

CODE COUPLING TO ENHANCE CFD ANALYSIS OF I.C. ENGINES

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Abstract. *Modeling internal combustion engines (I.C.E.) can be made following different approaches, depending on the type of problem to be simulated. 1D models can be used to study unsteady conditions of the engine or for those applications requiring a great number of cycles to be simulated. Such models can also be used to give boundary conditions for 3D codes since it is still computationally hard, for the latter, the simulation of the whole engine. The basic idea of this paper is to couple the two methods in order to use the peculiarity of both. The coupling is based on the transfer of the interface boundary conditions of the two codes at each time step. The 1D code is based on a finite volume high resolution TVD scheme while the 3D code is a modified version, able to model GDI full cycle, of the well known Kiva code. For the 3D code a boundary condition based on the mass flow rate and the pressure obtained from the 1D code, is applied. For the 1D code we have adopted an absorbing boundary conditions strategy to compute the flow state at the coupling interface. In this paper we present details of the implementation and results of a four cylinder engine where experimental measurements are available. In this problem the intake plenum is solved by the 3D code while the 1D code is used for the rest of the whole engine configuration. This development will be applied in the near future for engine design optimization.*

1 INTRODUCTION

Following Heywood¹ and Ramos² historically the researchers and engine designers have been using four different categories of internal combustion engine models:

- air standard cycle simulation,
- zero and quasi-dimensional thermodynamic models,
- a combination of zero dimensional and one dimensional models,
- multidimensional models

The first approach was used in the past when only human work were available with no computer capabilities. At most this model might be enhanced with some graphical technique for the gas dynamics in the intake and exhaust system if the scope of the work is to predict the whole indicated cycle, the power and pumping process. Following in complexity the zero dimensional thermodynamic models offer the possibility to include the unsteady behaviour of the system and the changing thermo-physical properties along the whole cycle. For the intake and the exhaust system the emptying and filling models³ may be an attractive technique because its simplicity. It consists of assuming a fixed volume for each manifold and follow their time evolution with some spatial average for the thermodynamic variables. In this sense this strategy represents a significant improvement relative to the earlier models because the gas charging process may be added to the whole computation and some sort of tuning may be predicted. However the traveling waves in the manifolds are not represented at all because the spatial averaging. In order to include this important effect that has a significant influence on the volumetric efficiency the following model includes a one dimensional representation of the gas flow inside the manifolds solving the mass, momentum and energy balance in each tube of the whole engine network^{4,5,6,7}. Therefore, a simple spatial discretization is adopted using some robust numerical scheme to solve the dynamical system. With the just above mention models it is possible to solve the entire engine configuration including several devices like cylinders, mufflers, manifolds, air intakes, tanks, junctions, carburetors, air cleaners, catalytic converters, and so on, with an accuracy level that depends strongly on some experimental measurements to calibrate the whole model^{3,8}. Multidimensional or CFD models extends the one dimensional spatial discretization presented before to the whole three dimensional domain with the added complexity of treating moving boundaries, turbulent and reactive flows with injection and combustion. This last kind of models deals with numerical techniques for more detailed and more accurate analysis but in this case only about an specific part of the engine. Historically Kiva code family was the pioneer in simulating internal combustion engines and currently its usage is very widespread in the scientific community⁹. However there are other commercial codes that may treat this kind of problems nowadays. Thinking about the simulation of the whole engine with a 3D approach is currently an unapproachable task, even though using powerful computer resources like parallel processing on supercomputers, cluster of workstations or personal computers. This is why a coupling between 1D codes and 3D codes is being seen as a promissory candidate to answer some complex problems of engine design. This paper focus on the numerical implementation of a 3D/1D codes coupling to be used in the future to solve industrial problems. In this work Kiva 3V⁴ was used as the 3D code and

for the 1D code we have chosen one developed by ourselves. Next sections are organized in the following manner: first a brief description of the one dimensional formulation of the gas dynamics equations and its numerical treatment, specially for the boundary conditions, next section includes how to build an interface between the code for the gas dynamics inside the tubes with the well known software KIVA and finally there is a section with some numerical results.

2 ONE DIMENSIONAL SIMULATION CODE

Current usage of 3D codes applied to internal combustion engines focus on an specific part of the whole configuration due to computational resources. So, they need in general a lot of experimental information to be used to impose boundary conditions. Very often this information is either very hard to obtain (in technical or economic terms) or impossible.

