1,t))^2 - d_{c_0}^2}{(\psi \cdot b)^2 - d_{c_0}^2} \right)$$ **Spherical**

$$\Phi(t) = \left(\frac{(d_c(1,t)) - d_{c_0}}{(\psi \cdot b) - d_{c_0}} \right)$$ **Cylindrical**

Konstandopoulos et al (2000, 2002)

Transient filtration numerical algorithm-1

Filter wall discretization



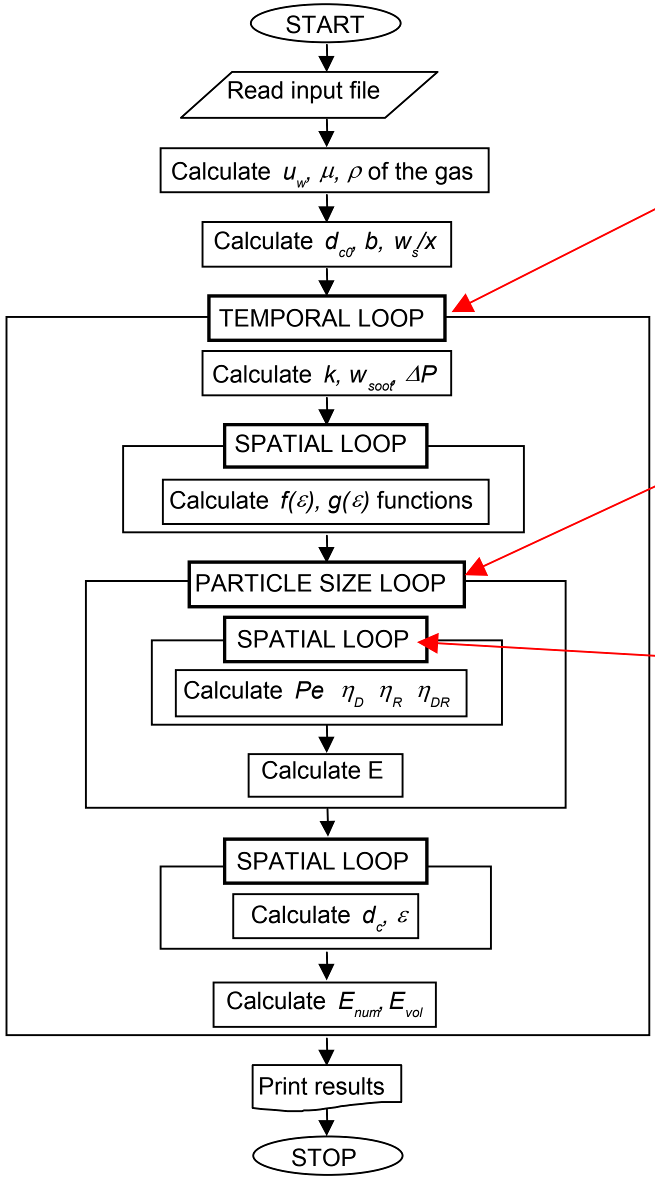
Particulate mass transport equations

$$\frac{\partial \dot{m}_p}{\partial x}+\frac{\partial m_c}{\partial t}=0 \qquad \frac{\partial \dot{m}_p}{\partial x}=-e_f(m_c)\dot{m}_p$$

Local collection efficiency

$$E(i,t)=\int_{x_i}^{x_{i+1}} e_f(m_c(x,t))dx=\begin{cases} 1-\exp\left[-\dfrac{3\eta(i,t)\cdot(1-\varepsilon(i,t))\cdot(x_{i+1}-x_i)}{2\varepsilon(i,t)d_c(i,t)}\right] & \textbf{Spherical} \\ \\ 1-\exp\left[-\dfrac{4\eta(i,t)\cdot(1-\varepsilon(i,t))\cdot(x_{i+1}-x_i)}{\pi\varepsilon(i,t)d_c(i,t)}\right] & \textbf{Cylindrical} \end{cases}$$

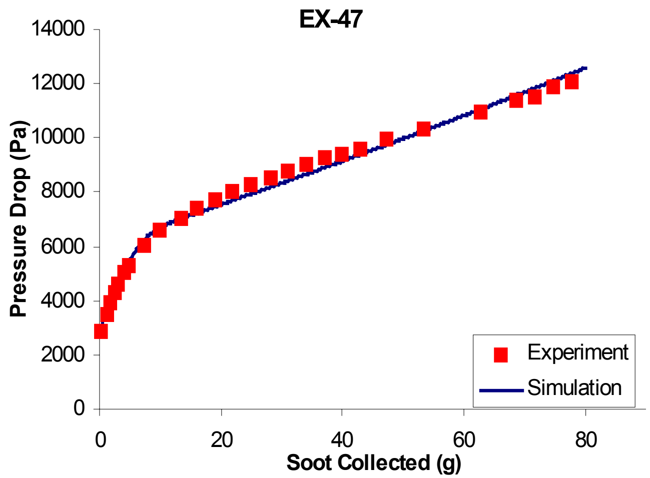
Transient filtration numerical algorithm-2

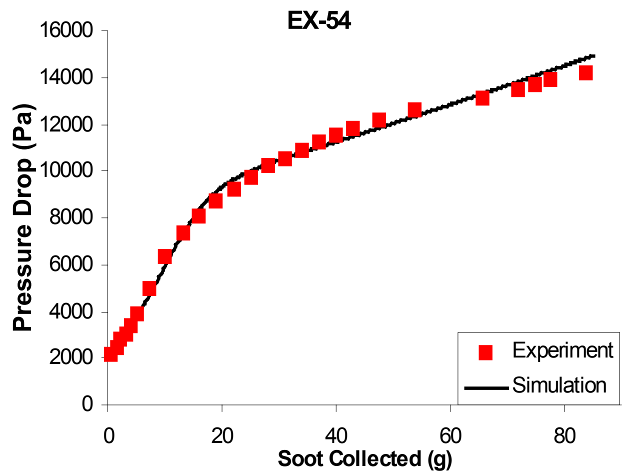


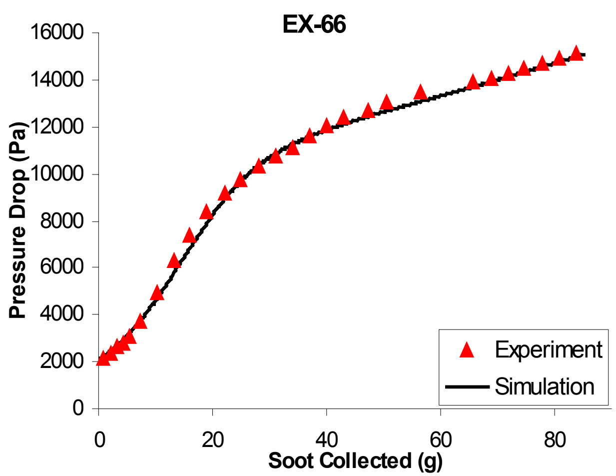
- **Temporal loop: repeat inner loops, recalculating collector properties as particulate matter accumulates in the layers.**
- **Particle size loop: calculate collected mass from each layer for given time-step.**
- **Inner spatial loop: calculation of flow parameters, unit collector properties and E for each layer.**

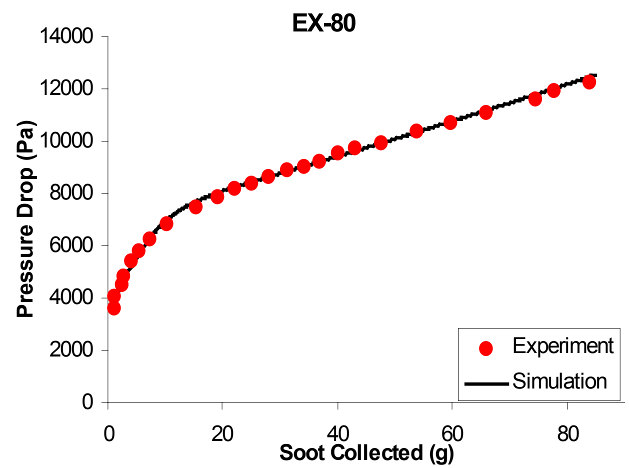
Transient Loading Model Validation

Cordierite Filters (Exper. Murtagh et al. 1994)



