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Trapping Efficiency of Diesel Particles Through a Square Duct

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***Abstract*—**Diesel Engines emit complex mixtures of inorganic and organic compounds in the form of both solid and vapour phase particles. Most of the particulates released are ultrafine nanoparticles which are detrimental to human health and can easily enter the body by respiration. The emissions standards on particulate matter release from diesel engines are constantly upgraded within the European Union and with future regulations based on the particles numbers released instead of merely mass, the need for effective aftertreatment devices will increase. Standard particulate filters in the form of wall flow filters can have problems with high soot accumulation, producing a large exhaust backpressure. A potential solution would be to combine the standard filter with a flow through filter to reduce the load on the wall flow filter. In this paper soot particle trapping has been simulated in different continuous flow filters of monolithic structure including the use of promoters, at laminar flow conditions. An Euler Lagrange model, the discrete phase model in Ansys used with user defined functions for forces acting on particles. A method to quickly screen trapping of 5 nm and 10 nm particles in different catalysts designs with tracers was also developed.

Simulations of square duct monoliths with promoters show that the strength of the vortices produced are not enough to give a high amount of particle deposition on the catalyst walls. The smallest particles in the simulations, 5 and 10 nm particles were trapped to a higher extent, than larger particles up to 1000 nm, in all studied geometries with the predominant deposition mechanism being Brownian diffusion. The comparison of the different filters designed with a wall flow filter does show that the options for altering a design of a flow through filter, without imposing a too large pressure drop penalty are good.

***Keywords*—**Diesel Engine trap, thermophoresis, Exhaust pipe, PM-Simulation modeling.

I. Objectives

To optimize particle trapping efficiency for an oxidation catalyst more specifically a squre duct monolith channel by altering the geometric shape and through the use of promoters in the channel. An important design parameter to consider was the resulting pressure drop in the channel which should be kept as low as possible or otherwise the engine efficiency might deteriorate and fuel consumption increase.

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1. Suggest a novel design for an oxidation catalyst that is optimized with respect to particle trapping efficiency.
2. Assess the possibilities to design such a catalyst in a way which is also beneficial from a heat and mass transfer perspective.

II. Introduction

At high temperatures most of the hydrocarbons are present in vapour-phase but during cooling in the exhaust pipe, increased adsorption onto carbon particles and condensation processes occurs with formation of nucleated droplets. The nuclei mode particles (carbon particles and nucleated hydrocarbon droplets) is centered near 0.01 mm and usually accounts for only a small fraction of the overall mass but up to 90% of the total number of particles [1].

A. Diesel PM Emission

Diesel particulate matter is measured by sampling gas from the exhaust system, diluting it with air and filtering diluted diesel exhaust at teparature lower than 52^0C. The current PM emissions standards are mass based, corresponding to the amount of mass left in the filter after the sampling procedure. Even though studies have shown that ultrafine particles (<100nm in diameter) and nanosized particles (<50nm in diameter) are detrimental to human health because of their capability to enter the body by respiration and penetrate cell membranes [2]. Diesel exhaust mostly contains hydrocarbons of C_{15} but also a significant amount which is larger than C_{25} [3]. The diffusivities of these larger molecular compounds are slow and results in poor mass transfer to the surfaces within a catalytic device. About 80% by mass of the particulate emission consist of solid carbon particles and sulfur compounds [4]. The solid part of diesel particulate matter, carbon particles (soot), hydrocarbons and sulfates is formed early in the combustion process and is relatively stable. Soot is formed due to air deficiency caused by incomplete mixing and soot emissions are strongly increased if the air-fuel mixture is enriched to near stoichiometry [5].

The solid carbon particles are spherical with diameters in the range of 0.01 to 0.08 μm; particulate matter is classified into three major size distribution modes: nuclei, accumulation and coarse mode.