As aforementioned the one dimensional code is able to simulate the engine operation giving its performance and also a detailed information about its thermodynamics and gas dynamics response. The reasonable accuracy in its results makes this kind of code a good candidate to provide for good boundary conditions for the 3D computation

In general the one dimensional codes for internal combustion engines treat a set of devices using either a thermodynamic (zero dimensional) approach or a gas dynamic (one dimensional) one. Our 1D engine simulator includes the following devices:

- the intake and exhaust manifolds
- a set of cylinders,
- the intake and exhaust ports and valves,
- air intake or tanks
- junctions
- EGR valves

2.1 Tubes modeling

For the tubes we use a computational gas dynamics approach under the hypothesis that the main changes in the state variables inside the tubes occur in the longitudinal direction. Then, a one dimensional model is adopted considering the domain as a spatial curve with the goal of determining the main variables along the tube and assuming some sort of averaging for them at the cross section

2.2 Conservation equations

A set of nodes are placed along the longitudinal domain with the purpose of getting the traveling waves developed inside the manifolds and therefore being possible to gain some insight about the engine tuning, one of the main responsible for the volumetric efficiency. In order to include some 3D effects like variable cross section, viscous friction and heat transfer close to the wall in a one dimensional description some source terms are defined. Then, an inviscid gas dynamic model represented by Euler equations enhanced with extra sources terms to take into account for these effects is used. This mathematical model may be written in an integral form as:

$$\frac{\partial}{\partial t} \int_{\Omega} U \, d\Omega + \int_{\partial\Omega} F \cdot n \, d\Omega = \int_{\Omega} Q \, d\Omega \quad (1)$$

where $U = \{\mathbf{r}, \mathbf{r} u, \mathbf{r} e_{total}\}$ represents the unknown state vector in conservative variables way including the density, the linear momentum and the total energy.

$F = \{\mathbf{r} u, \mathbf{r} u^2 + p, \mathbf{r} u h\}$ is the advective flux vector where h is the specific enthalpy and

$Q = \{0, \mathbf{r} f_e, -q_{ht} + \mathbf{r} f_e u\}$ is the source vector term where fe is the external force, in this case it is due to the wall friction and qht is the heat transfer at the tube wall. To closure the above system we adopt the ideal gas law and some thermodynamic definition for the total and the internal energy:

$$\frac{p}{\mathbf{r}} = RT \quad ; \quad e_{total} = C_v T + \frac{1}{2} |u|^2 \quad (2)$$

with R the gas constant for gas contents and Cv the specific heat at fixed volume. To take into account variation in the cross section S we modify the whole set of equations including it inside them.

2.3 Numerical scheme

The set of partial differential equations aforementioned is spatially discretized using a finite volume and for time evolution we adopt a simple explicit scheme based on finite differences, like Forward Euler. The current trend in one dimensional problems is towards high resolution schemes preserving monotonicity and positiveness like TVD (total variation diminishing) or ENO (essentially non oscillatory) in a finite volume method. The hyperbolic system of conservation laws (Euler equations) may be solved with TVD, a high resolution scheme where total variation in the numerical solutions is non-increasing with time. Therefore unwanted oscillations are prevented. Our solution procedure is based on a second-order explicit TVD method by Harten¹⁰. In this work we transform the original system of PDEs (partial differential equations) in three decoupled scalar transport equations, we apply the second order TVD scheme to each one and finally we return to the original basis.

2.4 Boundary conditions

This is a critical point in terms of numerical stability and accuracy. In general a computational boundary may reflect and transmit incoming waves in a way that may be very different to that based on physical principles, specially if no care is taken in the numerical design of boundary condition. In one-dimensional simulation in general we split the treatment in two parts, first one is applied to atmospheric boundary conditions and the second for internal one. For the former we fix some variables according to the topological position in the network configuration and for the latter we applied an absorbing boundary condition strategy. For the atmosphere at the intake side we fix density and pressure and for that placed at the end of the last exhaust tube we fix only the pressure. Relative to absorbing boundary conditions we compute the new state variable at the boundary in

terms of the old state variable at the boundary and a reference state variable computed in terms of the conditions at the device connected to the tube. To do this we first do a change of variables to that base that decouple the three state variables and fix the transformed variables according to the direction of the three different waves arriving to the boundary. Finally we transform back to the original system. This methodology shows be very efficient in terms of stability and accuracy.