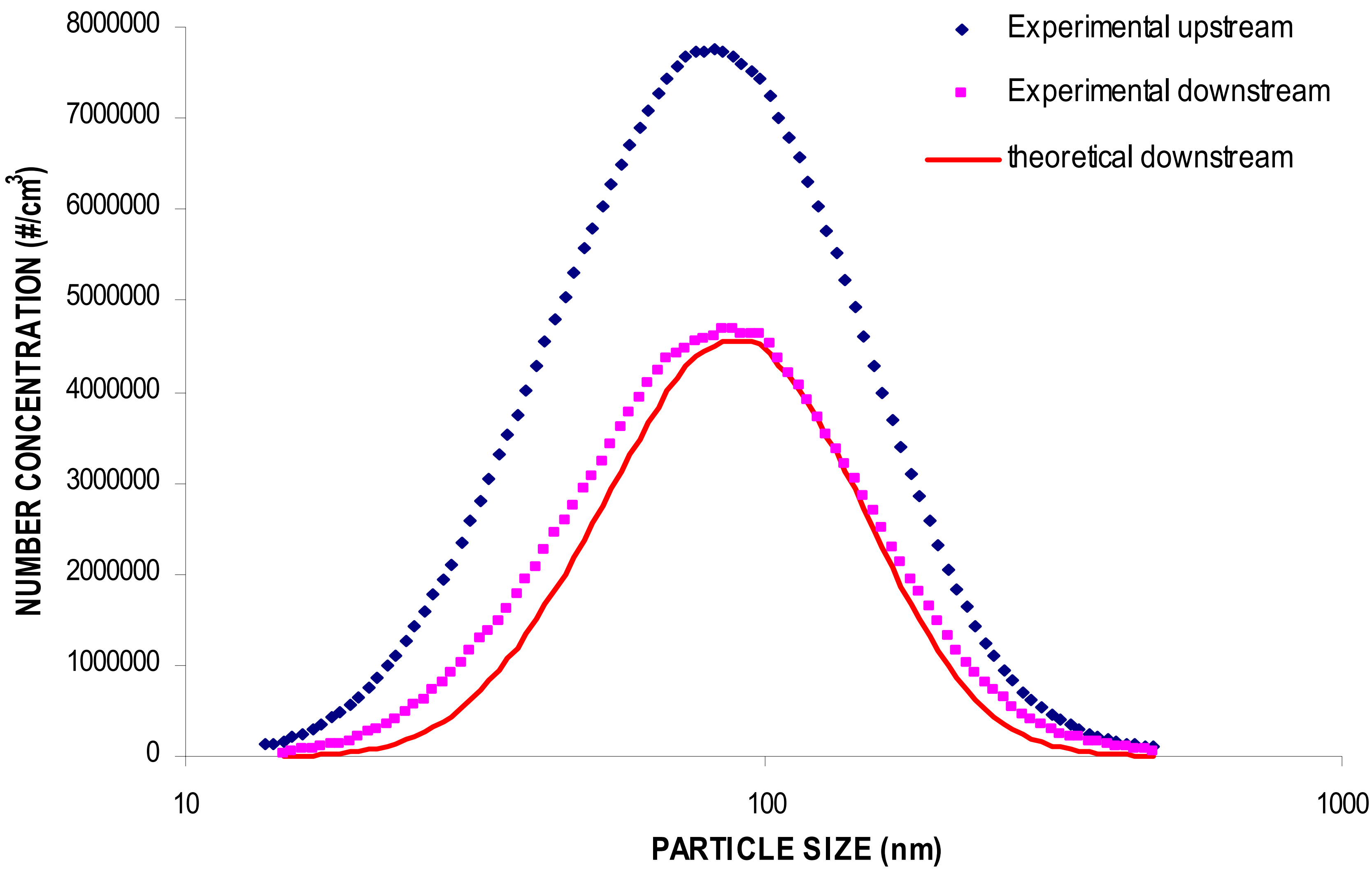




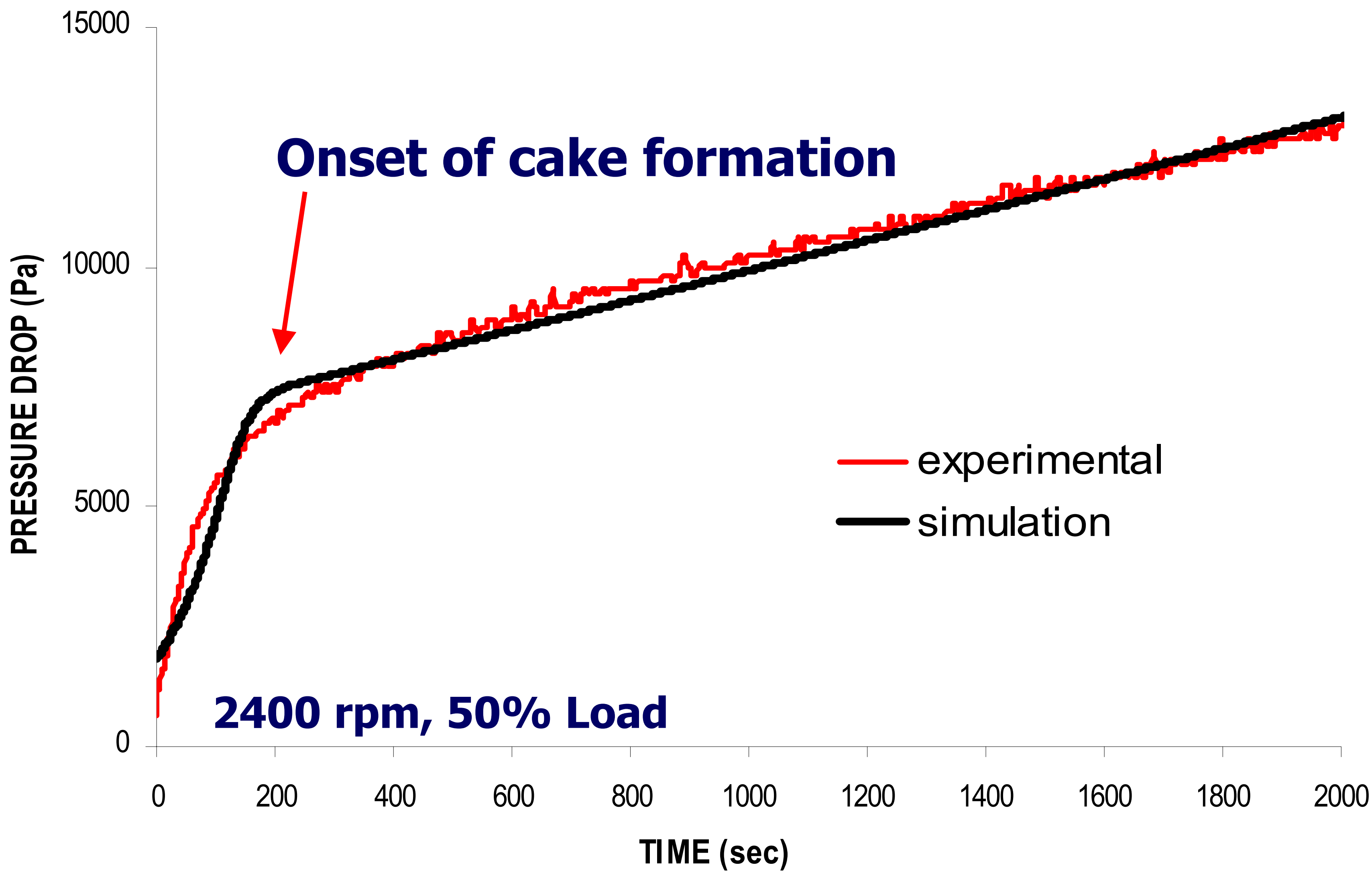


Konstandopoulos et al 1999

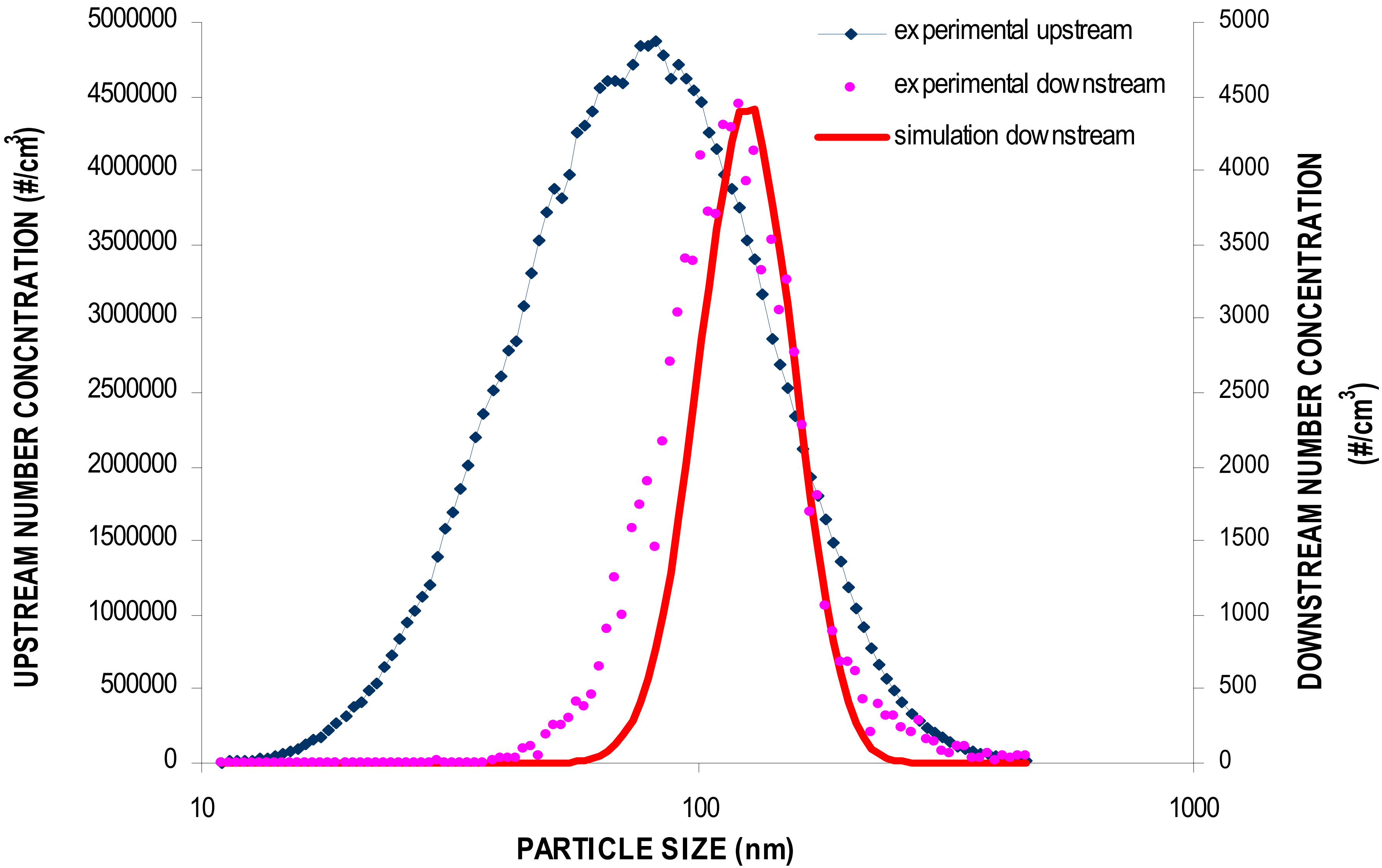
Cordierite wall-flow DPF – collection efficiency



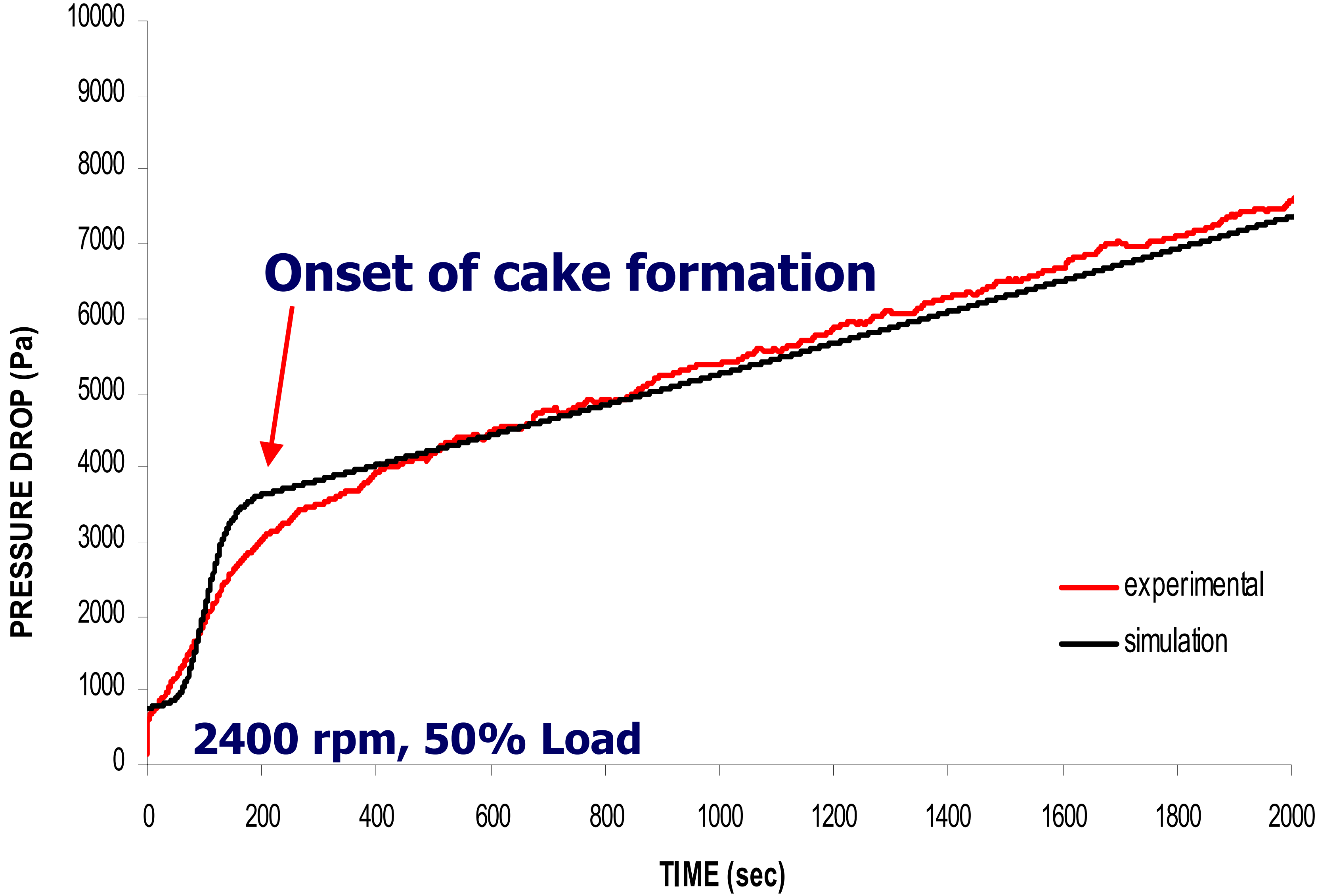
Cordierite wall-flow DPF – transient pressure drop



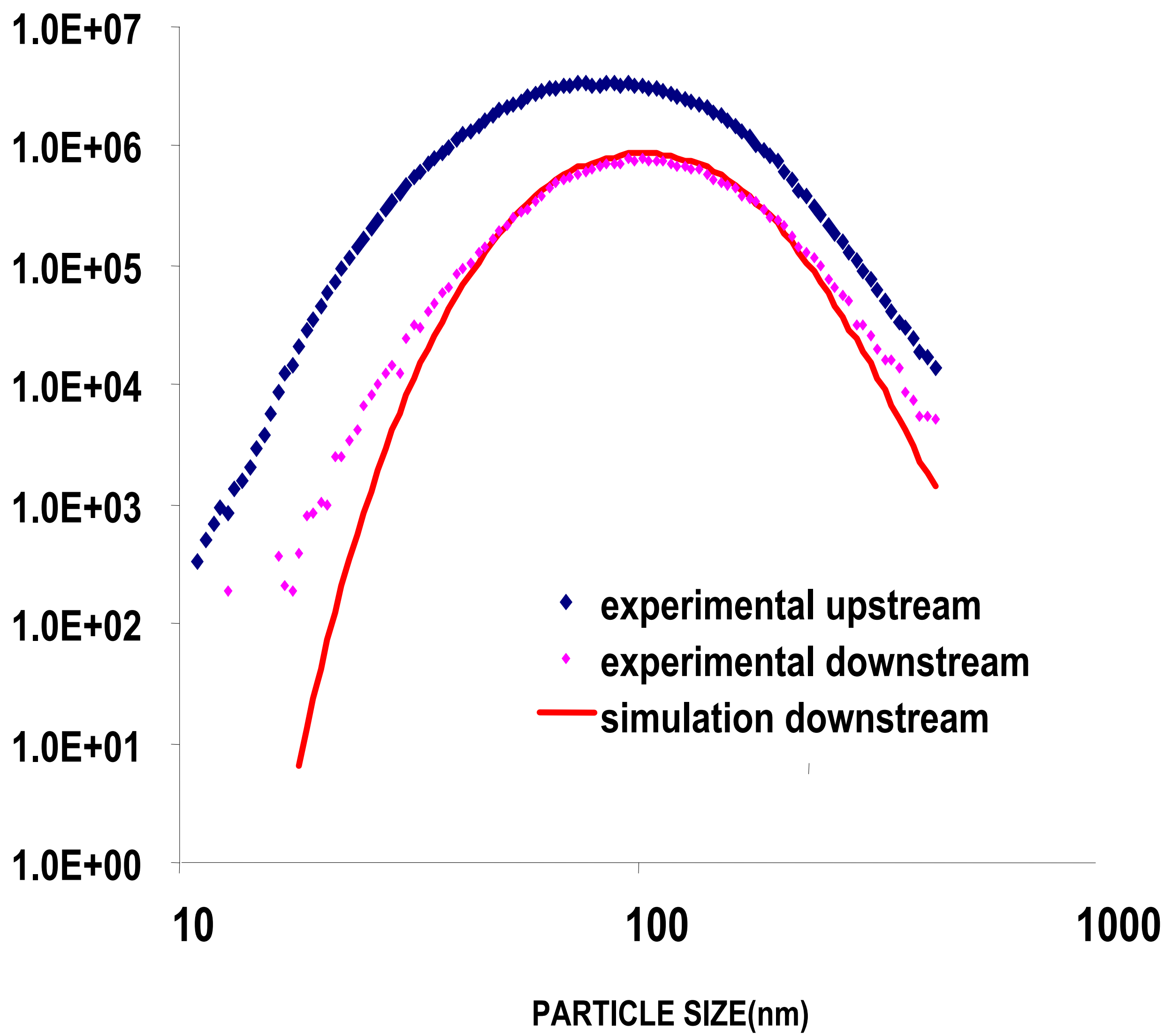
Silicon carbide DPF – collection efficiency



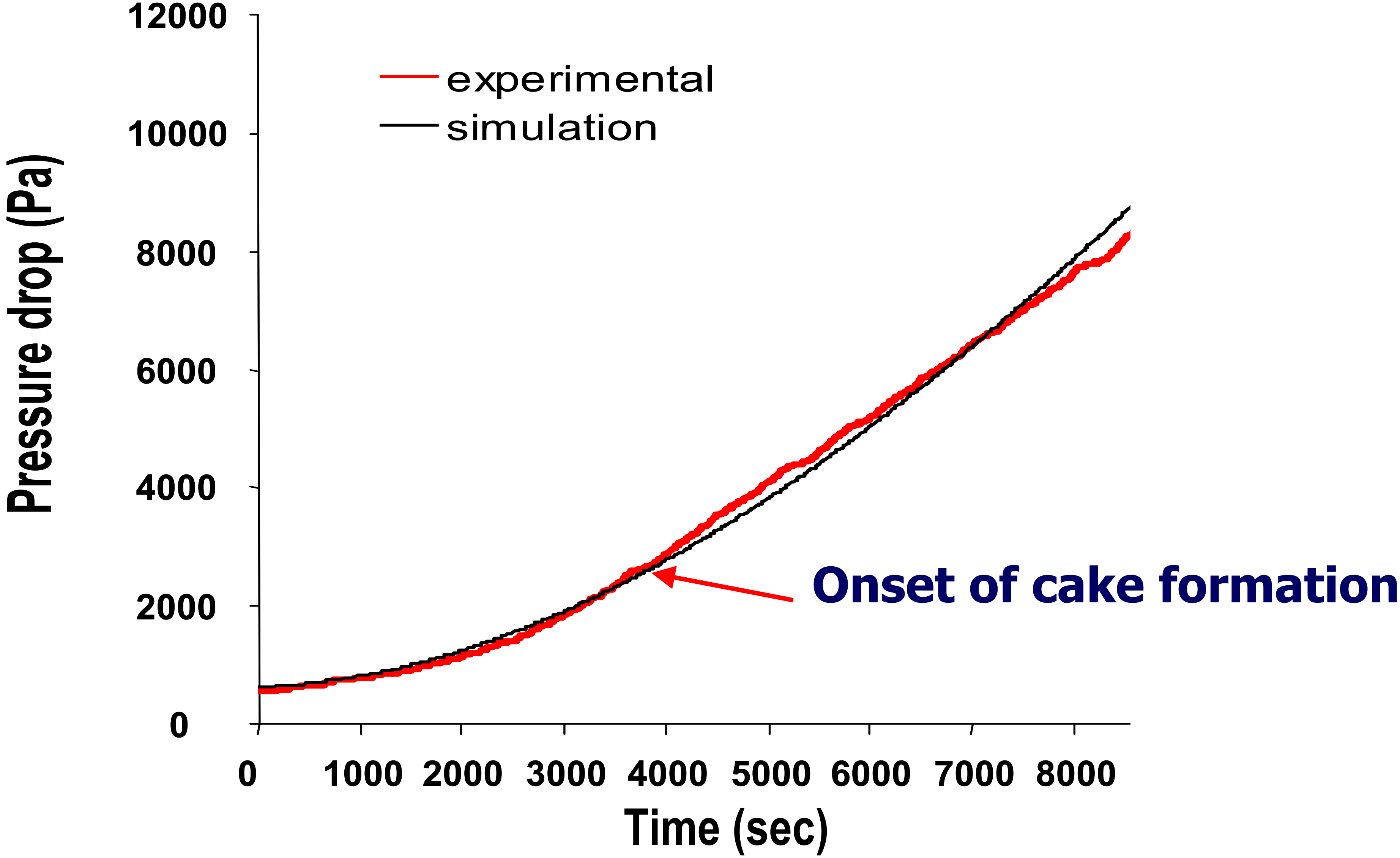
Silicon carbide DPF – transient pressure drop