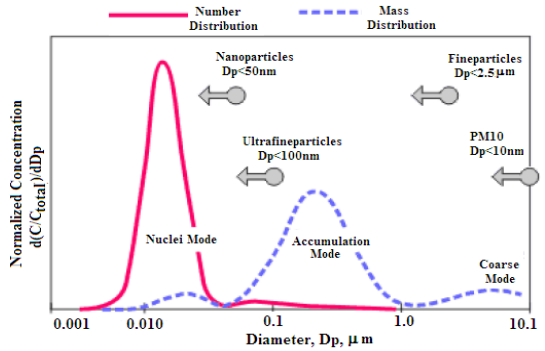

Fig. 1 Diesel Particulate size distribution[2]

B. Emission Legislation

The European emission regulations, Euro IV-VI in Table I apply for new heavy-duty diesel engines of compression ignition type, positive ignition natural gas and LPG engines. The emissions are normalized according to the total energy output of an engine over the specified driving cycle [6].

TABLE I
EMISSION STANDARDS FOR HEAVY DUTY DIESEL ENGINES, G/KWH

Tier	Year	Test	CO	HC	Nox	PM	Smoke
Euro IV	2005	ESC&	1.5	0.46	3.5	0.02	0.5
Euro V	2008	ELR	1.5	0.46	2.0	0.02	0.5
Euro VI*	2013		1.5	0.46	0.4	0.01	
*Proposal (2008)							

A rapid complete combustion decreases the particle emissions but on the other hand promotes NOx formation. The opposite, exhaust gas recycling (EGR), a procedure to lower NOx emissions instead generally increases particulate emissions. The coming Euro VI emision standards will be met by disel engine manufactures through different exhaust aftertreatment devices, most probably by particulate traps and NOx reduction catalysts which are only efective at low sulfur levels [7].The most common type of measure to reduce diesel particulate matter and clean exhaust gas for automotive applications are different filters and oxidation catalysts often of monolith structure. The possibility to modify filters and use promoters for increased particle trapping, heat and mass transfer propoerties will be described here. The drawback with a modification is usually an increased pressure drop. The equations for pressure drop determination and physical parameters for characterisation of exhaust gas characterization also have to be considered. The diesel oxidation catalyst (DOC) is designed to oxidize exhaust gases in the presence of oxygen. The most common pollutants oxidized are cabon monoxide (CO), hydrocarbons (HC) and volatile organic compounds in the form of soluble organic fraction (SOF). Nitrogen oxide (NO) is also oxidized to nitrogen dioxide (NO_2) at the temperatures of 270^0C to 470^0C [8], an important reaction which can be undesirable since nitrogen dioxide is more toxic than nitrogen monoxide in nature. However incineration of solid carbon particles (soot) mostly requires temperatures above 600^0C, temperatures diesel exhaust gases cannot reach during normal engine operation. Therefore a diesel particulate filter is often placed downstream from the DOC which utilizes NO_2 to oxidize soot and accumulated particle matters (PM) at temperatures below 350^0C[9]. Since the temperature of diesel exhaust is low, only a small amount of NO is oxidized to NO_2. The oxidation is further improved if the oxidation catalyst is placed closely to the engine or upstream from the turbocharger [10].

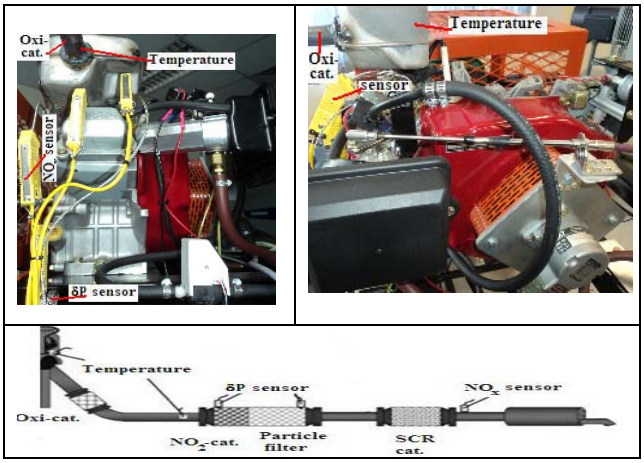

Fig. 2 Schematic view of a DOC

C. Diesel Oxidation Catalysts

The DOC is usually a honeycomb monolith structure coated with an active catalytic material, a wash coat of precious metals which effectively reduces CO and hydrocarbons emissions through oxidation. One of the most basic washcoat formulations is platinum on alumina (Pt/Al_2O_3) [9]. The effectiveness of the DOC is mostly dependent on the temperature. Below the light off temperature 250^0C for a common DOC of Palladium Rhodium [8], the surface reaction kinetics of the primary chemical reactions determines the performance. Above the light off temperature diffusion of chemical species from the exhaust gases to the solid surface determines the effect of the catalyst that is mass transfer resistances controls the reaction. The main reactions on the catalytic surface of the DOC are described by reaction 1-3 below where (1) represents the reactions of hydrocarbons to water vapour and carbon dioxide and (2) the oxidation of SOF compounds. Reaction (3) represents the oxidation of carbon monoxide to carbon dioxide [10].

