

Multi-Dimensional Modeling of the Soot Deposition Mechanism in Diesel Particulate Filters

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ABSTRACT

A computational, three-dimensional approach to investigate the behavior of diesel soot particles in the micro-channels of wall-flow Diesel Particulate Filters is presented. The *KIVA3V* CFD code, already extended to solve the 2D conservation equations for porous media materials [1], has been enhanced to solve in 2-D and 3-D the governing equations for reacting and compressible flows through porous media in non axes-symmetric geometries.

With respect to previous work [1], a different mathematical approach has been followed in the implementation of the numerical solver for porous media, in order to achieve a faster convergency as source terms were added to the governing equations. The Darcy pressure drop has been included in the Navier-Stokes equations and the energy equation has been extended to account for the thermal exchange between the gas flow and the porous wall. The mesh generator *K3PREP* and the code have been extended to define geometries having an arbitrary number of symmetry axis, in order to perform simulations of 3D sectors of the filter, where a sector represents a group of DPF channels.

Also, Lagrangian particles in the flow were used to represent the diesel soot particles. The increase of the soot cake layer thickness on the porous wall and its spatial distribution as a function of time have been determined by the fully coupled particle-hydrodynamics in the gaseous flow, since *KIVA3V* calculates in the computational domain the rates of mass, momentum, and energy exchange between the gas and particles. The influence of gas molecules-particle interaction on overall particle behavior is examined by including Brownian motion and partial slip in particle equation of motion. Simulations help to highlight three-dimensional non-uniform particle deposition, mainly due to flow distribution in the micro-channel; the soot packing density and thickness on each face of the computational

porous cells are calculated.

A set of unsteady simulations was run to steady state for wall-flow Diesel Particulate Filters having substrates with different geometrical and physical properties. Distinct types of diesel particulate matter (PM) in terms of chemical composition, concentration, and size distribution, known by the experiments carried out on a single-cylinder 2.3-liter D.I. heavy-duty diesel engine, were used in the simulations. The experimental distribution of particle sizes and density was injected through the inlet boundary of the computational domain and its deposition along the filter porous surface was monitored. A validation of the code has been carried out by the comparison with pressure drop measurements across the different DPFs studied.

INTRODUCTION

More stringent limits on emissions for Diesel engines adopted in Europe and in the US require the use of after-treatment devices both on heavy and light duty engines. In particular, Diesel Particulate Filters (DPF) are nowadays the most common technology used to reduce PM emissions in diesel-fuelled passenger cars; depending on their material, DPFs have shown high filtration efficiencies (frequently in excess of 92%) and thermal durability. The most important issue with diesel traps is filter regeneration: because of the fuel penalty resulting from the increased backpressure of the loaded DPF, it is necessary that the filter be regenerated, during the normal engine operation. Filter regeneration strongly depends on the hydrodynamic performance of the filter, which is strictly related to the soot deposition mechanism. Optimal filtering efficiency leading to longer regeneration cycles would be ensured by a uniform particle distribution in the filter cross-section [2]. To understand and possibly optimize particle deposition inside micro-channels, accurate local measurements are required; since measurements

are hard and costly, three-dimensional simulations may be helpful to characterize the particle behavior inside the flow field developing in the porous walls micro-channels.

Mathematical modeling of the hydrodynamics and regeneration in diesel particulate filters has been the subject of continuous research since the introduction of the wall-flow exhaust filtration technology. The modeling framework developed by Bisset [3] has allowed a single channel flow and thermal regeneration representation of the entire filter. Konstandopoulos et al. [4] built upon that framework and developed a wall filtration model so that the filtration could be studied; in the following years, models to simulate the oxidation of PM by NO_2 in the cake layer have also been developed by researchers [5; 6; 7; 8] and they were included in zero-dimensional codes [9], one-dimensional codes [10; 11; 12] or integrated models [13; 14]. One-dimensional and zero dimensional DPF channel models are certainly informative and they are able to provide information on the axial variations of flow, temperature and soot loading in the channel, by means of descriptors defined on the basis of the researchers' experience; on the other hand, the three dimensional simulation is the only way to obtain a detailed comprehension of the phenomena occurring in filter channels. A complete three-dimensional DPF simulation may require a high computational effort to describe a four-hour filter loading process, because the time step of the numerical solver is usually on the order of 10^{-8} seconds; hence, decoupling the fluid-dynamic processes and the soot load variation (by neglecting the particle inertia [15; 16]) represents a very common strategy for CFD simulations of diesel particulate filters.