3 CYLINDER MODEL

This model assumes that the cylinder is a variable volume reactor. In general it is an open thermodynamic system with the inlet and outlet represented by the intake and exhaust valves. The internal energy varies according to the thermodynamic first principle that may be written in a time dependent form as:

Energy balance at cylinder

$$\dot{E} = \dot{m}_{in} h_{in} + \dot{m}_{out} h_{out} - p \dot{V} + \dot{Q}_{chem} - \dot{Q}_{ht} \quad (3)$$

Mass balance at cylinder

$$\dot{m} = \dot{m}_{in} + \dot{m}_{out} \quad (4)$$

The cylinder unknowns are the time dependent density, pressure and temperature of the spatially averaged gas contents. In order to closure this system we add an state equation under the assumption of being an ideal gas. The left hand side of the energy balance equation at the cylinder represents the change of rate of the internal energy of the cylinder gas contents.

The first two terms in the right hand side consider the enthalpy flow rate through the intake and exhaust valve. The third term is the work change rate between the system and the environment, in this case, the piston work represented by the force exerted by the cylinder gas pressure over the piston crown surface times the pistonspeed. This term may be written in terms of the volume change rate. The last two terms represent the heat releases between the system and the environment. One of them is due to the combustion process that may

be seen as an external heat source and the other is due to the heat transfer between the cylinder gas and the engine cooling system. The equation named mass balance at cylinder expresses how to update the mass inside the cylinder and consequently the gas density. In this expression appears the mass flow rate through the intake and exhaust valves.

Having updated the temperature from energy balance at cylinder equation and the density from the mass balance at cylinder equation we update the pressure from the ideal gas law

Therefore, to closure this set of equations we need to add the following models:

- the classic crank rod mechanism to compute $\dot{V}(\mathbf{q})$ ¹
- a combustion model to compute $\dot{Q}_{chem}(\mathbf{q})$ following Wiebe function.¹
- a heat release model $\dot{Q}_{ht}(\mathbf{q})$ following Annand model¹¹.

- flow through ports and valves $\dot{m}_{in/out} = \dot{m}(\mathbf{q})$ following Benson approach ⁸

For brevity we do not enter into details about these models that may be found in the cited references. For the same reason we only mention that for tanks it is possible to use the cylinder model taking into account that no volume changes occur and no combustion model is necessary. For junctions we have used the Corberan approach ¹²

4 INTERFACE BETWEEN THE ONE DIMENSIONAL SIMULATION CODE AND KIVA CODE

At first we did a preliminary version of this 3D/1D coupling for an ad-hoc example consisting of solving a single cylinder engine. In this version the cylinder (with the intake and exhaust ports) is solved by Kiva code and the 1D code computes the two manifolds.

In order to use both codes with minimum modifications we have chosen a strategy based on a dialog between the KIVA main program and those routines of SIM1D included through the external intake and exhaust variables used when KIVA adds the corresponding ports in the computation. In this case KIVA looks for the external intake or crankcase (pcc) and exhaust (pex) pressure arrays with the corresponding angle arrays capcc and capex, the intake and exhaust species density spdin0 and spdamb, an array of nsp components, being nsp the number of species involved in the computation and the main turbulence parameters tkeamb and sclamb representing the turbulent kinetic energy and the turbulent length scale at the vicinity of both ports. All these variables should be defined by the user in the itape5 file and in a standard KIVA computation they remain unaltered during the whole computation. In this first part of the work we propose to change their values in a dynamic way from the SIM1D computation and also specify the boundary conditions needed by SIM1D from some KIVA variables. Therefore, we propose to include two main routines for the interface,

- bc_kiva2sim1d, where the state variables at the intake and exhaust ports are built from some Kiva variables and they are imposed as the reference state in the boundary conditions for the SIM1D computation.
- bc_sim1d2kiva, where we overwrite the pressure, the species density and the turbulent quantities for the intake and exhaust ports from the results obtained by the SIM1D at the node placed immediately close to the KIVA ports.

This interface is completed with the following routines:

- the solver for the one dimensional gas dynamic equations
- the computation of the critical time step for the gas dynamic problem
- input and output standard routines

In the following sections we present some details concerning with the implementation of the two boundary conditions routines above mentioned.