$$1.[HC] + O_2 = CO_2 + H_2 0$$

$$2.C_n H_{2m} + (n + \frac{m}{2})O_2 = nCO_2 + mH_2O$$

$$3.CO + \frac{1}{2}O_2 = CO_2$$

The oxidation reactions in the DOC produce some undesirable products, if sulphur dioxide is oxidized to sulphur trioxide and further reacts with water vapour, sulphuric acid is formed. In the tailpipe or in air, gaseous sulphuric acid adsorbs onto carbon particle and sulphur particles are formed and emitted from the engine.

D. Diesel Particulate Filters

Automotive filter used for particle trapping is the wall flow filter, a catalyst where some of the channels are blocked forcing the flow through porous walls into other channels. Wall flow filters made from ceramic or metallic substrates have a high efficiency; more than 90% of the particulates in the size range of 15 to 500nm can be captured [11]. Tests in non-blocking continuous flow catalysts have given particle trapping efficiencies ranging from 20-50% based on different operating conditions [12]. One of the major advantages with the continuous flow filter is the tendency to avoid clogging; in case of insufficient regeneration particles will merely flow through the device [13].

III. Modeled in Solidworks

The design is given below figure 3, the height and width, z and y direction was 2 mm and h=1.25 mm.

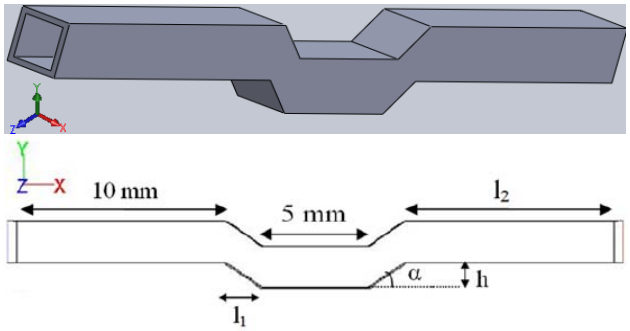

Fig. 3 Design of Catalyst with tortuous path

IV. FEA Procedure

A. Pre-Processing

To build a complete finite element mode, including physical and material properties and boundary conditions, and analysis the various behaviors of mechanical components and structure.

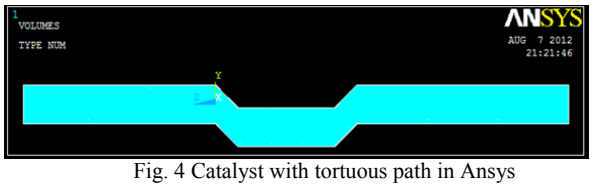

Fig. 4 Catalyst with tortuous path in Ansys

B. Meshing

Ansys offers a complete set of tools for automatic mesh generation including mapped meshing and free meshing can access geometric information in the form of point, curves and surface.

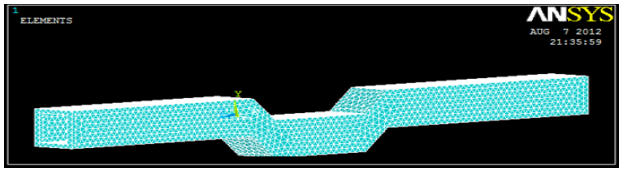

Fig. 5 Mesh model of Catalyst with tortuous path

The parameters altered in the study believed to affect the pressure drop and particle trapping efficience is shown in table II below.