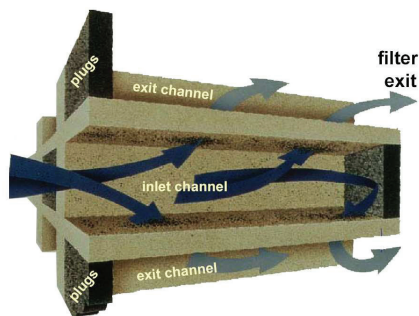


Figure 1: 3D schematic of the two channel system in a Diesel Particulate Trap (courtesy of [17]).

This paper shows some enhancements of the work previously published in [1] on the KIVA3V CFD code: the complete Lagrangian track of the particles in the flow has been simulated, in order to obtain detailed information in terms of mechanical and chemical properties of the soot particles building up the soot cake. Also the velocity flow field, and the particle Stokes numbers are investigated.

A specific soot particle-gas interaction model was implemented in the code; the Stokes-Cunningham slip correction factor [18; 19; 20] and the effect of the Brownian force [21; 19] were included in the expression of the drag coefficient, to account both for the increased resistance of the aerosol particles and for the effect of the kinetic energy of the gas molecule on particle trajectory.

A detailed description of the logic followed for the mesh generation of 2D and 3D filter geometries, for the implementation of the modified equations and of the boundary conditions for two phase-flow problems is given. An overview of the new numerical procedure used for the solution of the momentum equation for porous media is described; the result is a strong improvement of the computational accuracy and efficiency of the numerical solver, whose predictive capability is discussed. A user-defined soot particle distribution at the inlet section of the computational domain has been imposed and the composition of the soot cake at different locations of the channel has been studied, by monitoring the size distribution of the collected particles on the porous surface. While the three-dimensional solver has been tested for simulation of Diesel Particulate Filters, the mesh generator and the code, as well as the employed boundary conditions, were implemented for general applications.

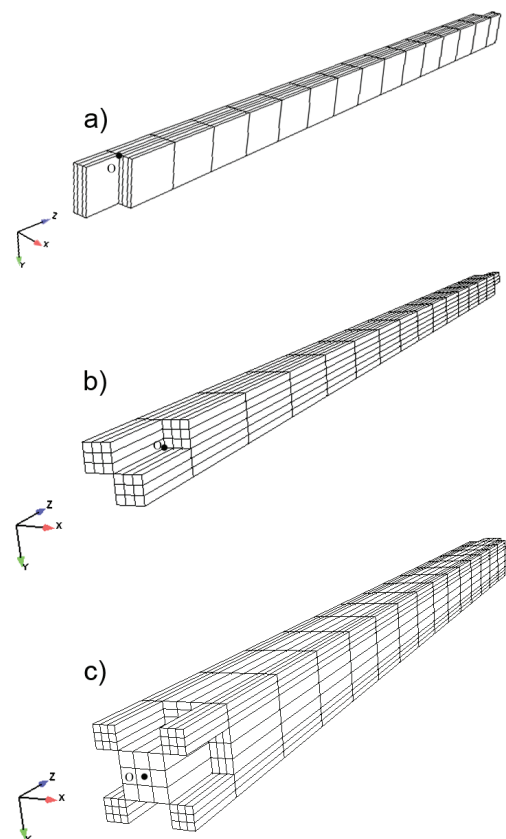


Figure 2: Different approaches to model Diesel Particulate Filters: a) 2-D modeling b) 3-D modeling by means of a four-channel geometry c) 3-D modeling by means of a nine-channel geometry. The boundary planes of the computational domain are symmetric. The axis origin is located in correspondence of point O.