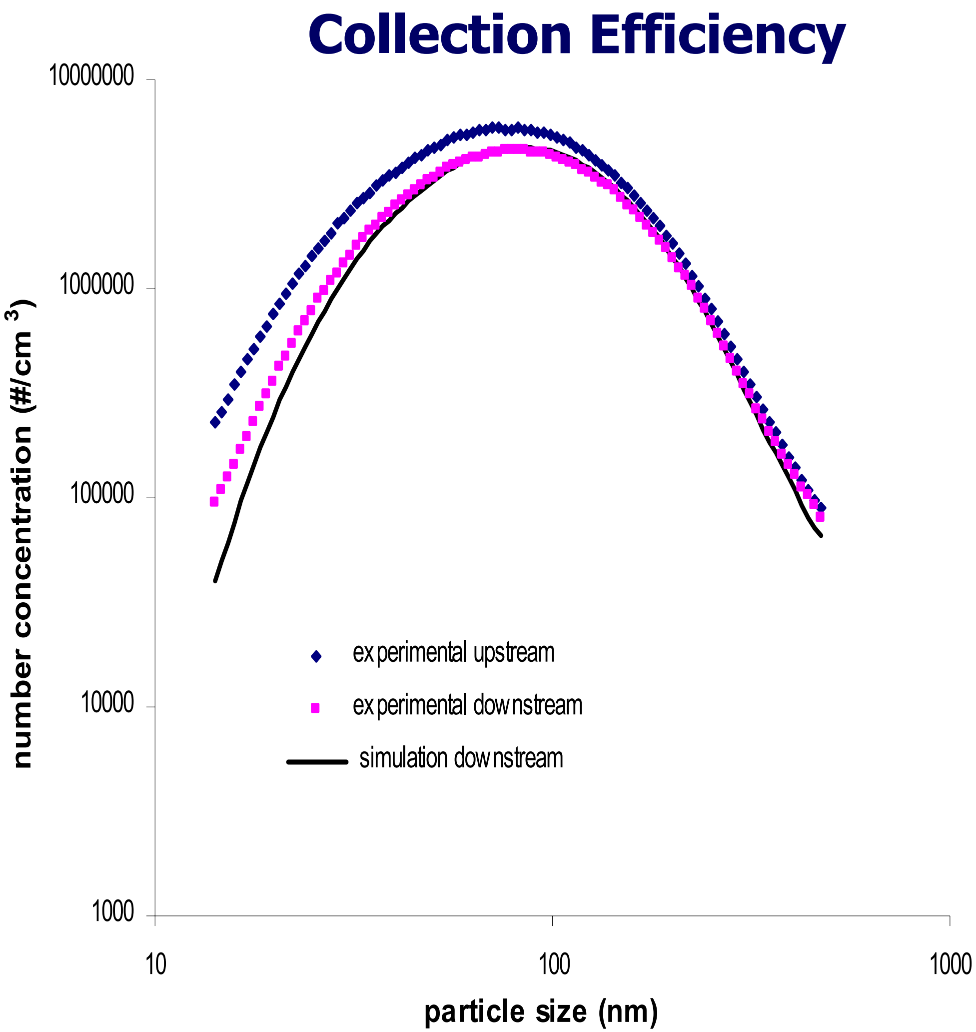
Fibrous filters – woven fiber filter collection efficiency

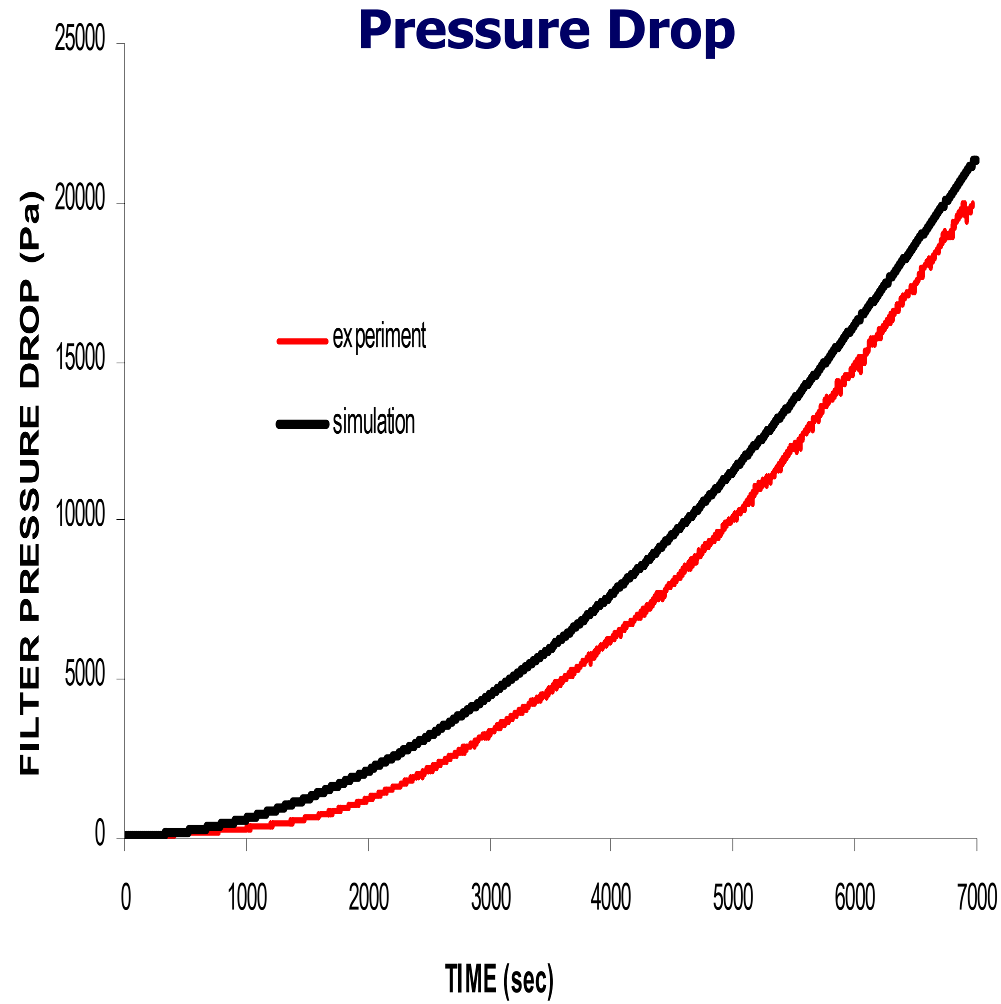


Fibrous filters – woven fiber filter pressure drop



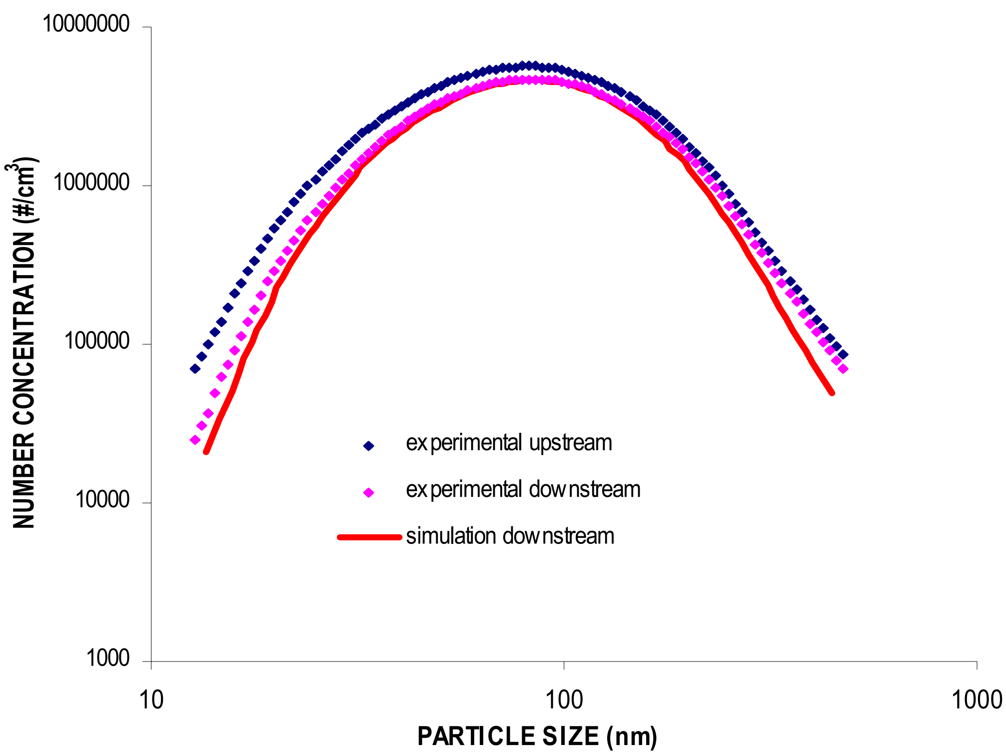
Fibrous filters – non-woven fiber filter