4.1 Bc_kiva2sim1d routine

In Kiva code the `bndpres` variable is used to impose inflow and outflow pressure boundary conditions at the corresponding ports. In this case we assert this variable because we need the user input this kind of boundary conditions in the `itape5` file to link KIVA with the SIM1D code. Next we compute the normal velocity of each vertex splitting in inflow and outflow groups and doing some sort of average in the following form:

$$\begin{aligned}
 (\bar{v}_n)_{intake} &= \sum_{i=1}^{nvlpres} \bar{v}_i \cdot \bar{n}_i c_i^{intake} + \sum_{i=1}^{nvfpres} \bar{v}_i \cdot \bar{n}_i c_i^{intake} + \sum_{i=1}^{nvbpres} \bar{v}_i \cdot \bar{n}_i c_i^{intake} \\
 N_v^{intake} &= \sum_{i=1}^{nvlpres} c_i^{intake} + \sum_{i=1}^{nvfpres} c_i^{intake} + \sum_{i=1}^{nvbpres} c_i^{intake} \quad \forall i \in V^{inflow/outflow} \\
 \overline{(\bar{v}_n)_{intake}} &= \frac{(\bar{v}_n)_{intake}}{N_v^{intake}}
 \end{aligned} \tag{5}$$

where $V^{inflow/outflow} = V^{inflow} \cup V^{outflow}$ are the sets of vertices belonging to the inflow and

outflow pressure boundary condition, $c_i^{intake} = \begin{cases} 1 & \text{if } i \in V^{inflow} \\ 0 & \text{else} \end{cases}$ is a identification function in order to choose which vertex belongs to the intake port and which one belongs to the exhaust one being `nvlpres`, `nvfpres`, `nvbpres` the number of vertices belonging to $V^{inflow/outflow}$ associated with left, front and bottom boundary condition faces according to Kiva requirements. \bar{v}, \bar{n} are the velocity and the unit normal vectors and therefore $\overline{(\bar{v}_n)_{intake}}$ is some sort of normal velocity average at the inlet port. The same remains valid for the exhaust port.

The intake and exhaust density are computed by the summation of the species density grouped in the `spdin0`, `spdamb` arrays respectively,

$$\begin{aligned}
 \mathbf{r}_{intake} &= \sum_{isp=1}^{nsp} spdin0(isp) \\
 \mathbf{r}_{exhaust} &= \sum_{isp=1}^{nsp} spdamb(isp)
 \end{aligned} \tag{6}$$

The intake and the exhaust pressure are taken from the effective pressure computed in the piston routine of Kiva code from the `pcc` and `pex` arrays,

$$\begin{aligned}
 p_{intake} &= pcceff = pcc(1) \\
 p_{exhaust} &= pexeff = pex(1)
 \end{aligned} \tag{7}$$

These two arrays are in general defined by the user as a table of pressure measured from experimental data. In this case we only need a pair of values for both `pcc` and `pex` (`numpcc=2`,

numpex=2) and these values are changing dynamically by the KIVA-SIM1D coupling. Finally we need to do some unit conversion because both codes manage different unit systems, cgs uses Kiva and SIM1D uses mks.

4.2 Bc_sim1d2kiva routine

For each tube, in this case for the intake and the exhaust one we need to update the following arrays:

- pcc,pex
- spdin0,spdamb
- tkeamb,sclamb

For the pressure arrays we only impose those values corresponding to the end node of the tube partition close to the Kiva ports, so

$$\begin{aligned} pcc &\leftarrow P_{nmod}^{intake} \\ pex &\leftarrow P_1^{exhaust} \end{aligned} \quad (8)$$

being P_{nmod}^{intake} the last node of the intake tube and $P_1^{exhaust}$ the first node of the exhaust tube, both in contact with their respective ports. In order to compute the species density array we write the mass balance at each port

$$\begin{aligned} \dot{m} &\approx \frac{\Delta m}{\Delta t} = \frac{m^{n+1} - m^n}{\Delta t} \\ m &= \sum_{isp=1}^{nsp} m_{isp} = \sum_{isp=1}^{nsp} m x_{isp} \Rightarrow \sum_{isp=1}^{nsp} x_{isp} = 1 \\ m^{n+1} &= m^n + \Delta t \dot{m} \Rightarrow x_{isp}^n m^{n+1} = x_{isp}^n m^n + \Delta t x_{isp}^n \dot{m} \\ m_{isp}^{n+1} &= m_{isp}^n + \Delta t \dot{m} x_{isp}^n \\ \mathbf{r}_{isp}^{n+1} \Big|_{intake} &= \frac{m_{isp}^{n+1}}{Vol} \Big|_{intake} \\ \Rightarrow spdin0(isp) &\leftarrow \mathbf{r}_{isp}^{n+1} \Big|_{intake} = \mathbf{r}_{isp}^n \Big|_{intake} + \frac{x_{isp}^n}{Vol} [\Delta t \dot{m}] \Big|_{intake} \\ \Rightarrow spdamb(isp) &\leftarrow \mathbf{r}_{isp}^{n+1} \Big|_{exhaust} = \mathbf{r}_{isp}^n \Big|_{exhaust} + \frac{x_{isp}^n}{Vol} [\Delta t \dot{m}] \Big|_{exhaust} \end{aligned} \quad (9)$$