MESH GENERATION

In the proposed approach, the gas entering the front face of the monolith is assumed as spatially uniform, so each channel of the Diesel particulate trap is supposed to be fed by a flow having the same thermo-fluid dynamic properties across the inlet section, but possibly time-dependent. So, the filter may be seen as a periodic arrangement of longitudinal, square-section micro-channels; ceramic plugs are placed in a chessboard arrangement either at the end or at the beginning of each channel. The exhaust gas flow is modeled as a particle laden flow; while it goes through the porous-ceramic walls, the gas soot particles deposit in the micro-pore network of the walls and build the soot cake. Under these assumptions, the fluid-dynamic behavior of the filter channels which are open on their inlet-end may be represented by the a single rectangular inlet channel; the same holds for the outlet channels, so the study of the trap may be reduced to the system shown in Figure 1.

In this work, the computational mesh has been created by the open-source mesh generator *K3PREP*, which has been extended by the authors to define DPF geometries. Since *KIVA3V* has been originally developed with applications to internal combustion engines in mind, it contains several features designed to facilitate such applications: the automated mesh generator allows to easily create 2-D or 3-D cylindrical grids for a wide variety of piston and head shapes but several modifications were required to extend *K3PREP* to define different geometries.

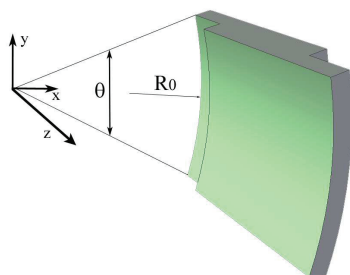


Figure 3: In *K3PREP* the generation process of the DPF geometry in two-dimensions is performed by rotating the azimuthal plane (where the two-channel system lays) about the symmetry axis by an angle $\theta = 0.5^\circ$ to form a cylindrical sector.

The simplest multi-dimensional approach to model a DPF consists of a two channel geometry in two-dimensions (Fig. 2-a). More detailed information, of course, may be obtained by three dimensional simulations of four-channel systems (3D-4, Fig. 2-b) and of nine-channel systems (3D-9, Fig. 2-c). For each case, the global right-handed Cartesian coordinate system in the computational grid has been chosen with the orientation of z-axis longitudinal (z is parallel to the filter-channel axis), while x-axis and y-axis have been oriented perpendicularly to the

porous surface. The exact location of the origin O and the orientation of the coordinate system vary with the geometry of the channel system modelled, as shown in Fig. 2-a, 2-b and 2-c. Note that since *KIVA3V* has been thought for cylindrical meshes, *K3PREP* treats the mesh generation as two dimensional; it initially creates the geometry for only one azimuthal plane xz, which is rotated about the axis z to create the remaining NYP azimuthal planes. With 2D geometries, only one plane is created by the rotation process.

The resulting grid is shown in Fig. 2-a; it looks similar to a three-dimensional grid, but it has just two planes in the y-direction where a periodic boundary condition is applied. The generation process of the DPF geometry in two-dimensions is shown in Fig. 3. The two-channels system lays on the azimuthal plane, which performs a rotation $\theta = 0.5^\circ$ about the symmetry axis to form a cylindrical sector. The symmetry axis is located at a distance R from the rotating plane; if R is assumed much greater with respect to the channel length, the curvature of the grid may be neglected.

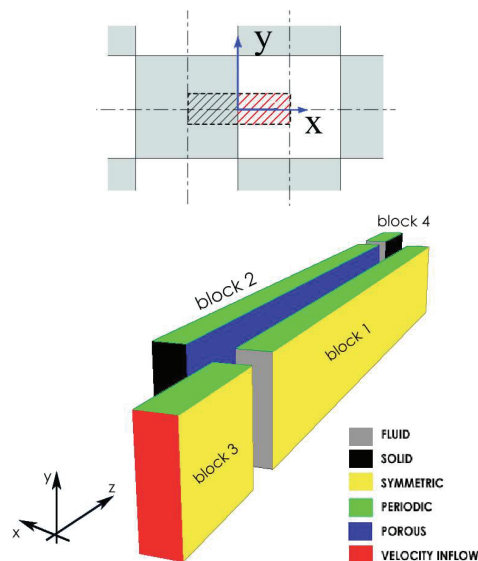


Figure 4: 2-D schematic of the two-channel DPF geometry. a) Boundary conditions used through the simulations; b) the CFD computational domain may be strongly reduced by considering the symmetries in the transverse plane xy.