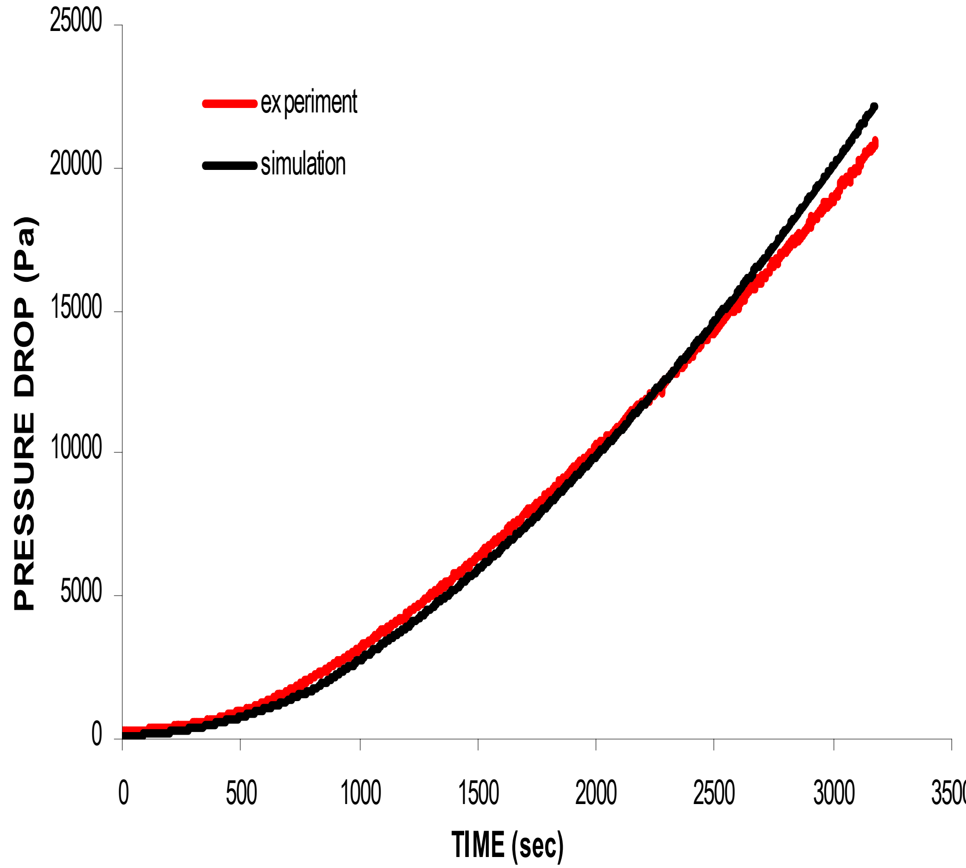


Fibrous filters – gradient porosity filter

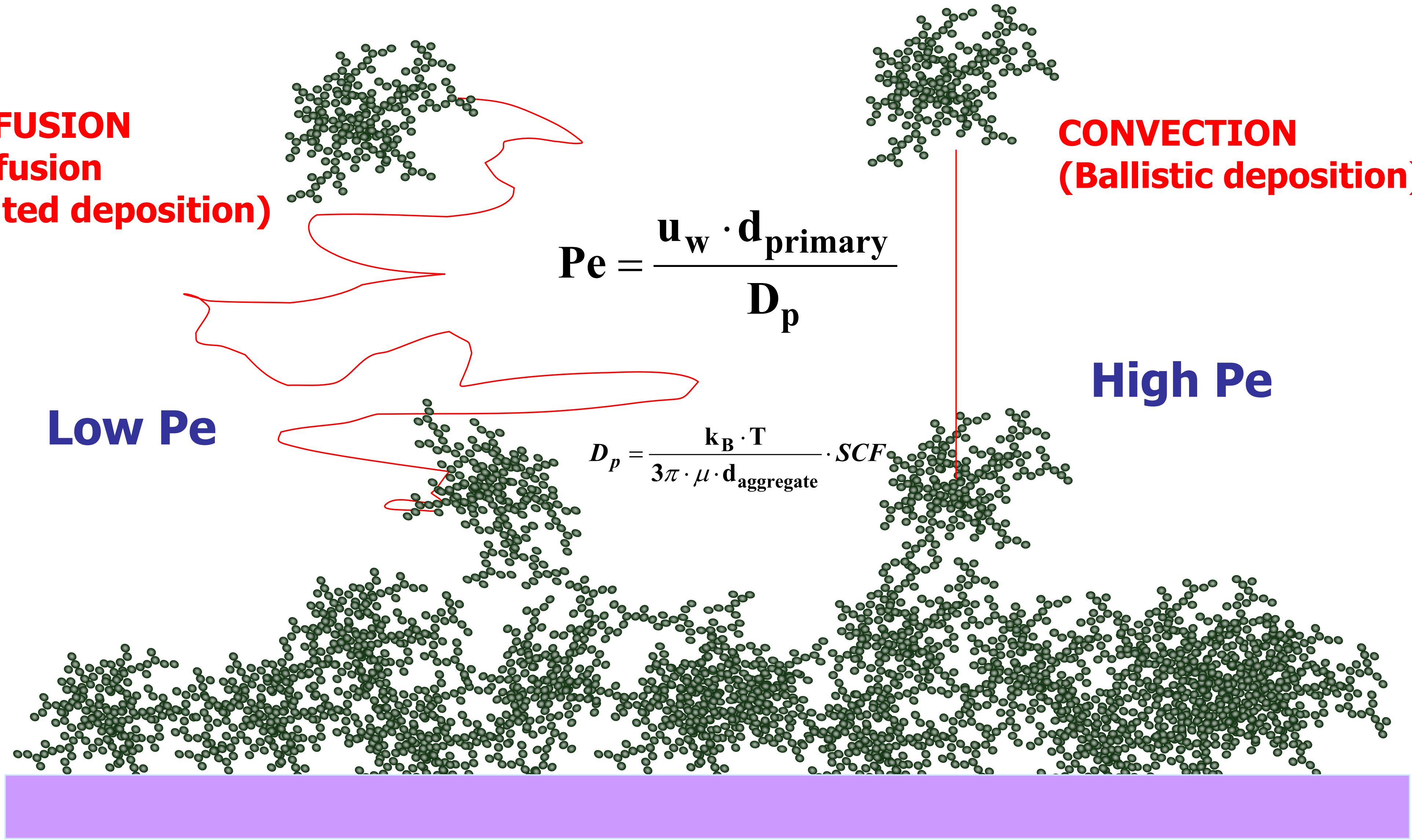
Collection Efficiency



Pressure Drop



Soot Cake Formation Mechanism

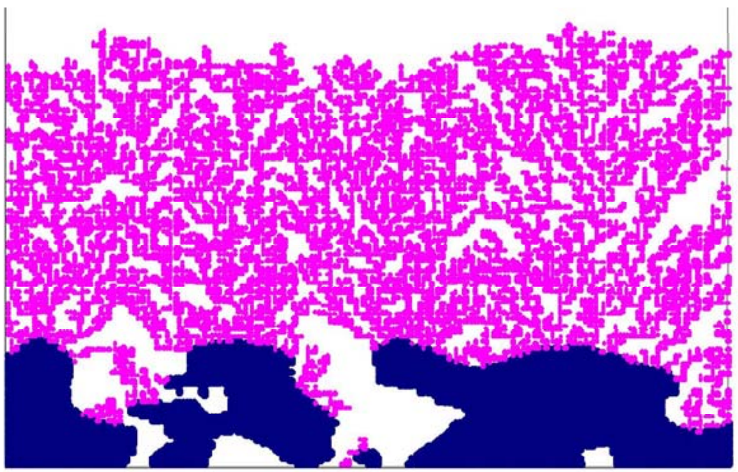


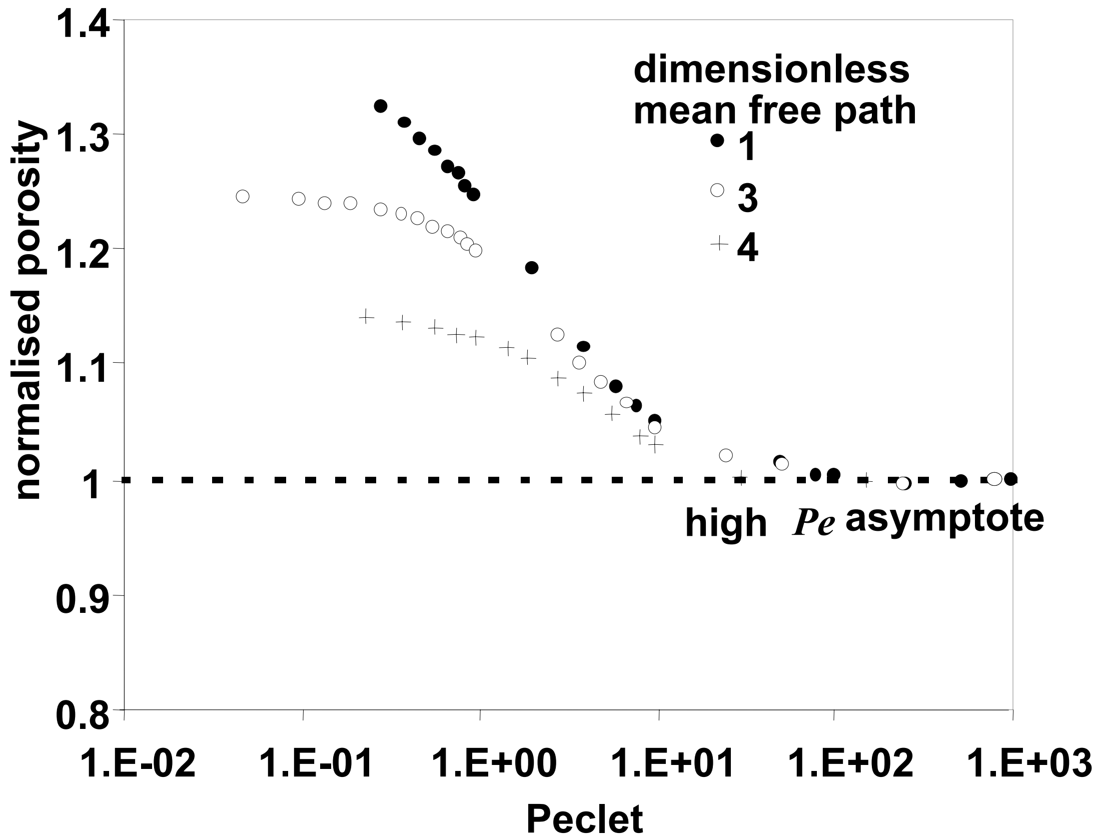
$$Pe = \frac{u_w \cdot d_{primary}}{D_p}$$

$$D_p = \frac{k_B \cdot T}{3\pi \cdot \mu \cdot d_{aggregate}} \cdot SCF$$

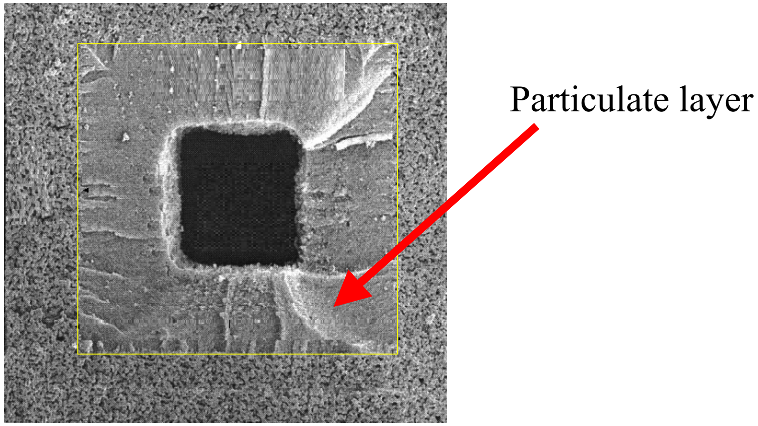
Discrete Particle Dynamics Simulation

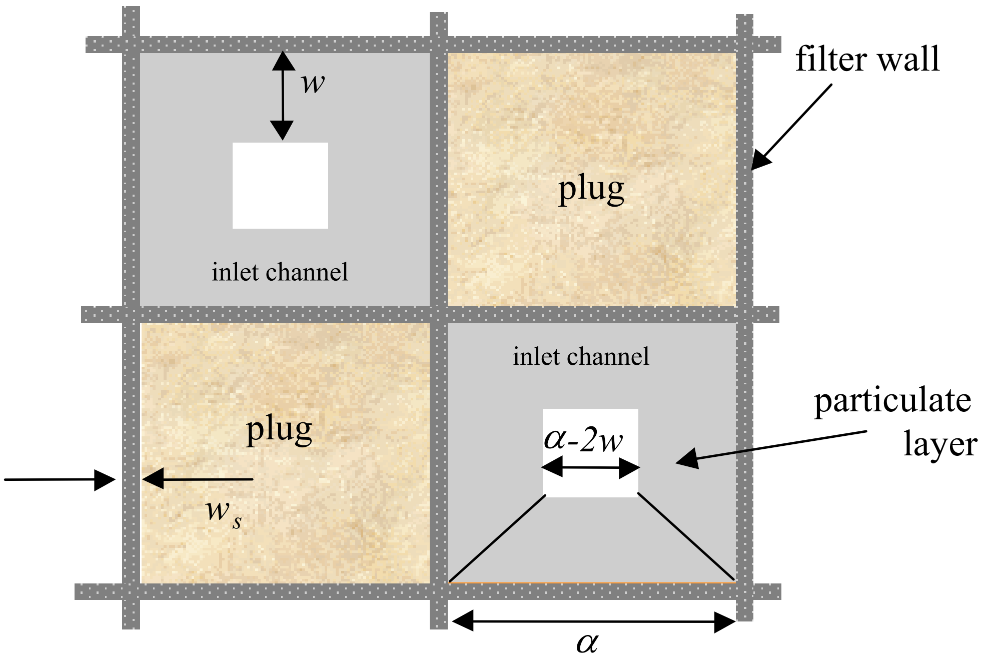
[Tassopoulos, 1991, Konstandopoulos, 1991].





Pressure Drop of Cake Wall Flow Filters-1

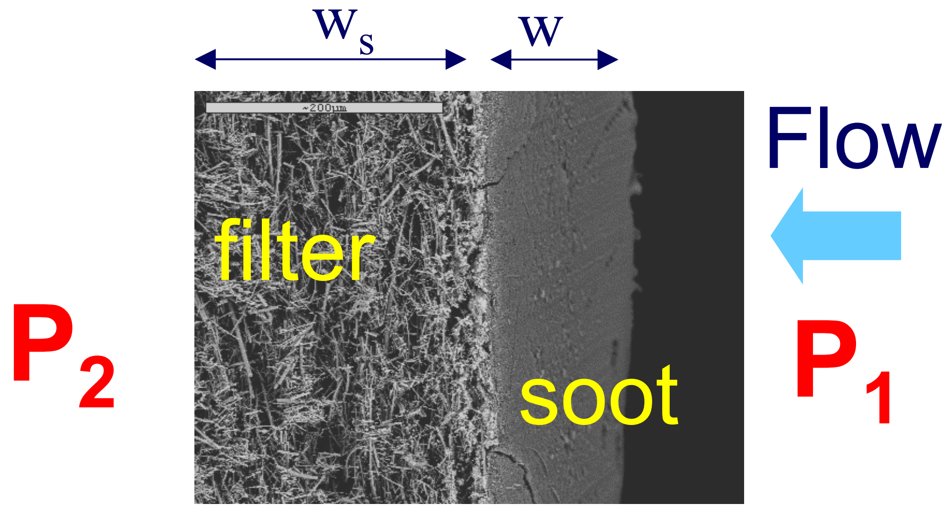




- m_{soot} : particulate mass collected in DPF
- N_{cells} : number of inlet cells of wall-flow filter
- σ: cell density
- Q : exhaust volumetric flow rate
- V_{trap} : filter volume
- L : filter length
- a: channel width
- w : particulate layer thickness
- w_s : filter wall thickness
- k_0 : filter wall permeability
- k_{soot} : particulate layer permeability
- $\rho_{soot,\,c}$: particulate packing density in cake deposit
- μ : exhaust dynamic viscosity
- F : factor equal to 28.454
- l_p : plug length
- β: Forchheimer losses coefficient
- ζ: contraction/expansion losses coefficient
- ρ: air density

Pressure Drop of Cake Wall Flow Filters-2

Konstandopoulos et al. 1989-2001



$$\Delta P_{loaded} = \frac{\mu Q}{2V_{trap}}(a + w_s)^2 \left[\frac{w_s}{k_o a} + \frac{1}{2k_{soot}} ln\left(\frac{a}{a-2w}\right) + \frac{4FL^2}{3}\left(\frac{1}{(a-2w)^4} + \frac{1}{a^4}\right) + \frac{4L_p^2}{a^4} \right] + \frac{Q^2}{4V_{trap}^2}(a+w_s)^4 \beta\rho \frac{w_s}{a^2} + \frac{1}{2}\zeta\rho u_{inlet}^2$$

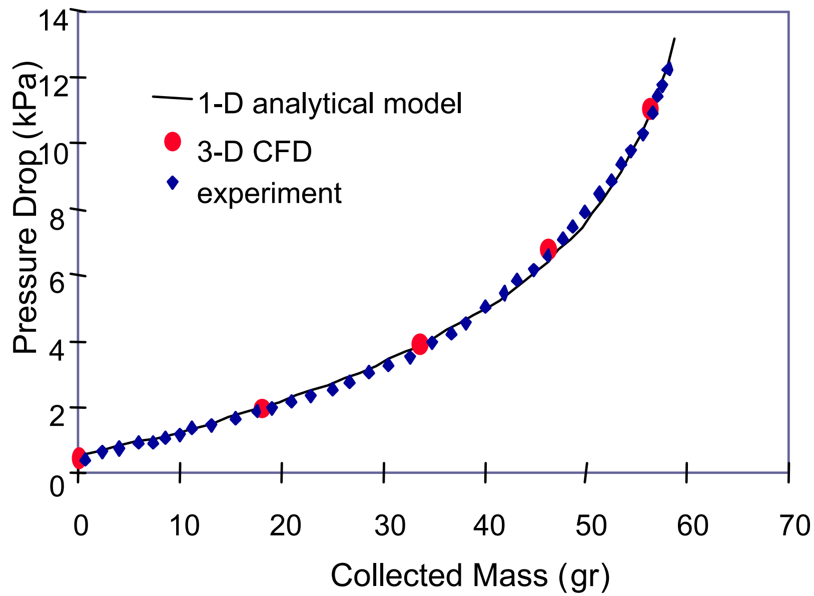
Darcian contributions term | Channel friction | Plug | Forchheimer term | Contraction & Expansion losses

where

$$w = \frac{\alpha - \sqrt{\alpha^2 - \frac{m_{soot}}{N_{cells} L \rho_{soot,c}}}}{2}$$