where Δt is the time step according to Kiva and Sim1d stability criteria, x_{isp}^n is the mass fraction of the isp species at the n-th time level, Vol is the manifold volume and \dot{m} is the mass flow rate at the

port. To compute x_{isp}^n we need to know the flow direction. If the flow is from the tube to the cylinder the mass fraction is taken from the `ispdin0` or `spdamb` array representing the species density at the whole intake and exhaust manifold under the assumption of instantaneous mixing inside each whole tube. In the other case, flow from the cylinder to the tubes, the mass fraction is computed from the species density at each vertex lying on the port section. Due to the Kiva code organization the species density arrays are available at each cell and we have to compute the corresponding values at each vertex of each cell.

$$x_{isp}^n \Big|_{intake} = \begin{cases} \frac{\mathbf{r}_{isp}^n \Big|_{intake}}{\sum_{isp=1}^{nsp} \mathbf{r}_{isp}^n \Big|_{intake}} & \text{if } \vec{v} \cdot \vec{n} > 0 \\ \frac{\overline{\mathbf{r}_{isp}^n} \Big|_{intake}}{\sum_{isp=1}^{nsp} \overline{\mathbf{r}_{isp}^n} \Big|_{intake}} & \text{if } \vec{v} \cdot \vec{n} \leq 0 \end{cases} \quad (10)$$

Where the density is computed through the following expression:

$$\overline{\mathbf{r}_{isp}^n} \Big|_{intake} = \frac{\sum_{v \in V^{inf low}} \mathbf{r}_v^n Vol_v}{\sum_{v \in V^{inf low}} Vol_v} \quad (11)$$

In the same way for the exhaust we have

$$x_{isp}^n \Big|_{exhaust} = \begin{cases} \frac{\mathbf{r}_{isp}^n \Big|_{exhaust}}{\sum_{isp=1}^{nsp} \mathbf{r}_{isp}^n \Big|_{exhaust}} & \text{if } \vec{v} \cdot \vec{n} > 0 \\ \frac{\overline{\mathbf{r}_{isp}^n} \Big|_{exhaust}}{\sum_{isp=1}^{nsp} \overline{\mathbf{r}_{isp}^n} \Big|_{exhaust}} & \text{if } \vec{v} \cdot \vec{n} \leq 0 \end{cases} \quad (12)$$

$$\overline{\mathbf{r}_{isp}^n} \Big|_{exhaust} = \frac{\sum_{v \in V^{outflow}} \mathbf{r}_v^n Vol_v}{\sum_{v \in V^{outflow}} Vol_v} \quad (13)$$

where \mathbf{r}_v^n, Vol_v is the vertex density and volume, respectively. To compute them we have used a cell to vertex routine

$$\begin{aligned} \mathbf{r}_v &= cell \rightarrow vertex(\mathbf{r}_c) \\ V_v &= cell \rightarrow vertex(V_c) \end{aligned} \tag{13}$$

For $[\Delta t \dot{m}]$ we have used the Kiva array called `fxv` at each vertex lying on the port sections. Having updated the species density at the intake and exhaust port we may return to a new Kiva time step computation.

Remarks

1. At each Kiva time step the one dimensional tube solver is called with a number of substeps being chosen according to the CFL stability criterion.
2. In this preliminary version the `tkamb,sclamb` parameters have been assumed as fixed values input by the user. In the future we may update these values according to some correlation formula taking into account the kinetic energy of the gas inside each tube.
3. The specific heats ratio \mathcal{g} for the tube computation is frozen to some original value input by the user. In the future we may update it according to the species density array at each manifold and the temperature.
4. In the future a one dimensional $\mathbf{k} - \mathbf{e}$ turbulence model may be included in the tube solver.