Figure 4 shows the boundary conditions applied to the two-dimensional grid representing the two-channel geometry. Being the computational domain an elementary part of a periodic arrangement, in the two-dimensional schematization periodic conditions (labeled as "symmetric") were applied to all computational cell faces laying on the two azimuthal planes xz, where also a free-slip condition was applied; no-slip and no-cross boundary conditions were applied to the solid surfaces. With respect to previous publication [1], a different approach has been followed to model porous media, that now are treated as a boundary condition applied to cell faces. At the inlet boundary, an

uniform flow velocity (normal to the xy plane) is imposed; at the outlet channel end, mass conservation is ensured by a non-reflecting outlet boundary condition. Ad-hoc periodic boundary conditions were developed in *KIVA3V* to deal with the particle motion across the porous media and through periodic-symmetric boundaries and it will be discussed further in this paper. Several enhancements were required to extend the preprocessor *K3PREP* for the definition of three-dimensional DPF channel geometries, displayed in Fig. 2-b and 2-c. As it will be discussed further, the choice to model the 3D DPF geometry by a four channel system (Fig. 2-b) rather than by a nine-channel system (Fig. 2-c) strictly depends on the kind of periodic boundary condition used with multiphase flows.

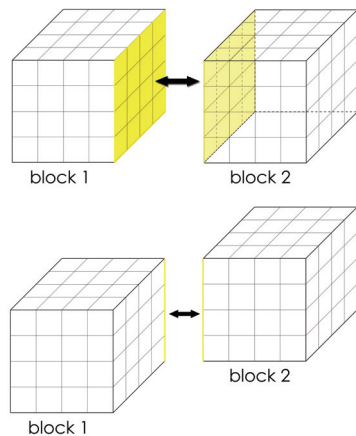


Figure 5: In the original version of *K3PREP*, different blocks in the computational grid may be patched only through common surfaces (a). In order to create 3-D DPF channel grids, *K3PREP* has been extended by the implementation of a new algorithm to patch blocks through edges (b).

In *K3PREP*, the computational grid may consist of several blocks and, in the original version, blocks can be patched only through their surfaces (Fig. 5-a). In order to create 3D multi-channel geometries (and non-cylindrical geometries, in general), the mesh generator needed to be extended to patch blocks through edges; this feature is not included in the original version of *K3PREP*, where a grid connectivity error occurs anytime edges of different blocks are connected. Hence, *K3PREP* has been extended by the implementation of a new algorithm that ensures the correct grid connectivity between different blocks connected by edges. In Fig. 6 a particular of the application of the patch algorithm to the three-dimensional DPF four-channel grid is displayed. In Fig. 7 the logic followed by *K3PREP* to create the four channels mesh and the boundary conditions defined for the computation in *KIVA3V* are shown; the computational domain is displayed in the transverse direction in Fig. 7-a. The four channel geometry is built by patching eight different blocks; blocks 6 and 8 represent the inlet plug ends where a uniform inlet velocity is applied as boundary condition, blocks 5 and 7 are the outlet plug ends

where an outflow boundary is set.

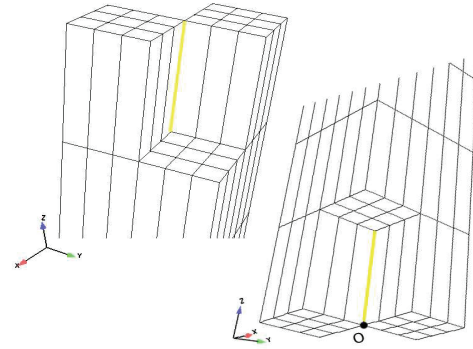


Figure 6: Application of the algorithm implemented in *K3PREP* to patch blocks sharing an edge to a DPF 3-D four channel geometry.

Yellow surfaces in Fig. 7 are periodic surfaces, black surfaces indicate solid walls (where a no-slip condition will be applied by the code). The porous surfaces (where the Darcy pressure term is added as a sink in the Navier-Stokes equation) are blue. For the 3-D simulation of wall-flow monolith channels arranged in a regular repeating pattern, the domain topology described is applicable to any channel cross-section.