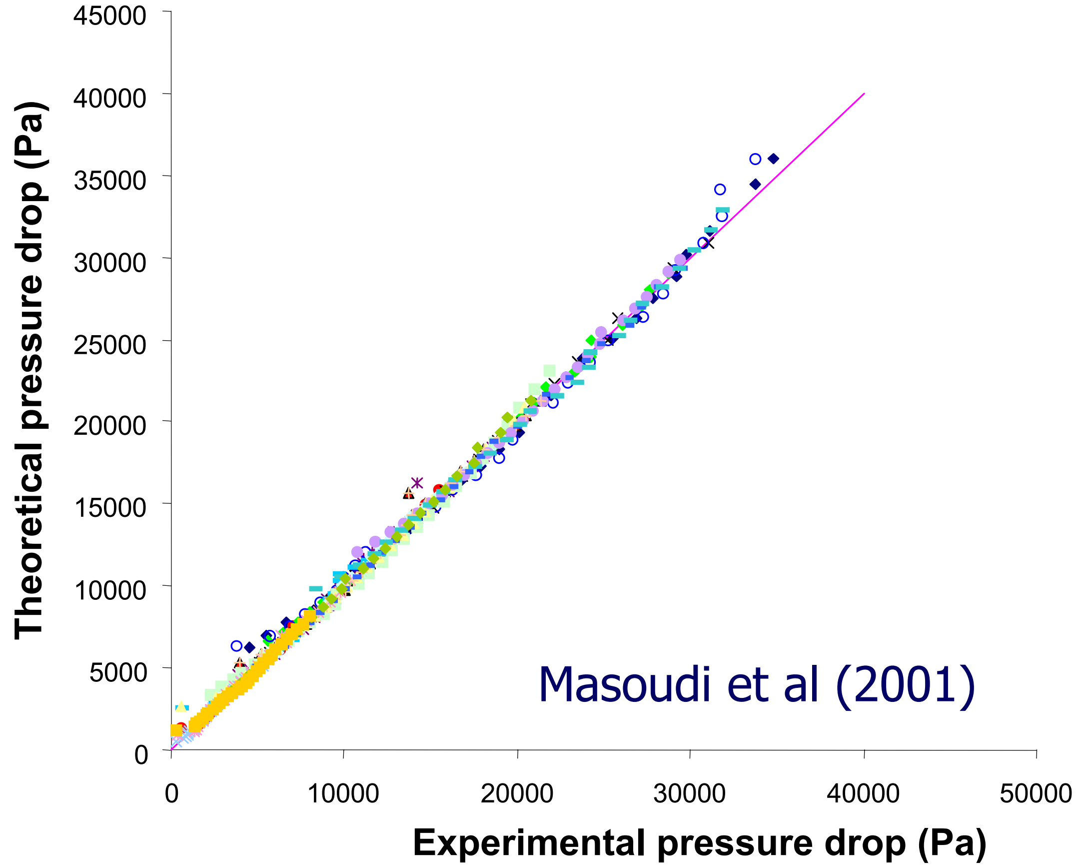
$$u_{inlet} = \frac{8Q}{\pi\sigma D^2 a^2}$$

Validation of Cake ΔP model



Parameter	Min-Max. value	Unit
Filter size (diam.xlength)	4.66x6 – 12x15	in x in
Filter cell density	100 – 200	cpsi
Filter wall thickness	12- 17	mil
Filter geometry	Round, Oval	-
Engine flow rate	97.5 – 790	kg/hr
Engine flow temperature	240 – 370	°C
Particulate emission rate	1.45 – 20.8	gr/hr
Loading duration	1.3 – 118	hr

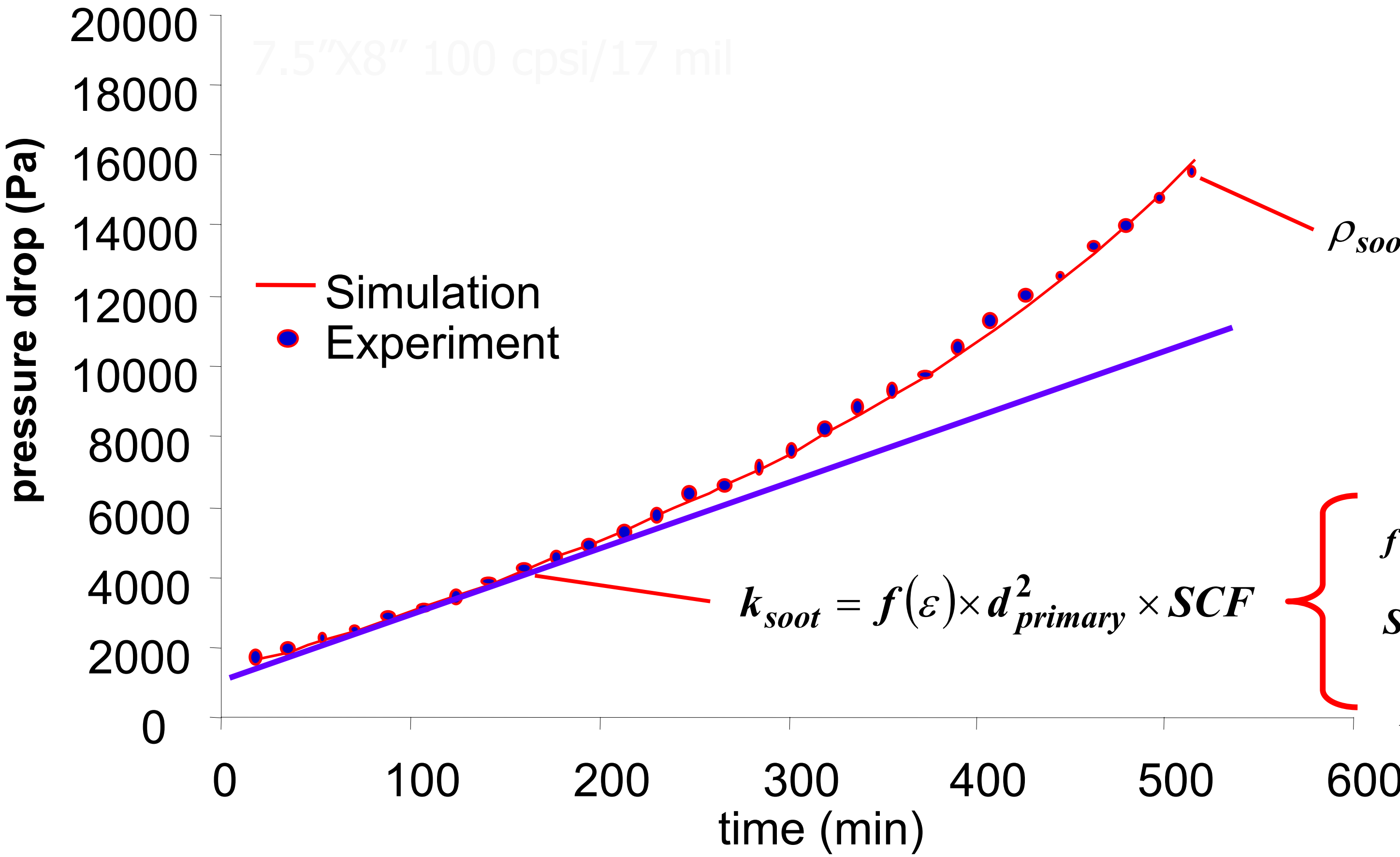
10 filters in 31 experimental runs with light and heavy duty engines



Masoudi et al (2001)

Soot Cake Microstructural Desriptors

In-situ measurement of soot cake permeability and packing density (or equivalently primary particle size and porosity)



$$\rho_{soot} = \rho_{solid} \times (1-\varepsilon)$$

$$k_{soot} = f(\varepsilon) \times d^2_{primary} \times SCF$$

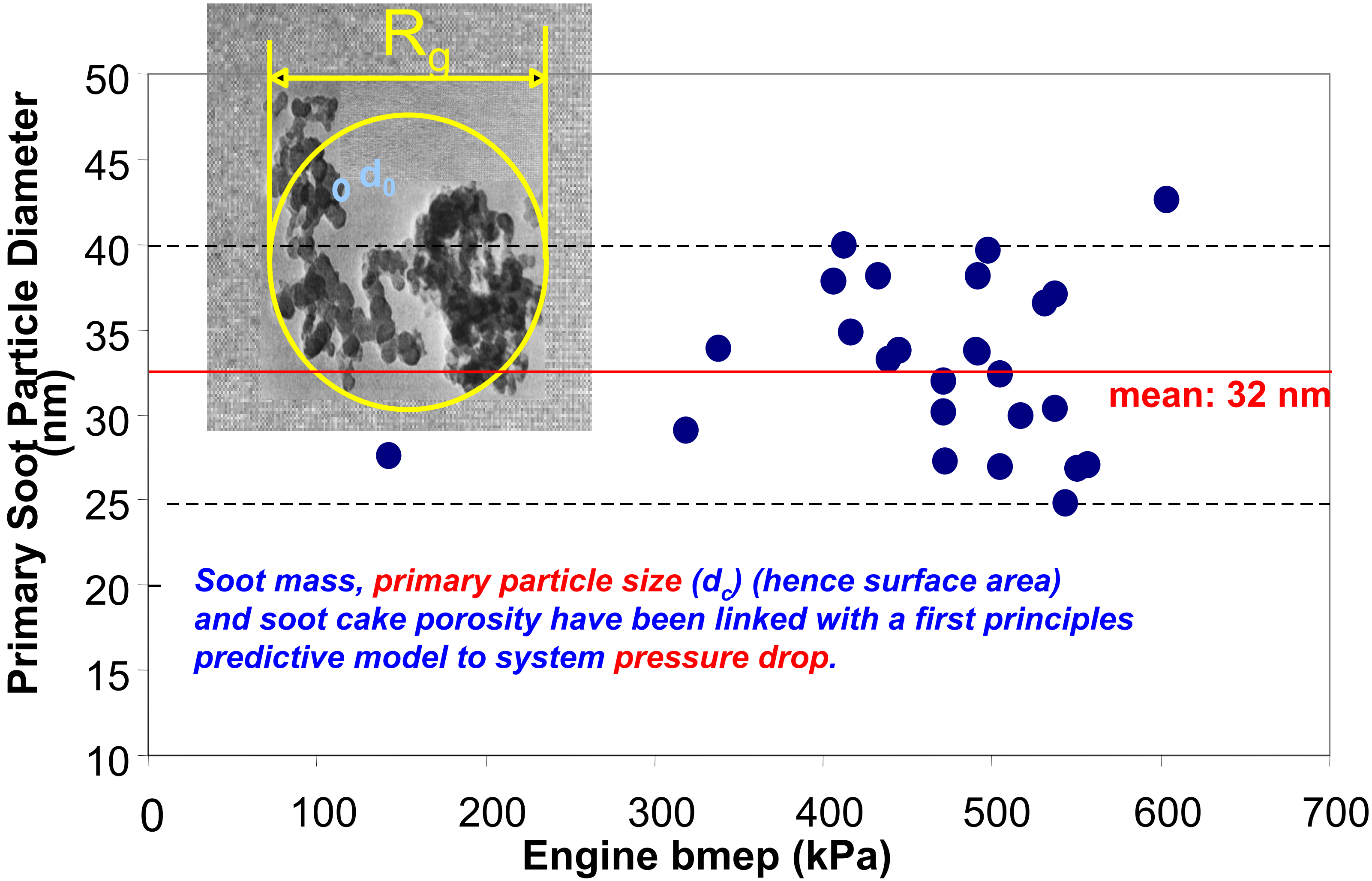
$$f(\varepsilon) = \frac{2}{9} \cdot \frac{\left[2 - \frac{9}{5}\cdot(1-\varepsilon)^{1/3} - \varepsilon - \frac{1}{5}\cdot(1-\varepsilon)^2\right]}{(1-\varepsilon)}$$