TABLE II
CATALYST WITH TORTUOUS PATH WITH FOLLOWING CASE DESIGNS

Case	Angle α (^{0})	Length l_1 (mm)	Length l_2 (mm)	Total length (mm)
4.0	-	-	10	28.42
4.1	35	1.71	10	28.42
4.2	45	1.2	11.02	28.42
4.3	55	0.84	11.74	28.42

V. Computational Fluid Dynamics

A. Fundamental Equations

CFD provide insight on the flow and pressure fields for both single and multiphase flows. In the following section the most imporatnt forces acting on soot particles in exhaust gas and the particle depostion mechanisms are introduced. The equations solved for particle simulation with Euler Lagrange model and its limitation is discussed. Most commercial CFD codes rely on a finite volume solver to numerically solve discretized equations for a domain divided into small computational cells. The Navier stokes equations describing the transport of fluid flow, derived over control volume consists of the continuity equation and the momentum equations [14].

$$\frac{\partial \rho U_i}{\partial t} + \frac{\partial \rho U_i U_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\mu \frac{\partial U_i}{\partial x_j}\right) - \frac{\partial \mathrm{P}}{\partial x_i} \quad (1)$$

Simulating turbulence requires the addition of turbulence model.

$$\frac{\partial^2 \mathrm{P}}{\partial x_i \partial x_j} = -\frac{\partial^2}{\partial x_i \partial x_j}\left(\rho U_i U_j\right) \quad (2)$$

Multiphase flows are more complex and there are many computional models available to choose from. The parameters for flow characterization can be good aid in determining the suitable model.

B. Euler Lagrange Particle Tracking

The Lagrangian approach to describe the particle motion or trajectory in a fluid is centered on the solution of three ordinary differential equations given by:

$$\frac{dx_p}{dt} = u_p \;;(3) \quad m_p \frac{du_p}{dt} = \sum F_i \;;(4) \quad I_p \frac{d\omega_p}{dt} = T \;;(5)$$

Where: $m_p = \rho_\rho \left(d_p\right)^3 \frac{\pi}{6}$ and $I_p = 0.1 m_p \left(d_p\right)^2$

These equations describe the particle location, angular and linear velocities, where m_p is the mass of a spherical particle or droplet while up=the linear velocity [15]. The particle are treated as point-wise rigid spheres, represented by source terms and possibly a volume fraction [14]. The number of depostion efficiency for particles deposited in a channel or pipe is governed by the forces acting on the particles [3].

$E = 1 - \left(\frac{n_{outlet}}{n_{inlet}}\right)$; n= number concentration of particles

Particles hitting a wall may either adhere or are reflected. At the wall of a catalyst agglomeration of soot particles can transpire which makes reentrainment of particles, mainly caused by vibrations and fluid shear forces [16].

VI. Methodology

A. Simulation

Two major computational approaches were taken to determine uncoated monolith catalysts effectiveness in trapping soot particulate matter. One used an Euler Lagrange model-discrete phase mode (DPM) which solves the Lagrangian equations of motion for particles. The major forces governing particle depostion, Brownian duffusion and drag were the only forces solved for with this model. The other method is based on tracking tracers or species with an assigned diffusivity throughout the flow field. Since Brownian diffusion is the predominant depostion mechanism for 5nm and 10nm particles only, those sizes were expected to give accurate values in simulations with the species method. The major advantage with the species method is the faster simulation time compared to the DPM.

B. The Discrete Phase Model and UDF

The model chosen for tracking particles of a wide size range in Ansys simulations was the discrete phase model. The flow of the gas in the domain was solved prior to injection of particles and the particles tracked in the frozen flow field, assuming one way coupling to be valid. For the discrete phase model, four user defined functions: where applied to solve for ***drag***, ***particle injections***, ***force*** and the ***time*** step. The user defined function calculates **drag** and the Cunningham correlation

$$C_c = \left(1 + Kn_p * \left(2.514 + 0.8e^{\left(\frac{-0.55}{Kn_p}\right)}\right)\right)$$

The gas molecules do not stick to the particles surface instead a partial or full slip condition occurs which in turn reduces the drag coefficient. Rarefaction effects can be estimated from the ratio of the mean free path of gas molecules to the particle diameter with is the particle Knudsen number.

$$Kn_p = \frac{\lambda}{d_p} \text{ Where: } \lambda = \frac{\mu_f}{0.499\,\bar{c}_{Mol\,\rho f}};\ \bar{c}_{Mol} = \left(\frac{8P}{\pi\rho_f}\right)^{1/2}$$