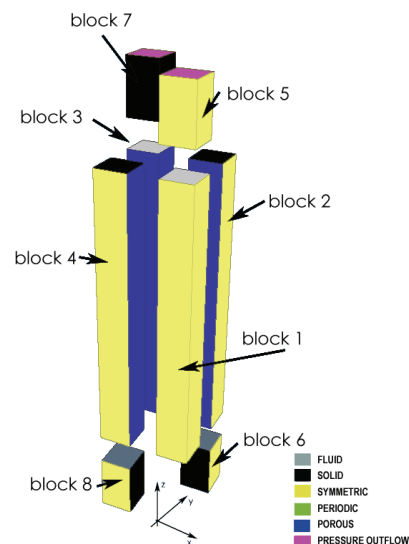
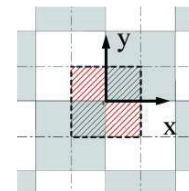


Figure 7: 3-D schematic of the four-channel DPF geometry modelled via a finite-volume CFD code for the solution of the NavierStokes equation in *KIVA3V*. a) the CFD computational domain may be strongly reduced by considering the symmetries in the transverse plane xy ; b) Boundary conditions used in the simulations.

As it will be stated further, a four-channel schematic can lead to satisfying results when the hydrodynamics of a clean trap is studied; on the other hand, a specific boundary condition must be implemented to correctly describe the particle motion across the periodic boundaries of the computational domain, as simulations with multiphase flows are performed.

The main features of the filter modeled are described in Tab. 1; experiments on this filter were performed at the test bench of the Engine Research Center and they were subject of previous publications [22; 23].

The overall length of the filter channel is $L=152$ mm, the plug length is 10 mm and the channel width is 2.28 mm. In the generated computational grids, 2 cells/mm in the transverse direction and 1 cell/mm along the axial direction have been set; this leads to have 5x152 hexahedral finite volumes (giving an overall amount of 760 cells) in the two-dimensional grid along x and z-axial directions respectively (just one finite volume is defined along the y-direction) and up to 40x40x152 hexahedral finite volumes in the three dimensional domain, displayed in Fig. 2-b.

Table 1: Specification of the Diesel Particulate Filter used in the Experiments and Simulations [22].

substrate	Cordierite
channel length	152 mm
plug length	10 mm
channel width	2.28 mm
porous wall thickness, w_s	0.432 mm
cell density	88 CPSI
porosity	48.8%
mean pore size	12.8 μ m

The physical domain of the CFD model must include sufficiently large regions upstream of the inlet channel, to make sure that the flow field inside the filter is independent from the inlet boundary condition; the inlet velocity boundary condition has been set therefore on a section located twenty-five channel sides (about 50 mm) upstream of the filter face. No regions were included downstream of the outlet section, since a non-reflecting boundary was imposed.

POROUS MEDIA SOLVER

KIVA3V numerically integrates the equations of motion of a chemically reactive mixture of fluids, coupled to the equations representing a single-component spray (of soot, in the simulations of this work). With respect to previous work [1], a more efficient numerical technique has been employed to enhance the Navier-Stokes solver to deal with porous media materials. *KIVA3V* makes use of a coupled implicit diffusion calculation for pressure wave propagation. The discretization of the governing equations involves a combination of the *Arbitrary Lagrangian-Eulerian* method [24] for spatial discretization, and variably implicit time-discretization methods (or variable *theta-methods*). In particular, all the time derivatives are approximated by

the first order difference:

$$\frac{\partial f(t)}{\partial t} \approx \frac{f^{n+1} - f^n}{\Delta t^n} \quad (1)$$

where $f=f(t)$ is a function of time, $f^n = f(t^n)$ and $\Delta t^n = t^{n+1} - t^n$. The subscript n indicates the values at the current time iteration.