$$SCF = 1 + Kn\left(1.257 + 0.4e^{-1.1/Kn}\right)$$

$$Kn = \frac{2\lambda}{d_{primary}}$$

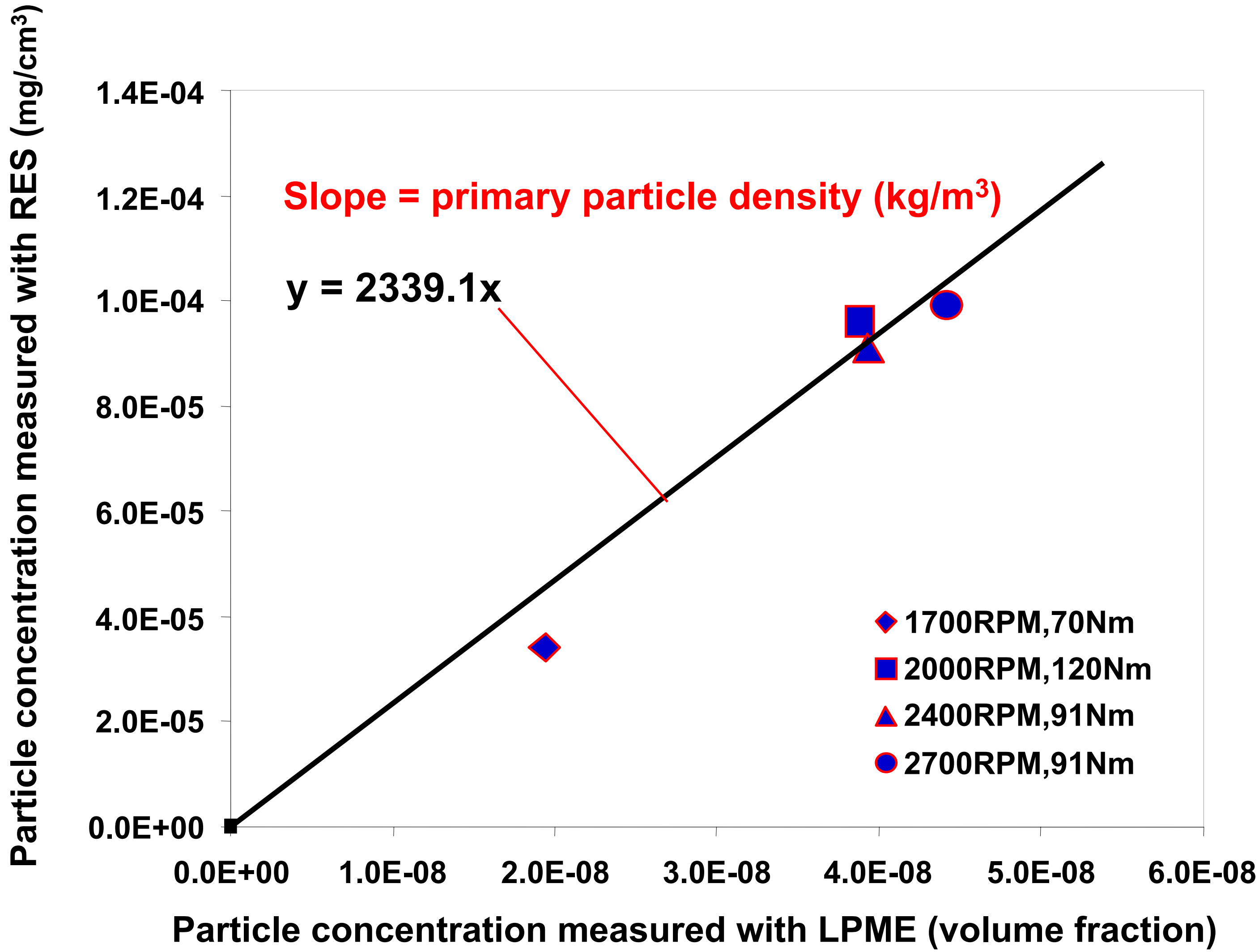
Soot Primary Particle Size

COMPUTED FROM PERMEABILITY



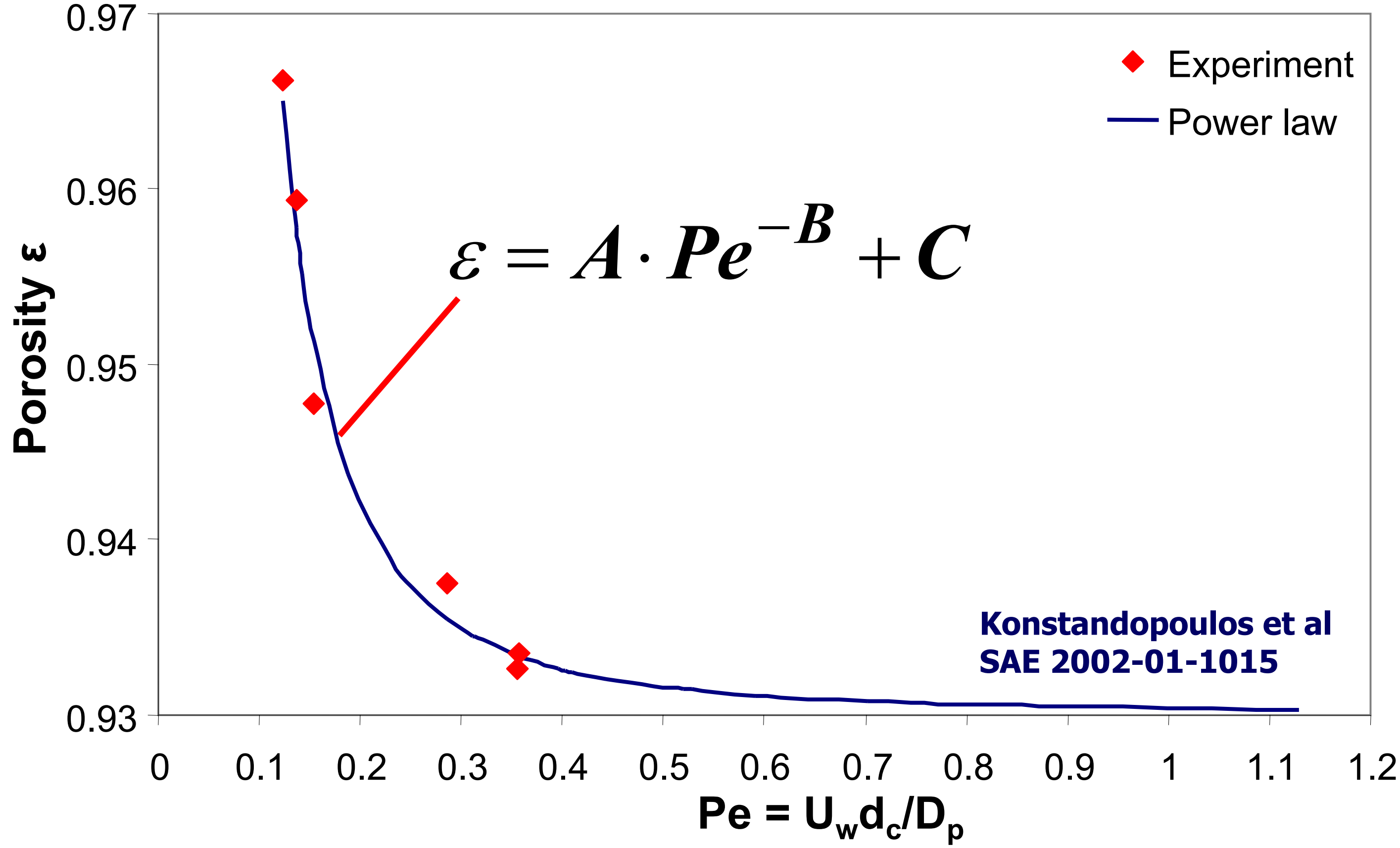
Soot mass, primary particle size (d_c) (hence surface area) and soot cake porosity have been linked with a first principles predictive model to system pressure drop.

Primary Particle Density

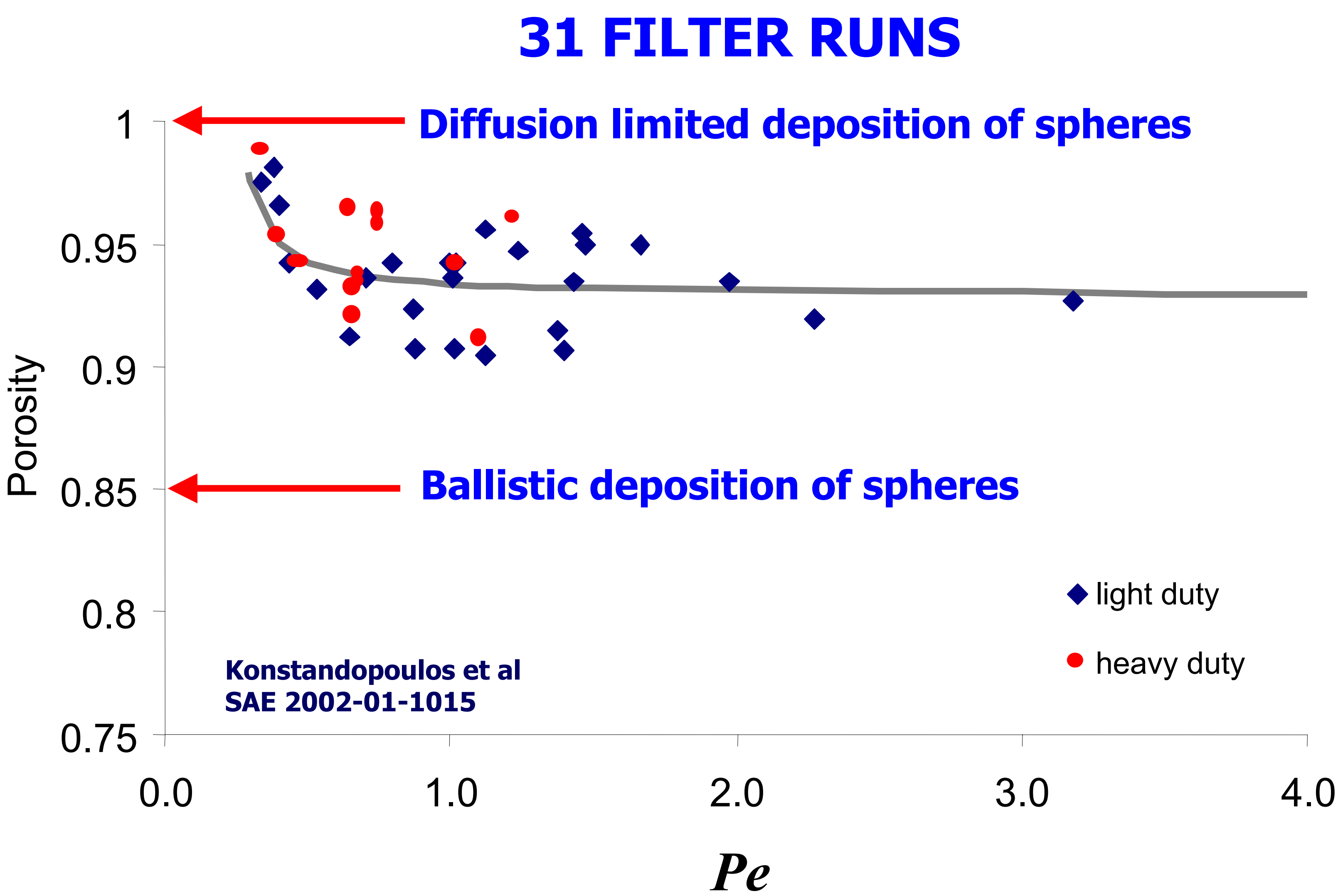


Soot Cake Porosity Variation with Pe number

Soot Packing Density and Porosity were for the first time measured in-situ and are found as power laws of Peclet number in agreement with discrete particle dynamics calculations [Tassopoulos, 1991, Konstandopoulos, 1991].

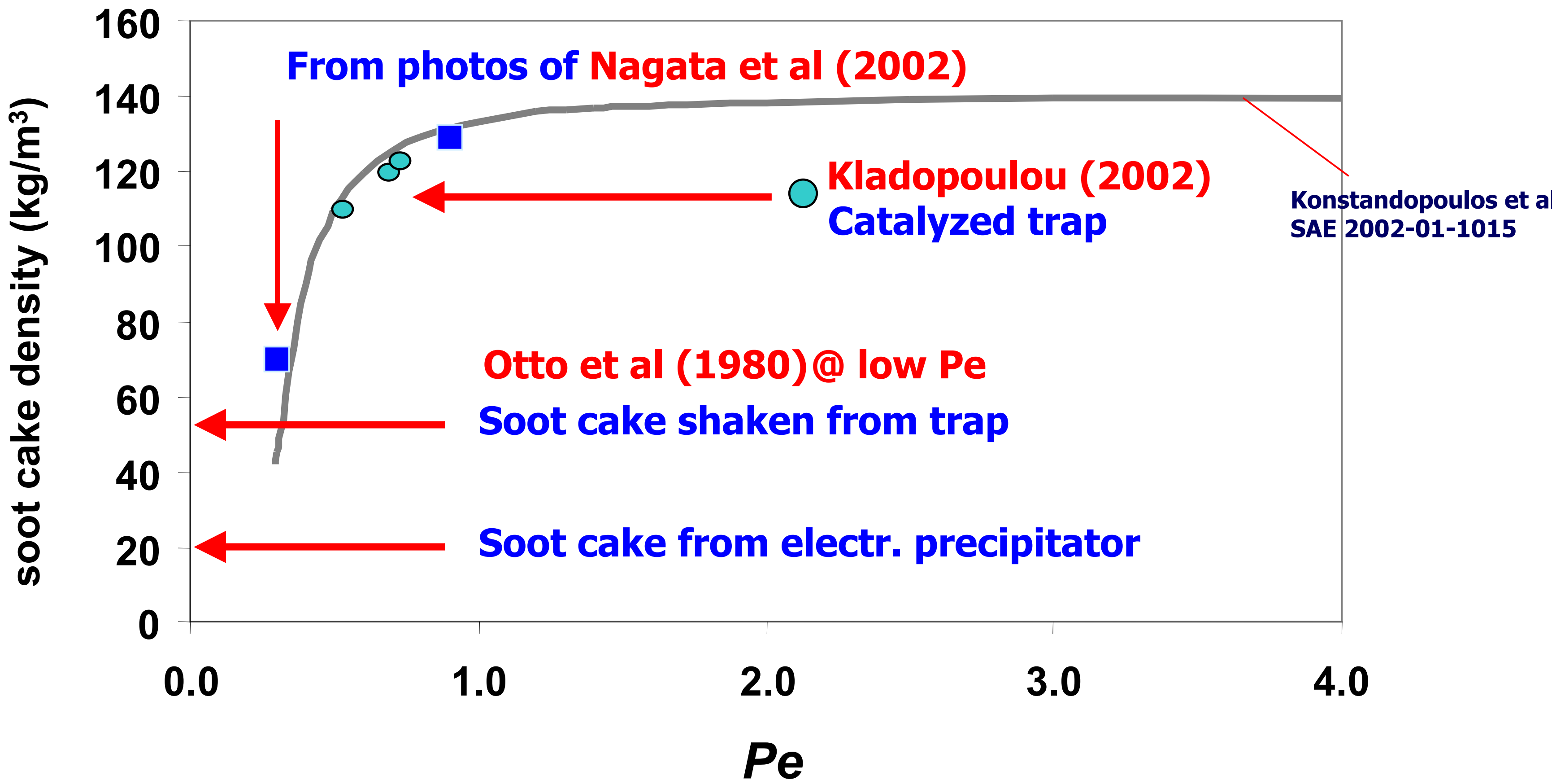


Soot Cake Porosity Variation with Pe number



Soot Cake Density Variation with Pe number

COMPUTED FROM POROSITY



Soot Cake Thickness Variation with Pe number

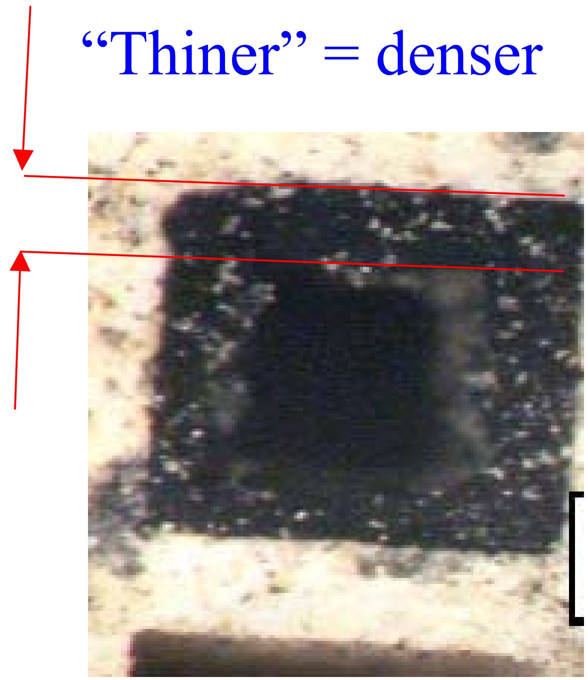
At similar soot loads (24 gr in trap)