4.3 An extension to the general case

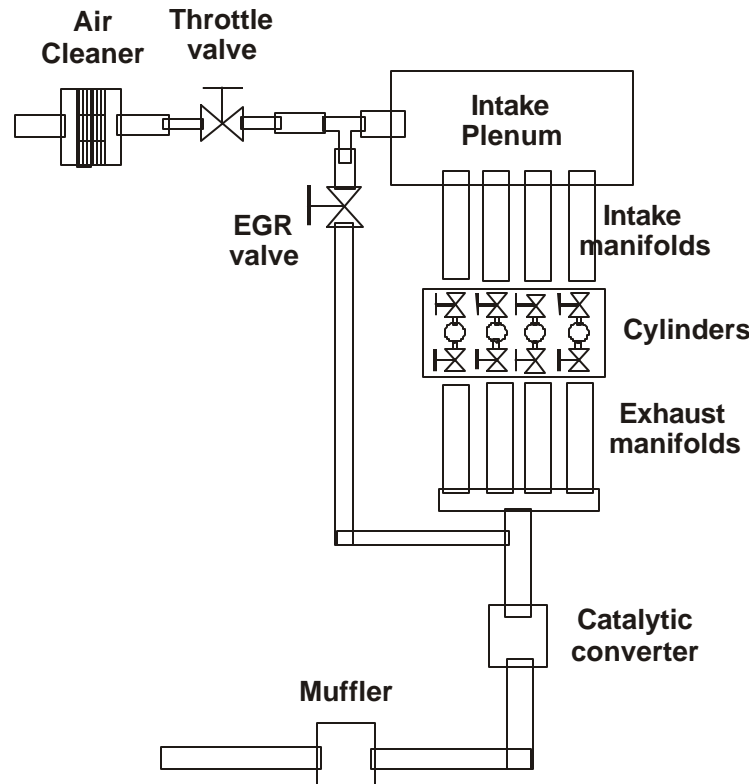
In general the coupling should consider the possibility to treat as three dimensional some part of the whole configuration defined by the user without imposing that the cylinder be the only device to be solved in this way. This generalization makes the coupling slightly more difficult because some routines of Kiva needs to be modified.

Briefly this generalization consists of replacing the `pcc` and `pex` one index arrays (vector) by the two index arrays (matrix) in order to include the possibility of having more than one inflow and outflow pressure boundaries. For the species density some modification is introduced in `bccfl` Kiva routine before calling `bcccin` routine, doing some loop over all the inflow and outflow pressure boundaries using only those vertex that belong to each specific pressure boundary in the computation.

5 NUMERICAL RESULTS

In this section we present only one example for brevity reasons to check the physical and numerical behavior of the KIVA-SIM1D coupling. This example is taken for code validation because we have some experimental records about it. It is a gasoline direct injection (GDI), 4 cylinder with 1.6 liters Fiat engine with EGR illustrated in the following figure.¹ The final goal of this simulation is to model mixture formation, combustion and the evaluation of EGR mass flow from inlet duct to the cylinders. Due to the great complexity in the simulation of this problem we divide the problem in two steps, the first one considers as three dimensional only the flow inside the intake plenum and the rest of the whole engine configuration is treated with the one dimensional code. In

this way an smaller problem like this makes feasible the test of the coupling without requiring huge computational resources. Once this example is solved we might add also the cylinders treatment as three dimensional in order to enhance the approximation including more physical phenomena involved in the operation of an internal combustion engine. An external view of the surface mesh for the intake plenum is observed in the figure 2. The 3D mesh is obtained using KIVA multi-block mesh generator.