For each time step, the calculation of the governing equations is performed in three phases [25]; the Lagrangian phase A calculates explicitly the contributions to the mass, energy and momentum equation due to the spray droplets and takes into account the effects of the gravitational forces. Phase B calculates by an implicit method the acoustic mode terms (pressure gradient in the momentum equation and velocity dilatation terms in mass and energy equations), the spray momentum source term, the terms due to the diffusion of mass, momentum and energy and the remaining source terms in the turbulence equation (that are neglected in this work, since the flow in DPF channels is assumed as laminar). In the third phase (C), the flow field is frozen and rezoned or remapped onto a new computational mesh. Results of the first phase, f^A , are used in the second phase (B), which produces f^B as result. At the end of the phase C, the value at $n+1$ is calculated.

$$f^n \rightarrow f^A \rightarrow f^B \rightarrow f^{n+1} \quad (2)$$

Time discretization of the governing equations in the code is performed by a variably implicit fashion by the use of implicitness parameters, denoted by ϕ ; the spatial discretization is a standard FV discretization for arbitrary hexahedrons. Since in *KIVA3V* thermodynamic quantities (cell volume V_{ijk} , cell pressure p_{ijk} , internal energy I_{ijk} , mass density ρ_{ijk}) are located at the center of the cell ijk , while velocities are located at the vertices, the numerical solver makes use of a staggered grid for the velocity components. Hence, spatial discretization is performed on the momentum cells (cell centered about the vertices), by converting the volume integrals to surface integrals by the divergence theorem. Once this is done, the volume integrals are approximated by function values at the cell center. The momentum equation

$$\frac{\partial(\rho \vec{u})}{\partial t} + \nabla \cdot (\rho \vec{u} \cdot \vec{u}) = -\frac{1}{\alpha^2} \vec{\nabla} p + \nabla \cdot \vec{\sigma} + \rho \vec{g} + \vec{F}^s \quad (3)$$

is written in the integral form as:

$$\begin{aligned} \frac{\partial}{\partial t} \left[(M')_{ijk} \vec{u}_{ijk} \right] = & g_{ijk} (M')_{ijk} - \frac{1}{\alpha^2} \sum_{\beta} p_{\beta} (A')_{\beta} \\ & + \sum_{\beta} \vec{\sigma}_{\beta} (A')_{\beta} + \vec{F}_{ijk}^s V'_{ijk} \end{aligned} \quad (4)$$

where α is the PGS parameter, that is used to artificially raise the Mach number in subsonic flows [25]. $\vec{F}^s$ is the spray source term. Since the flow is laminar in DPF channels, the source term for the turbulence in Eq. (4) has been neglected in this work; similarly, the alternate node coupler, that controls the parasitic pressure modes, has not been used, because it did not provide any significant improvement to the solution accuracy in our computation. As the momentum equation is solved for porous cells, another source term is added to the momentum equation to account for the Darcy pressure loss through the porous media. In *KIVA3V* time discretization is employed by a generalized form of the theta-method, where theta is represented by the implicitness parameters ϕ_p and ϕ_D , which are computed automatically from stability considerations [25]. The resulting discretized form of the momentum equation is:

$$\begin{aligned} \frac{(M')_{ijk}^B u_{ijk}^B - (M')_{ijk}^n u_{ijk}^n}{\Delta t} &= g_{ijk} (M')_{ijk} + (F_{ijk}^s V_{ijk}')^n \\ &- \sum_{\beta} [\phi_p p^p + (1 - \phi_p) p^n]_{\beta} (A')_{\beta}^n - \frac{1}{\Delta t} (R'_{ijk} + S'_{ijk} \vec{u}_{ijk}^p) \\ &+ \sum_{\beta} [\phi_D \vec{\sigma}(\vec{u}^p) + (1 - \phi_D) \vec{\sigma}(\vec{u}^n)]_{\beta} (A')_{\beta}^n \end{aligned} \quad (5)$$

M' , V' , A' are respectively the flow mass, the volume and the surface area of the momentum cell ijk , belonging to the staggered grid. ϕ_D and ϕ_p are the variable implicitness parameters, used in differencing the mass diffusion terms and the pressure gradient term respectively. The terms R'_{ijk} and S'_{ijk} concern with the coupling of the gas and droplets velocities and they come from the discretization of the source term $\vec{F}^s$ in Eq. (5); their value is set during the explicit calculation of the spray droplet interactions between particles and fluid (phase A). Analytical expression of R'_{ijk} and S'_{ijk} are given in Appendix H of [25].

Computation of the body forces and of the effects of chemical reactions and spray droplets interactions due to the species injected into the fluid in Eq. (5) is performed explicitly in phase A.