λ=Gas molecules, $\bar{c}_{Mol}$=average relative velocity between gas molecules and P is the pressure of the sysem and at for instance atmospheric condition with a temperature of 293 k and pressure of 1 bar, the mean free path is approximately 0.06μm. In the Stokes regime is valid for small particles, and drag coefficient has to be reduced and corrected by the Cunningham correlation. The user defined function calculates $\bar{c}_{Mol}$, λ and the Knudsen number and depending on the particle Reynolds number different correlations are used to obtain the drag. Stokes law is given the first equation below followed by different forms of correlations.

$$C_D = \frac{1}{C_C}\left(\frac{24}{\mathrm{Re}_p}\right) \qquad \mathrm{Re_p} < 0.1$$

$$C_D = \frac{1}{C_C}\left(\frac{22.73}{\mathrm{Re}_p} + \frac{0.0903}{\mathrm{Re}_p^{\,2}} + 3.69\right) \qquad 0.1 \leq \mathrm{Re_p} < 1$$

$$C_D = \frac{1}{C_C}\left(\frac{29.1667}{\mathrm{Re}_p} + \frac{3.889}{\mathrm{Re}_p^{\,2}} + 1.222\right) \qquad 1 \leq \mathrm{Re_p} < 10$$

The function enforces a limit on the **time** step, if the time step controlled by ordinary differential equations solver exceeds the limited value; it is set equal to the limit in equation. However if the time step never exceed the limit, it is left unmodified. Hence the time step is always smaller than the particle response time which is necessary for the Brownian force equation to be valid. The Brownian **force** utilizes randomization routines to impose a random velocity component to the particle movement as it moves through the flow field and collides with other particles. A normal distributed randomized number is multiplied to the Brownian force

$$F_{Brownian,i} = \zeta_i \sqrt{\frac{216\,\rho_g \nu_g k_B T}{\pi d_p^5 \rho_p^2 C_c \Delta t}}$$

Where: T=absolute temperature of the fluid;
V_g=kinematic viscosity of the gas; k_B=Boltzmann constant
C_c=Cunningham correction factor.

The function injects particles of 12 different diameters, from 5nm to 1000nm (1μm), to obtain reliable statistic values an equal number of particles, 2000 of each particles size are injected.

TABLE III
Particles of Different Diameters Used in CFD Simulations

PM type	Particle diameter (nm)	Normalized number concentration
Small particle in nuclei mode	5	0.0241
Typical particle in nuclei mode	10	0.3131
Typical particle in nuclei mode	20	0.5010
Large particle nuclei/accumulation mode	30	0.0722
Large particle nuclei/accumulation mode	50	0.0144
Large particle nuclei/accumulation mode	100	0.0289
Typical particle in accumulation mode	150	0.0193
Typical particle in accumulation mode	200	0.0120
Large particle in accumulation mode	250	0.0096
Large particle in accumulation mode	300	0.0048
Large particle in accumulation mode	500	0.0005
Particle in coarse mode	1000	-

C. The Species Method

Particle simulations with the Euler Lagrange discrete phase model can be time demanding since it requires extensive computational power to compute the trajectories of each individual particle. Therefore a method to screen the particle trapping efficiency for different catalyst design was applied. A Brownian diffusion is the predominant mechanism for depostion of particle on catalyst wall, at least for small particles with diameters of 5-10nm. To simulate tracers or

species released from the inlet of the channel which are asigned a Brownian diffusivity representative for a specific particle diameter. A user defined function where the diffusivity of each species is set according to the below Table IV was applied. The exhaust flow to be simulated in CFD simulations will then be represented as amixture of air and six different species.