Engine configuration

Fig. 1: Engine configuration

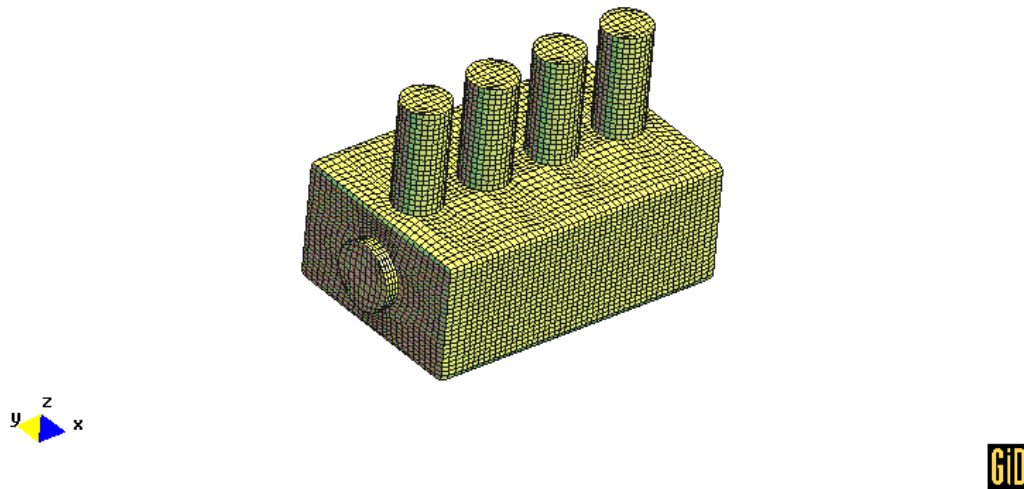


Fig. 2: Three dimensional intake plenum surface mesh

In the next figures we show some of the main fields solved by KIVA at the intake plenum. First the temperature in three cut planes showing a dissimilar spatial distribution due to the interaction between the intake system and each one of the cylinders.

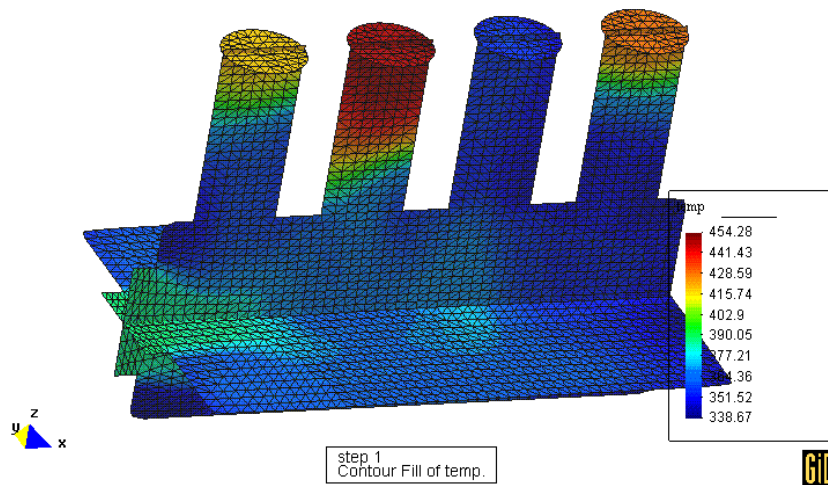


Fig. 3: Three dimensional temperature field at the intake plenum

Figure 4 shows some velocity fields in some cut planes where at this precise time step the intake valve of the third cylinder is open and a significant gas flow is being admitted by the corresponding cylinder.