Low Peclet Deposit

“Thicker” = less dense

High Peclet Deposit

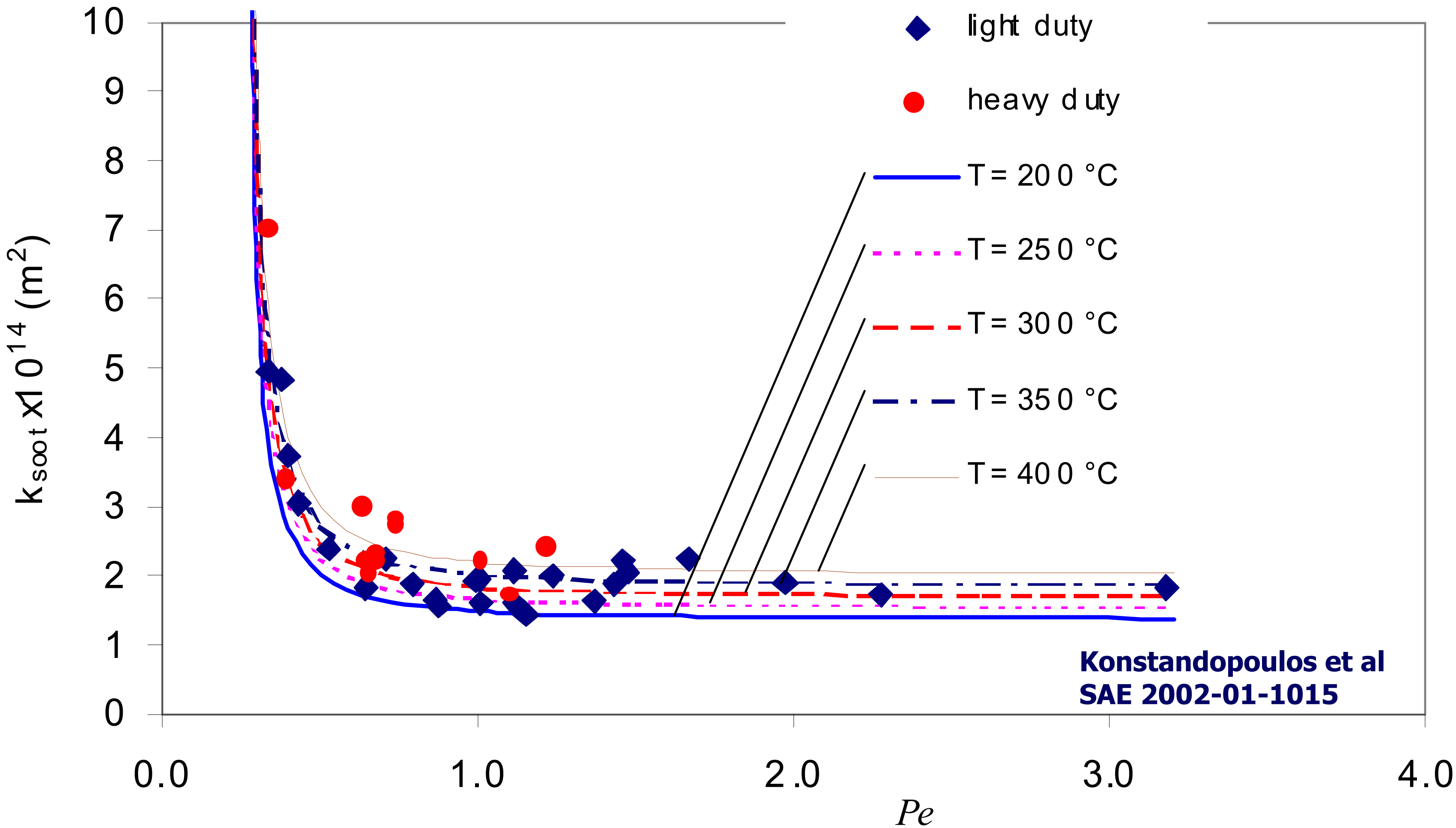
“Thiner” = denser



Nagata et al. SAE 2002-01-1013

Soot cake permeability variation with Pe

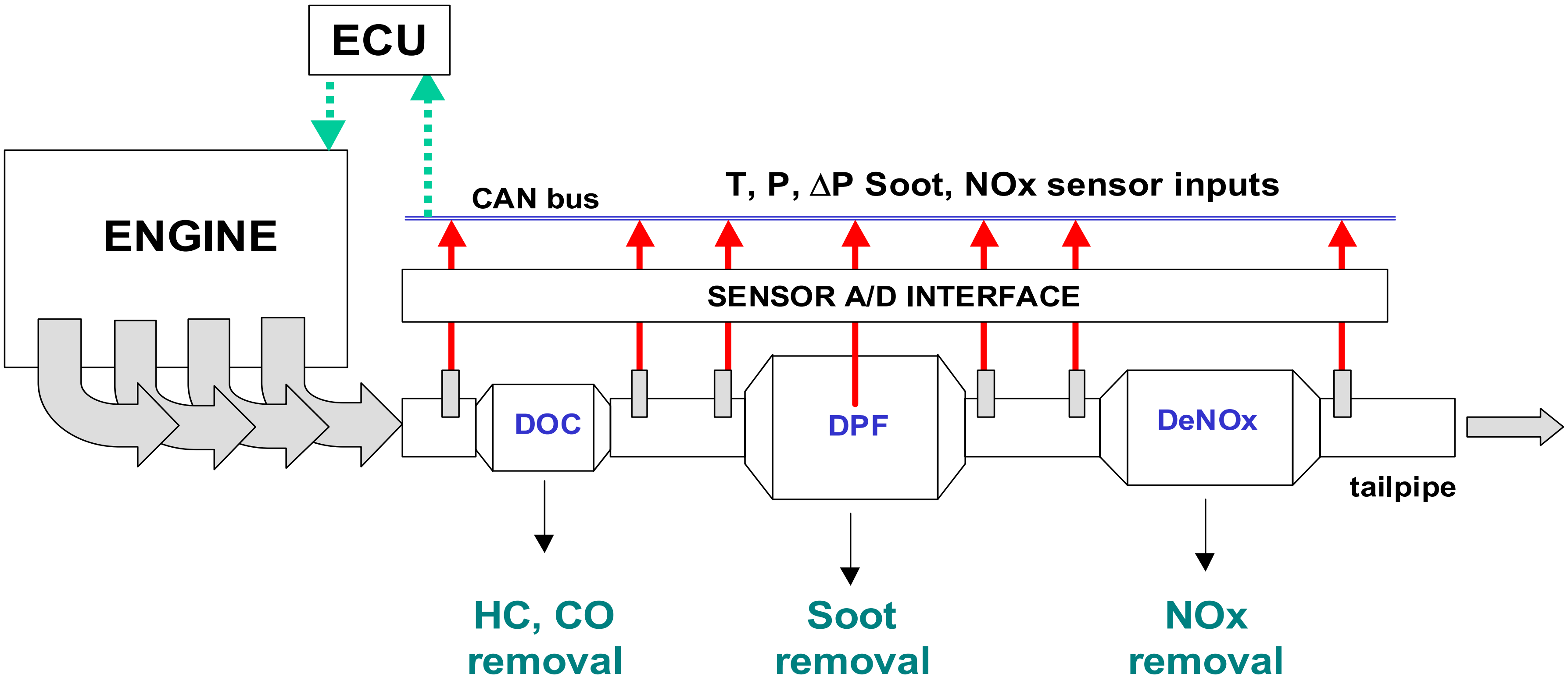
THEORY vs. EXPERIMENT



Unrealistic permeabilities (by a factor of 10 or more) are employed in many modelling studies!

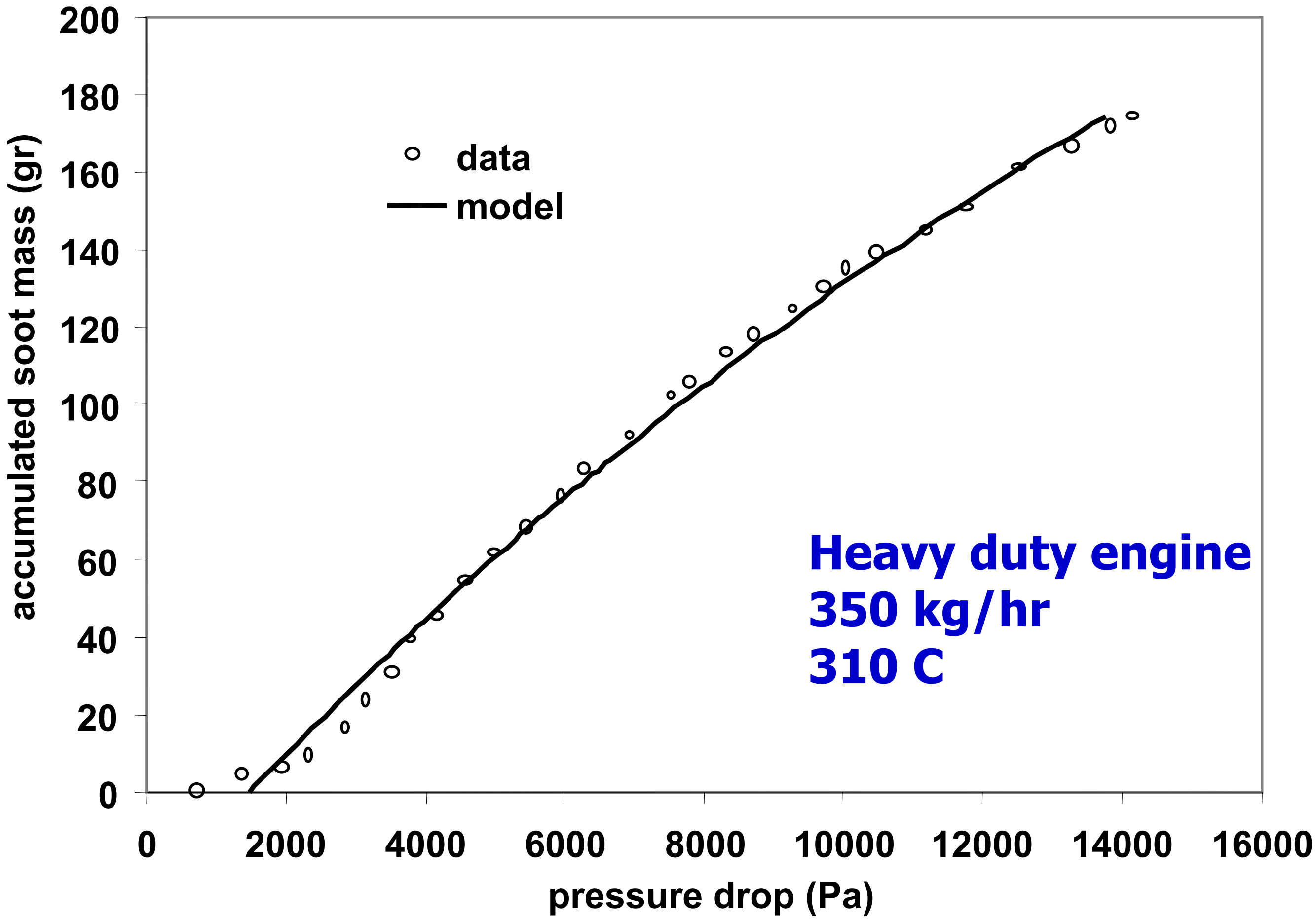
On-Board Soot Sensing

FUTURE EMISSION CONTROL SYSTEMS:
Assemblies of reactors, hardware and virtual sensors



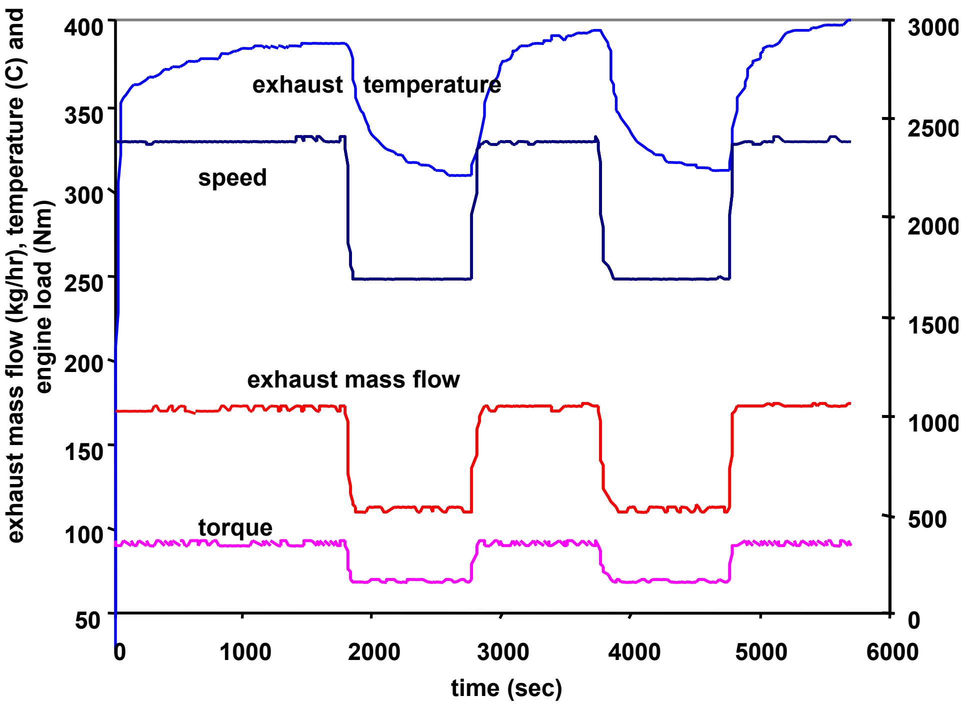
Estimation of Trap Soot Load (st. state)

Experimental data Johnson et al (1987)
SiC filter 9"x12" 60cpsi/31mil

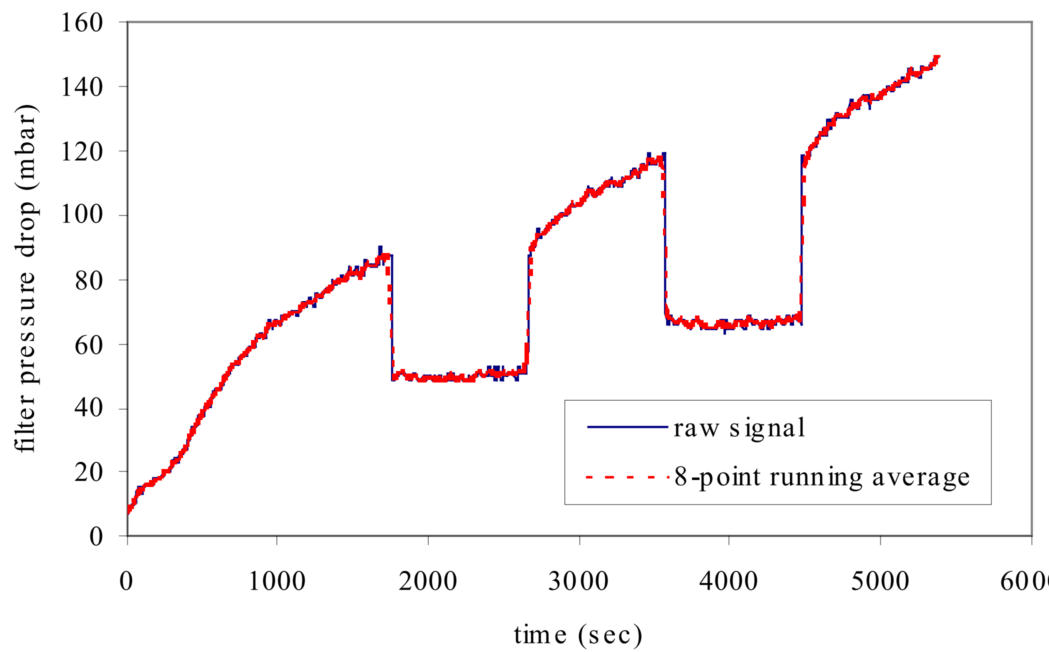


Model estimation of trap soot load (transient)