TABLE IV
BROWNIAN DIFFUSIVITIES ASSIGNED AS A DIFFUSIVVITY FOR DIFFERENT SPECIES IN A USER DEFINED FUNCTION, AT 300^{0}C AND ATMOSPHERIC PRESSURE

Species	Particle diameter (nm)	Brownian Diffusivity (m^2/s)
A	5	8.337×10^{-7}
B	10	2.100×10^{-7}
C	100	2.390×10^{-9}
D	150	1.137×10^{-9}
E	500	1.535×10^{-10}
F	1000	5.848×10^{-11}

D. General Conditions and Boundary Conditons

The exhaust gas simulated where given the same conditions as air at 300^{0}C: a dynamic viscosity of μ=2.93×10^{-3} and density of ρ=0.61 kg/m^3. A viscous laminar model was used for soot particle motion. Transient thermal effect such as thermophoresis and temperature gradients were neglected and isothermal conditions assumed. The standard velocity inlet boundary condition was used with a velocity of 10m/s and a pressure outlet boundary condition. A laminar velocity profile is expected to be developed after 5mm in the monolith channel therefore the first promoter was always positioned at least 10mm from the inlet. The distance from the last promoter and channel outlet had to be a minimum of 20mm to avoid convergence difficulties due to large variation in the velocity profile. The wall boundary conditions was set to instant trapping for particle simulations, the position of all particles injected in to the channel were then obtained once they encountered a wall or moved through the outlet. Each particle hitting a wall was considered trapped in the catalyst, reflections and reentrainment effects were not considered. All the simulations on the catalysts where made in three dimensions with double precision.

E. Simulation of Forces Acting on a Particle in a Vortex

The monolith channel width corresponded to 2 mm, therefore the vortex radius was set to 0.5 mm and a cylindrical coordinate system with coordinate zero in the vortex center applied. Assuming an initial particle position at 0.25 mm from the wall and also from the center of the vortex, the angular velocities required for particles of the twelve different sizes to reach the wall were calculated. Assuming initial conditions: zero radial velocity for the particle and position 2.5×10^{-4}m.

All the cases were also tested with different inlet flow velocities: 5, 10 and 15 m/s. The four promoters were placed to create a rotational flow or swirling flow so fluid elements would be exchanged and particles deposited on the walls due to the formed vortices. The expected flow pattern can be viewed in Figure 6 and should be compared to the velocity profiles for planes placed 10 mm behind the promoters.

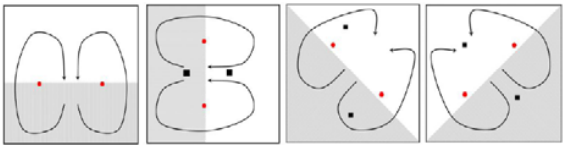

Fig. 6 Flow loops in sequence

Expected flow pattern observed downstream from the obstacle (shaded grey). The arrows indicate the fluid motion after the obstacle. Red circular dots indicate centers of fluid rotation and black square boxes indicate where the previous centers of fluid rotation were positioned.

VII. RESULTS

Solving the equation of motion, centrifugal and drag equations gives the result plotted in Figure 7 for the movement of particles in a vortex. The response time for a 5 nm particle is roughly 9.5 ms and for a 1000 nm particle 1.89 s

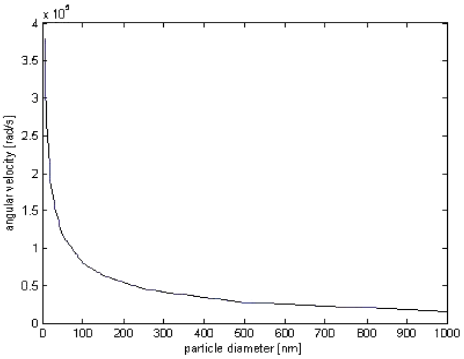

Fig. 7 Particle movements in a Vortex

Angular velocity in radians/s required for particles to move 0.25 mm in radial direction in a vortex and thereby hit a monolith channel wall. Calculation based on the assumption of a particle retention time of 20 ms. The values created with promoters are thus at least 10 smaller than the required for particles to move 0.25mm during 1 ms and deposit on the catalyst walls. The trapping efficiency and pressure drop increases with the angle α from 35-55^0. Hence there is a trade off between trapping efficiency and allowed pressure drop.