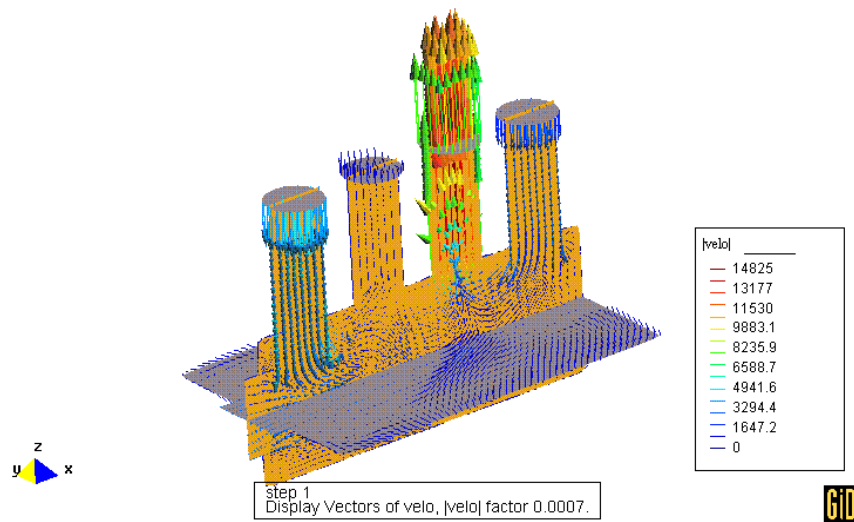


Fig. 4: Three dimensional velocity field at the intake plenum

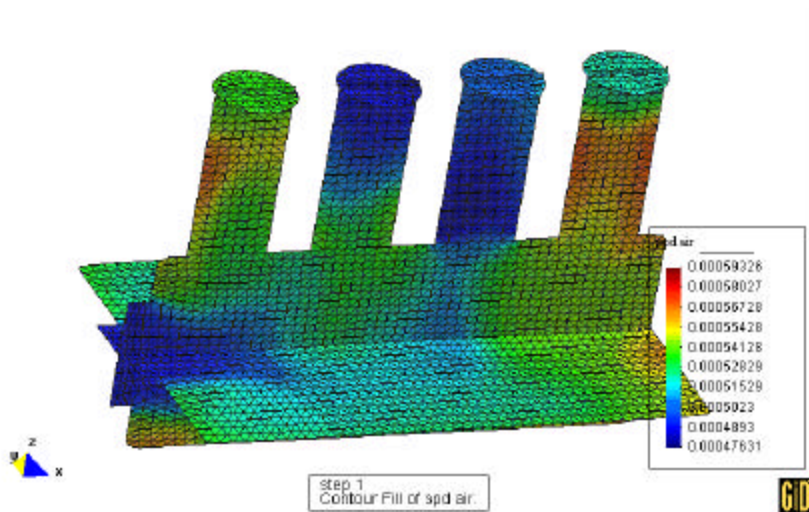


Fig. 5: Three dimensional fresh mixture density at the intake plenum

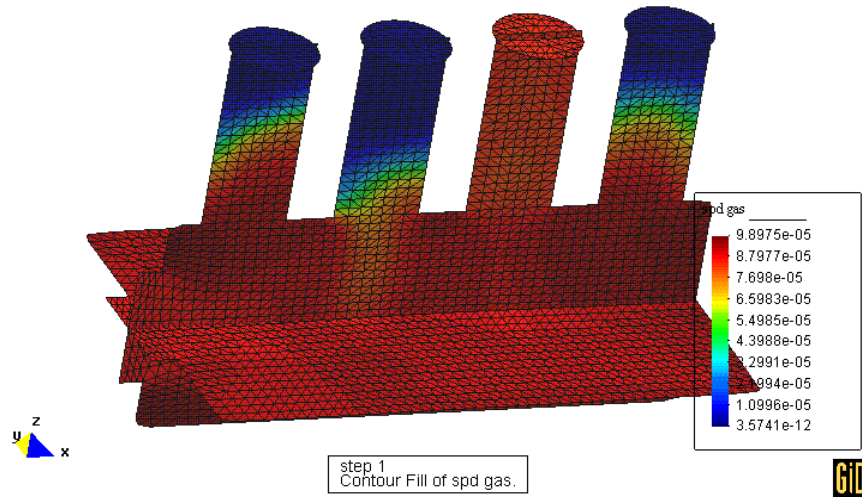


Fig. 6: Three dimensional residual gases density at the intake plenum

Fig 5 and 6 show the spatial distribution of fresh air and residual gases for a fixed time step where it is observed the heterogeneous density field established. Finally the last figure shows the time history of the EGR at each engine cylinder where it may be noted how the engine setup is working and how the emission indices may be controlled.

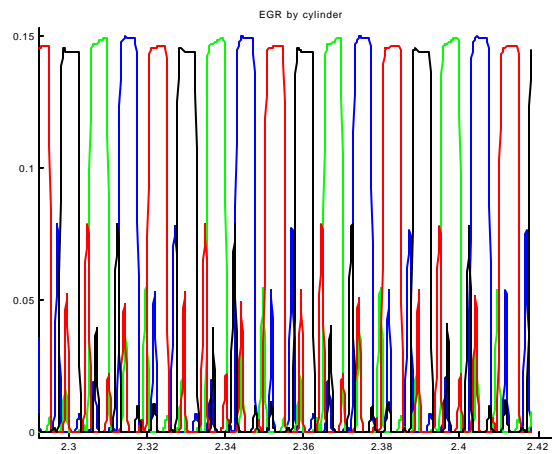


Fig. 7: Time evolution of EGR at each cylinder

6 CONCLUSIONS

The goal of this paper is to put in evidence the possibility of doing some coupling between the standard KIVA code with our own one dimensional gas dynamic code. After this first step we can advice that this kind of strategy may be extensively used in the future to combine the accuracy of three dimensional models with the efficiency of simple one dimensional codes. This work, currently under development, seems to be very promissory even though a lot of work should be done to produce a general coupling that allow to link arbitrary 3D/1D codes. The efforts should be also placed on including species transport and turbulence modeling of the one dimensional code.

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