ENGINE DATA



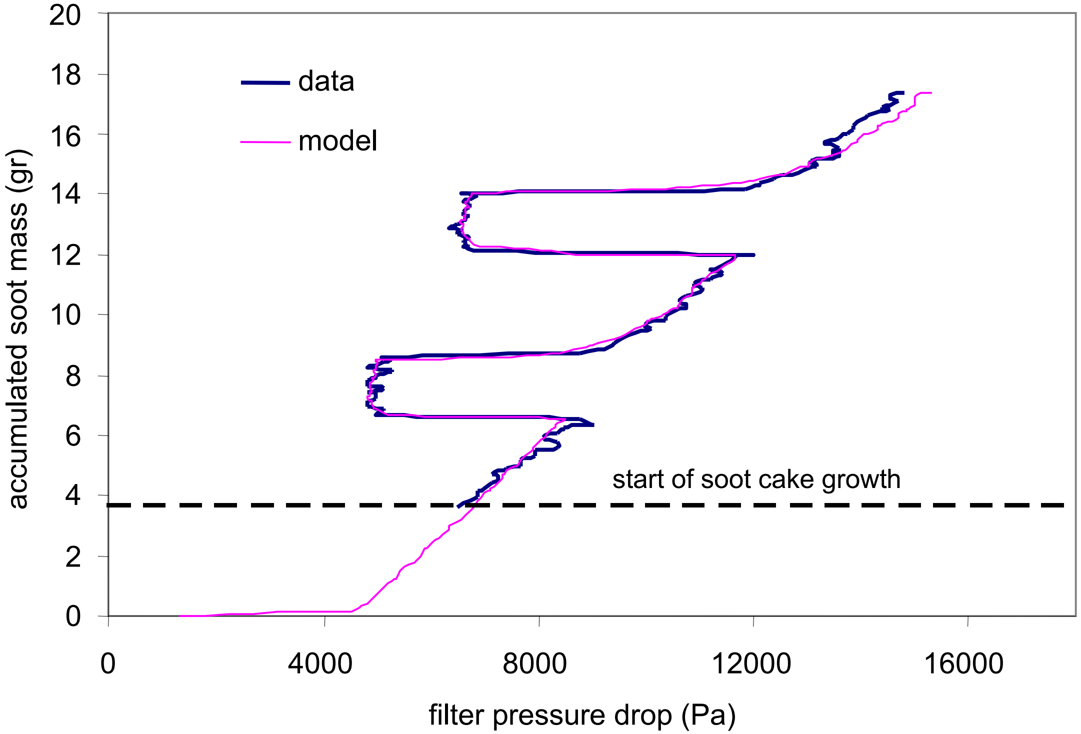
PRESSURE DROP

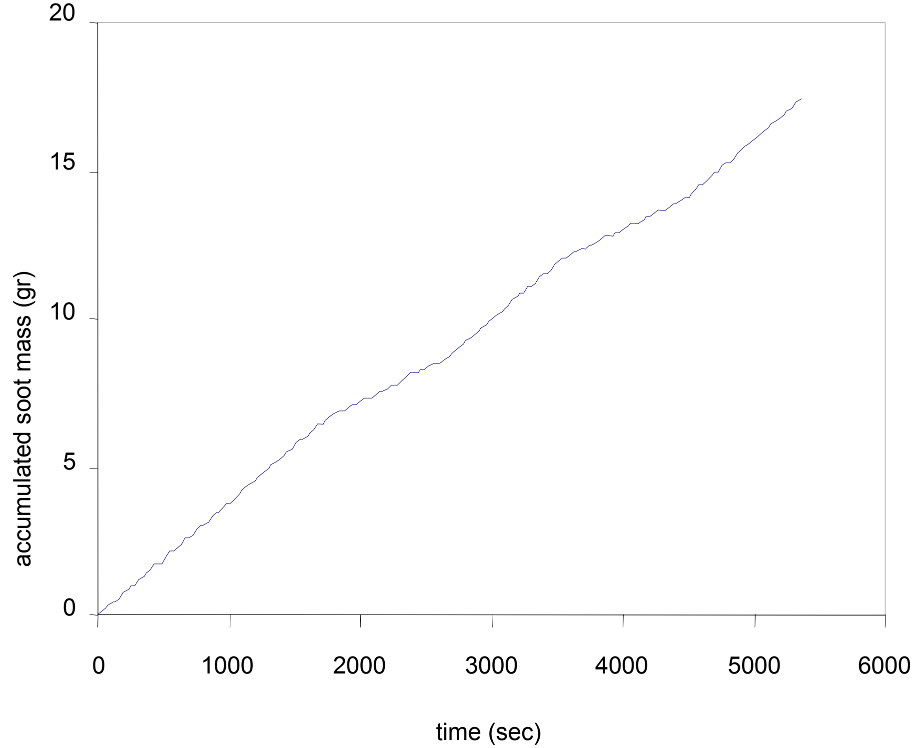


Experimental data CPERI, light duty 1.9 L engine
SiC filter 5.66"x7" 70cpsi/31mil

Model estimation of trap soot load (transient)

ACCUMULATED MASS ESTIMATION = 17.4 gr
MEASURED MASS = 15.2 gr





NEXT STEP: Microscale Flow Modelling

Kikkinides, Vlachos & Konstandopoulos (2002, in preparation)

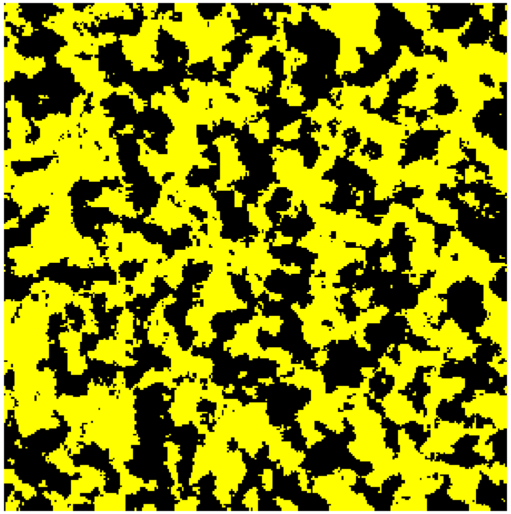
SEM picture

↓

Reconstruction computational engine matching:
- porosity, pore size
- autocorrelation function

↓

Binary representation of porous wall

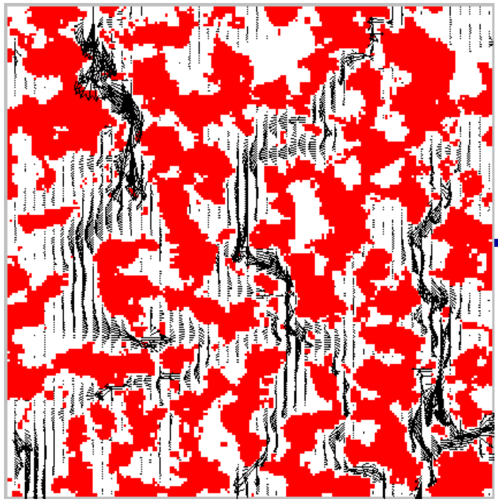


→

- Microstructure simulation
- Explore variations around a particular design
- Connected vs. non-connected porosity etc.
- Design desired material picture before making it

↑

Flow simulation



→

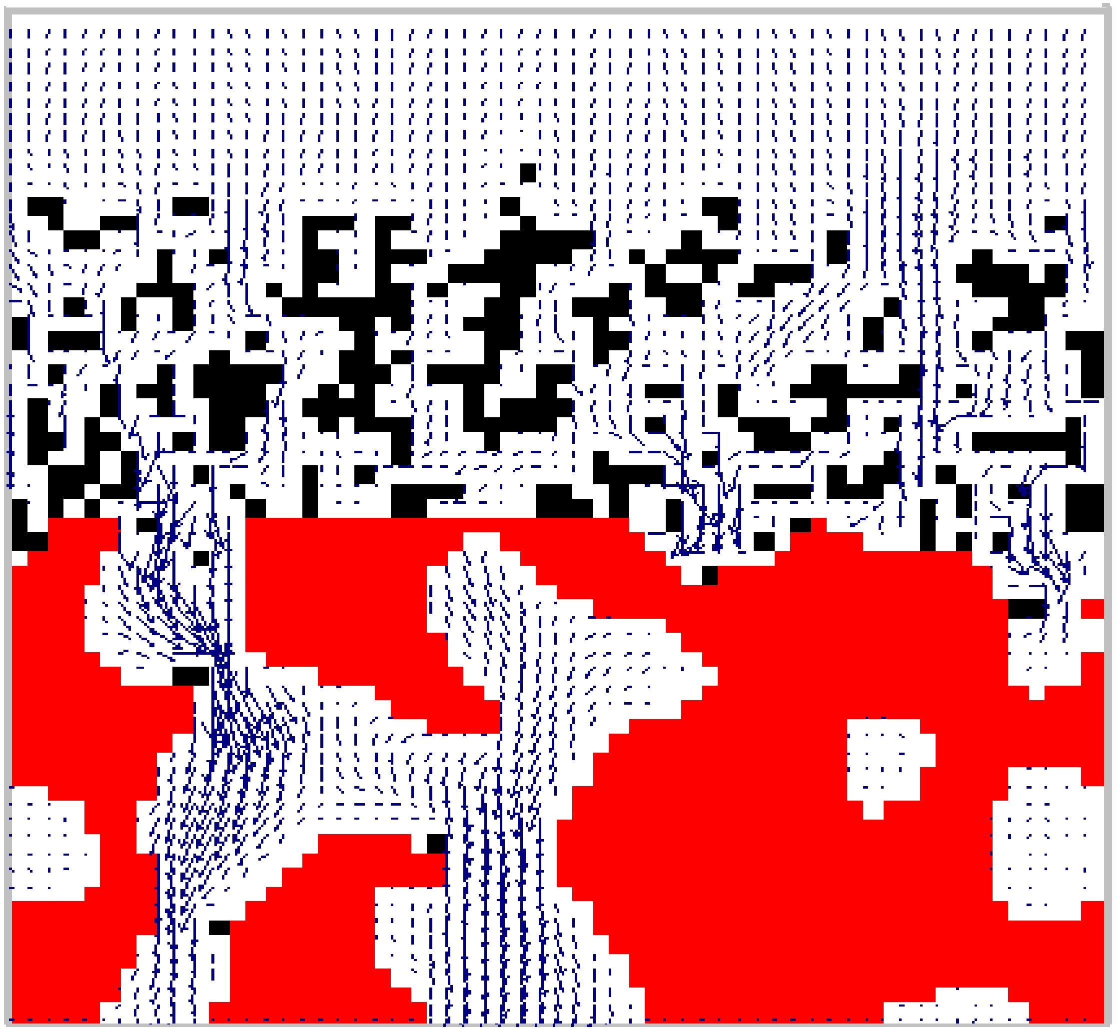
- Permeability Prediction
- Permeability Design from first principles

Microscale Filtration Modelling - 1

Kikkinides, Vlachos & Konstandopoulos (2002, in preparation)

Monte Carlo Diffusion-Convection Filtration Simulator

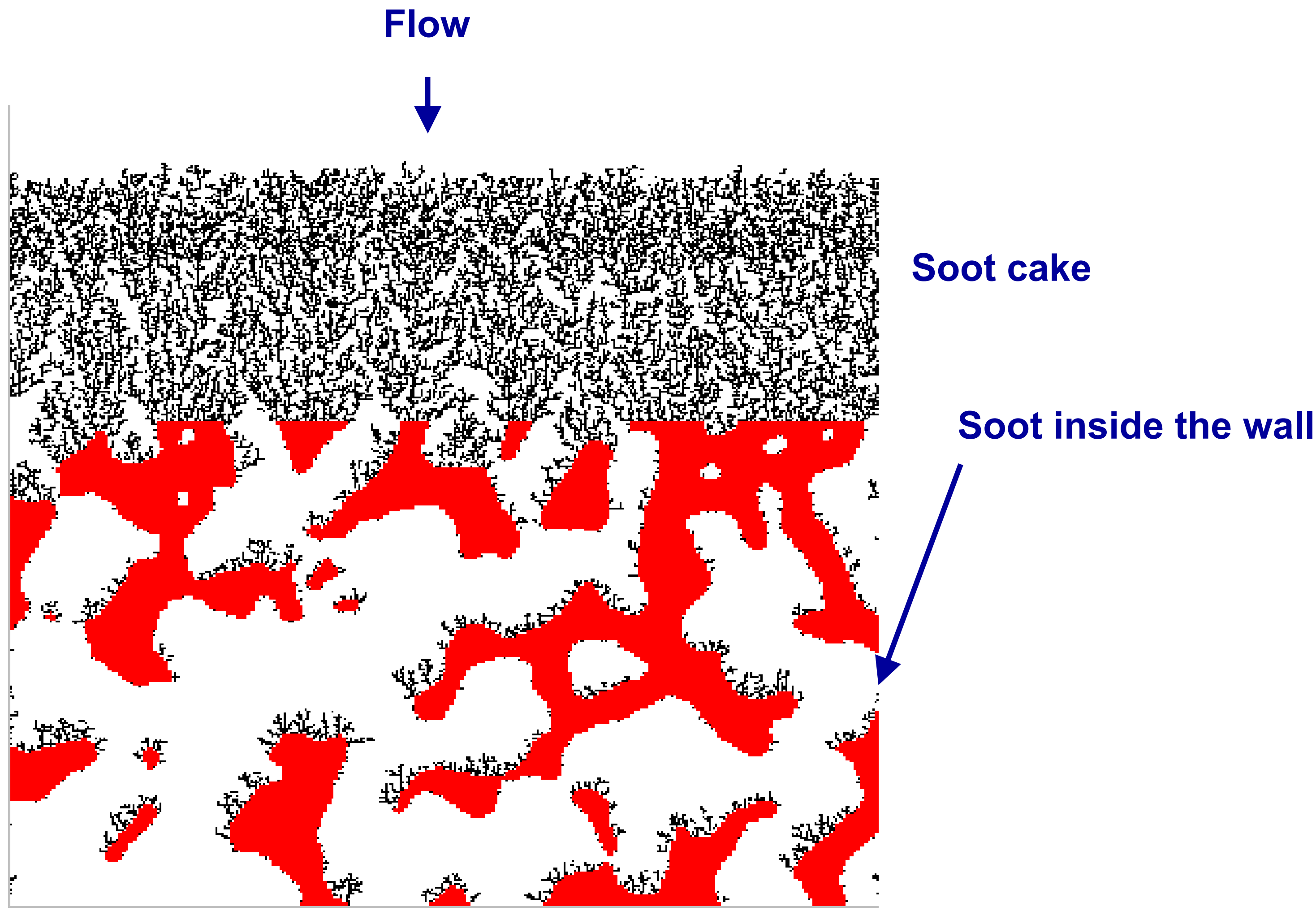
Flow ↓



Microscale Filtration Modelling - 2

Kikkinides, Vlachos & Konstandopoulos (2002, in preparation)

Monte Carlo Diffusion-Convection Filtration Simulator



Conclusions

- Understanding the structure of the soot cake is a prerequisite for the intelligent operation of Diesel filters and the practical estimation of their pressure drop for field applications.
- A key parameter that determines the resulting microstructure of the soot cake is the Peclet number for mass transfer.
- A non-destructive methodology has been developed for the measurement of soot packing density and permeability and their correlation to the prevailing Peclet number. The correlation is self consistent permitting the estimation of soot cake permeability from a knowledge of the soot primary particle size and vice-versa.
- The developed methodology can be adapted for on-board estimation of the trap soot load in real time

End

Thank You For Your Attention