TABLE V
OBTAINED PRESSURE FROM SIMULATIONS, % COLUMN IS THE INCREASE IN PRESSURE COMPARED TO AN EMPTY CHANNEL

Case	δ P	% increase
4.0	102.4	-
4.1	137.3	34.1
4.2	160.4	56.6
4.3	192.7	88.1

The trapping efficiency in the geometry with 45^0 angle reached 7.5 % for 5nm and 3.1% for the 10 nm particles. This angle was further evaluated with DPM simulations with the Brownian diffusion turned off since the commercial available catalyst had the same angle. The highest particle trapping was achieved for case 4.3 (55^0 angle), 7.8 % and 3.5% for 5nm and 10 nm respectively.

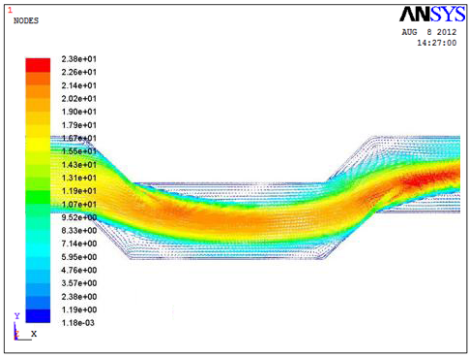

Fig. 8 Velocity vectors case 4.2

Without Brownian diffusion all the particles in the considered size range end up on 0.75 to 1% in trapping efficiency. The DPM failed to capture inertial effects for larger particles the current simulation. The larger particles are prone to hit the walls directly since it takes longer for them to respond to flow changes. In Figure 8, the velocity vectors show small recirculation zones, which can prove beneficial for distributing of particles on the wall.

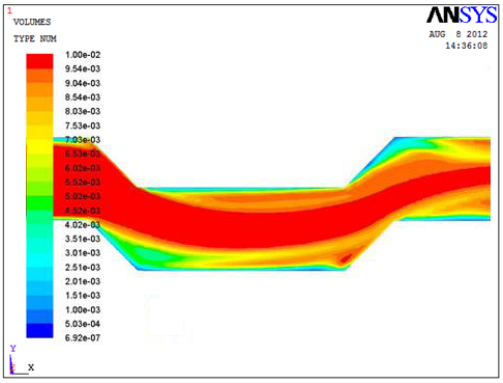

Fig. 9 Countour of mole fraction case 4.2

The trapping efficiency for all the case series were simulated and is show in Figure 10 where it is clearly observed that cases with higher angle α and steeper descent of the walls captures more particles directly on the walls.

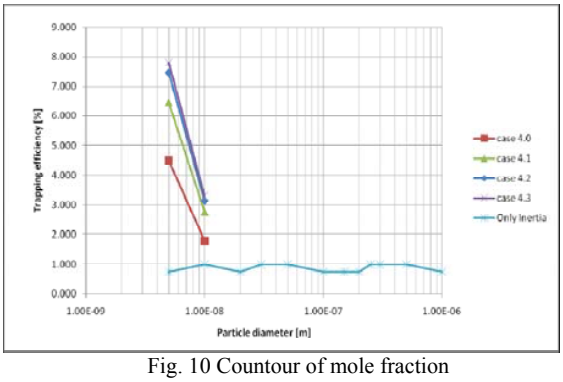

Fig. 10 Countour of mole fraction

VIII. Conclusion

The result of the discrete phase model is dependent on the injection routine used, distances from walls and between particles and on the number of particles injected. At the same time it is the only method to attain information of inertial effects and to model different forces causing particle deposition and is not limited to a certain particle size. The results provide support for using the species method for quick screening of catalysts designs. Despite from the fact the method is restricted to smaller particles (5 and 10 nm particles) with a prominent Brownian diffusion, it provides better accuracy and shorter simulations times than the DPM method. Particles of smaller size, 1-10 nm were trapped to a larger extent than other considered, with modified monolith catalysts. However trapping 100-1000 nm proved to be more difficult and no increase in deposition of larger particles due to inertial effects were observed.

Data on angular velocities in vortices from the simulated designs clearly show that creating strong enough vortices with promoters for particles to deposit on the walls is difficult. Improving the fluid element mixing with more turbulence would also have to be weighed against the increase in exhaust back pressure. The principle of forcing the flow and particles near walls for instance through the use of planes in a channel, is rather the main option to consider. The comparison of the different designs with a wall flow filter does show that the options for altering a design of a flow through filter, without imposing a too large pressure drop penalty are good.

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