Time-advanced pressures p^p are calculated by an implicit diffusion iteration, referred to as *outer iteration*, which is the most time-consuming phase. The *outer iteration* includes the momentum equation, the internal energy equation and the pressure equation; for each iteration of the *outer iteration*, the predicted pressure is first initialized according to the extrapolation formula, in order to reduce the number of iterations required to solve the pressure equation:

$$p_{ijk}^p = (p_{ijk}^B)^{n-1} + \frac{\Delta t^n}{\Delta t^{n-1}} [p_{ijk}^B]^{n-1} - p_{ijk}^B]^{n-2} \quad (6)$$

Eq. (5) is linear in $\vec{u}^B$ and may be written as follows:

$$\begin{aligned} \sum_{\beta} [\phi_D \vec{\sigma}(\vec{u}^B) (A')_{\beta}^n] + [(M')_{ijk}^B + S'_{ijk}] \vec{u}_{ijk}^B \\ = \vec{F}_u(\vec{u}_{ijk}^n, p^B, p^n, \dots) \end{aligned} \quad (7)$$

The linear system $Ax=B$ (where $x = \vec{u}^B$) written in (7) is solved by the preconditioned conjugate residual method [26; 27]. The conjugate residual method implemented in *KIVA3V* is an equivalent to the implementation of the Omin algorithm; this numerical method converges in n steps (where n is the dimension of the coefficient matrix A), only if the coefficient matrix A , the preconditioner C (where C in *KIVA3V* is the *Jacobi preconditioning*, a diagonal matrix containing the reciprocal of the diagonal elements of the implicitly defined matrix A) and the matrix $B=ACA$ are symmetric positive definite (spd). The addition of source terms and the boundary conditions may create nonsymmetries in the resulting discretized operators, so the conjugate residual method is not guaranteed to converge.

The numerical method used in the code is quite robust, but the nonsymmetries in the coefficient matrix A make the numerical solver slower to converge; this may also happen as the porous media source term is added to the momentum equation (4):

$$\Delta P_{porous} = - \left(\frac{\mu \cdot w_w}{k_w} - \frac{\mu \cdot w_{soot}}{k_{soot}} \right) u_W + \beta \rho u_W^2 w_w \quad (8)$$

Note that the pressure drop across the porous wall is a function of the wall flow velocity (flow velocity component in the transverse direction), which changes for each iteration of the conjugate residual method. The second term on the RHS of Eq. (8) is the Forchheimer term [28].

Formally, the most accurate solution of the linear system describing the velocity was followed in [1], where the source term representing the pressure drop was calculated as follows:

$$\Delta P_{porous} = - \left(\frac{\mu \cdot w_w}{k_w} + \frac{\mu \cdot w_{soot}}{k_{soot}} \right) \vec{u}^p - \beta \rho (\vec{u}^p)^2 w_w \quad (9)$$

where $\vec{u}^p$ is the wall flow velocity, defined as the component of the flow velocity normal to the the porous face of the momentum cell; the superscript p indicates that it is calculated at the current iteration of the current time step by the conjugate residual method implemented in *KIVA3V*.

In [1], the porous source term was added as an implicit volume term and this seemed to increase the nonsymmetries in the resulting discretized linear operators when the system was solved iteratively; this caused that the convergency of the solver was slow to obtain and that it was not always guaranteed, in particular as very low permeability for the porous media were used

in the simulations.

If the wall flow velocity calculated at the previous time step is used in Eq. (8), the porous media source term is explicit:

$$\Delta P_{porous} = - \left(\frac{\mu \cdot w_w}{k_w} + \frac{\mu \cdot w_{soot}}{k_{soot}} \right) (u_W)_{ijk}^n - \beta \rho [(u_W)_{ijk}^n]^2 w_w \quad (10)$$

where $(u_w)_{ijk}^n$ is the wall flow velocity across the porous media cell calculated at the previous time step n . For porous cells, the momentum equation takes the form:

$$\begin{aligned} \frac{(M')_{ijk}^B u_{ijk}^B - (M')_{ijk}^n u_{ijk}^n}{\Delta t} &= g_{ijk} (M')_{ijk} + (F_{ijk}^s V_{ijk}')^n \\ - \sum_{\beta} [\phi_p p^p + (1 - \phi_p) p^n]_{\beta} (A')_{\beta}^n &- \frac{1}{\Delta t} (R'_{ijk} + S'_{ijk} \tilde{u}_{ijk}^p) \\ + \sum_{\beta} [\phi_D \tilde{\sigma}(\tilde{u}^p) + (1 - \phi_D) \tilde{\sigma}(\tilde{u}^n)]_{\beta} (A')_{\beta}^n \\ + \sum_{\beta} \Delta P_{porous} (A')_{\beta}^n \end{aligned} \quad (11)$$

As the momentum equation for porous media cells is solved, the explicit porous source term is added to the right hand side of the linear system (7), which takes the form:

$$\begin{aligned} \sum_{\beta} [\phi_D \tilde{\sigma}(\tilde{u}^B) (A')_{\beta}^n] + [(M')_{ijk}^B + S'_{ijk}] \tilde{u}_{ijk}^B \\ = \tilde{F}'_u(\tilde{u}_{ijk}^n, p^p, p^n, \Delta P_{porous}, \dots) \end{aligned} \quad (12)$$

Theoretically, the use of the wall flow velocity of the previous time step would not be the best choice for the calculation of the porous source term; anyways, since the magnitude of the time step in the computation is of the order of $10^{-7} \div 10^{-8}$ s, the variation of the wall flow velocity is small ($\tilde{u}_{ijk}^{n+1} \simeq \tilde{u}_{ijk}^n$), and the committed error may be considered as negligible. Also, if steady state engine operating conditions are simulated, the velocity flow field does not vary with time ($\tilde{u}_{ijk}^{n+1} = \tilde{u}_{ijk}^n$) as the steady state operating condition is reached by the numerical solver.

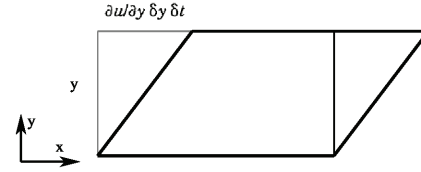


Figure 8: Cell distortion due to the velocity gradient after the phase B.

The cause of the small timesteps used by the numerical solver implemented for porous media may be found by looking at the automatic time step control of KIVA3V. In the code, the temporal difference scheme is implicit in the Lagrangian phase (B), for the diffusion terms and for the terms associated with the wave propagation. Conversely, temporal difference scheme is explicit when convection in the rezone phase are calculated; in this case, the convection timestep is a submultiple of the main computational timestep in order to satisfy the Courant stability condition. The timestep Δt during the implicit calculation (phase B) is varied to test for temporal accuracy:

$$\Delta t^{n+1} = \min(\Delta t_{acc}^{n+1}, \Delta t_{rst}^{n+1}, \Delta t_{ch}^{n+1}, \Delta t_{sp}^{n+1}, \Delta t_{gr}^{n+1}, \Delta t_{max}, \Delta t_{maxca}) \quad (13)$$

Each term Δt_i in the right hand side of Eq. (13) represents a different accuracy condition upon which the automatic selection of Δt is based.

Δt_{acc}^{n+1} is dependent on the mesh size; it is defined as :

$$\Delta t_{acc} = \min_{ijk} \frac{f_{\alpha} \Delta x_{ijk}}{|\tilde{u}_{ijk}^B - \tilde{u}_{ijk}^B|} \quad (14)$$

The accuracy constraint (14) is the only one in which the cell size Δx appears; according to it, the timestep must be reduced as the mesh is refined. This accuracy constraint, together with the Δt_{rst} , represents a serious restriction for the timestep for the DPF channel simulation. Since the DPF channel is very thin (the square channel side for a typical Cordierite wall-flow Diesel Particulate Filter may be about 2 mm and the porous media thickness for the same filter is smaller than 0.5 mm), the computational grid must be very fine in the transverse direction.

Also, a big constrain for the timestep used in DPF simulations is given by the accuracy condition:

$$|\lambda| \Delta t_{rst}^n < 1/\sqrt{3} \quad (15)$$

where λ is originally an eigenvalue of the rate of strain tensor $\tilde{\sigma}$ and it is correlated to the spatial distortion of