Study on Heat Transfer and CFD in a SCR Reservoir

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Abstract. According to an industrial demand of the simulation of the heat transfer in a SCR reservoir by Plastic Omnium, we firstly developed a 3D numerical model written in C++. Subsequently, the computational performance of the model was analyzed with both laboratory and industrial experiments. Besides, it was optimized by implicating certain advanced numerical methods, for instance, a gas-liquid flow simulation based on three dimensional VOF method was implicated in order to simulate the phase change coupling sloshing condition.

Keywords: SCR system; heat transfer; simulation; CFD; three-dimensional numerical model.

1. Introduction
Since the norms EURO6 and EPA2010 (The Environmental Protection Agency) have issued, the Selective catalytic reduction (SCR) system is selected as a general solution to limit the diesel engines’ pollution emissions by automobile. In the system of a company, the Urea solution of 32.5%, also called Adblue, is used as the reductant. However, this Urea solution freezes at temperature about -11.5°C which will impact the NOx reduction performance and propose many problems.

On account of the power of numerical solutions, many studies have been realized for modeling the thermal behaviors inside the tank, however, even in some recent researches[1][2], the geometries are still defined on two dimensional and few comparisons are done with tests using a real automotive SCR tank. That is the reason why the group has developed a software written in C++ and C#, which is a three-dimensional numerical model for the heat transfer problem with phase change utilizing the Finite Volume Method. The software is also compatible with MATLAB Simulink for data exchanges. The computational performance of the model was analyzed with laboratory and industrial experiments and it was optimized by implicating advanced numerical methods. In detail, the spatial differencing scheme is switched from HYBRID scheme to QUICK scheme considering of its higher order accuracy. The linear system solver of pressure correction equation is altered from Gauss Seidel method to Preconditioning Conjugate Gradient method for faster computation speed. And the gas-liquid flow simulation on the basis of three dimensional VOF method is implicated for simulating the phase change coupling sloshing condition.

2. Change of Spatial Differencing Scheme
In the former model, the convection-diffusion equation solved by hybrid difference scheme, which is a combination of central difference scheme and upwind difference scheme by exploring the favorable properties of both schemes [3][4]. However, the accuracy of it is only first-order in terms of Taylor series truncation error (TSTE). Therefore, in order to improve the transportiveness property on convection terms, a higher order accuracy scheme is entailed. Hence, the Hayase et al. QUICK scheme which replaces the troublesome negative coefficients in source term is ultimately utilized.

In the program, a circle of cells is expanded outwards as new boundaries and the definition of boundary conditions for all calculated field is removed inwards a circle of cells. Additionally, the exchange of data including inputs and outputs is also altered likewise. Another important part having
to consider following the alteration of differencing scheme is the pressure-velocity calculation process which corrects velocity field by correcting the pressure field. The processes utilized in our numerical model is optional among SIMPLE, SIMPLEC, SIMPLER and PISO, by solving a pressure correction equation deduced from continuity equations. Whilst the second-class neighbor field variables have been considered into the source term in the conservation law, pressure correction equations could be remained.

Figure 1. Solid fraction with time for different grid size.

One comparison results of solid fraction as a function of time (Figure 1) for an academic model is showed hereby as an instance: x-symmetric 2D model (150mm*106mm) with constant heat power(50W) at lateral face and initial temperature at -23°C (Adblue is solid). Theoretically, their difference is that the solutions achieved by Quick scheme with coarse grids are often deemed more accurate than those of hybrid schemes [4]. According to the Figure, we observe that for fin grids as 0.5mm and 1mm, two schemes have almost equal results, however for coarse grids, the solutions achieved by Hybrid scheme deviates more from those of fin grids, especially for the solution of 3 mm and 4 mm. In contrast, the solutions achieved by Quick scheme are close. Hence, it is deemed that Quick scheme is more accurate on coarse grids for phase change problem.

3. Change of Linear System Solver
The rate of convergence was a significant defect for the former solver, Gauss Seidel (‘GS’) method, when solving the large systems. This problem primarily embodied in two ways in our numerical model, due to the difficulty of solving pressure correction equations for convection:
1. Computation stagnation due to tiny time step

Figure 2. Computation algorithm of the program.
In the program, the next time step is controlled by the ‘adaptive time step setting’ process (see Figure 2). It is multiplied with the time step slower coefficient when the loop number for solving discretizing equations is bigger than a prescribed value. In consequence, the time step could be shortened into an extreme tiny span when the solver still has the convergence woe with a large iteration number, and that would ultimately result in a stagnation.

2. Computation break-down due to momentum continuity disagreement

The break-down state is principally depending on the momentum continuity disagreement. The calculation restarts with 0.5 times (this value can be modified) smaller time step when the continuity condition disagrees. Ergo, when the continuity is always unsatisfied within the maximum iteration number and given maximum restarting number (see Figure 2), the user would be required to modify the numerical parameters, otherwise the simulation computation would stop.

Figure 3. Restarting calculation and stagnation computation are concomitant.

The Figure 3 shows that the continually erroneous solution in the restart calculation process often goes together with a computational stagnation.

To conclude, in our former numerical model, the difficulties arise on computations with fin grid or on certain difficult calculating points occurring frequently in three-dimensional computation. In order to solve this problem, the Preconditioning Conjugate Gradient (‘PCG’) is taken into account owing to property of pressure correction equations. It can be derived mathematically that the equations result in a symmetric, positive definite matrix for our linear system, which corresponds with the conditions for application of PCG method.

The comparisons of a SCR 2D model (the mid-section of SCR 3D model) and a HDCC 3D model are presented hereby as instances:

- **SCR 2D Model**
  - Figure 4. Time consumed as a function of Time simulated-SCR-2mm-RN1000.
  
  The time consumed in GS method sharply escalates around 5000s. Since it stagnates with a 10e-8 s tiny time step length, the computation is enforced to stop after its time consumed length goes beyond that of PCG method which completes the computation smoothly.

- **HDCC 3D Model**
The model is extracted from a HDCC (another sort of SCR tank) 3D model where the GS method runs into computation difficulty. The comparison of continuity deviation (divergence of velocity field) and pressure system’s residual is plotted after 300 iterations. The result for \( dt = 3 \times 10^{-6} \) s is showed as an instance.

In order to illustrate more clearly the difference of these two methods on the iteration numbers for continuity agreement for different time step length, we plot it in Figure 6.

For all the time steps, we observe that on residual of pressure system, PCG method converges much more rapidly than GS method which becomes more and more flat. The continuity deviation of PCG method is much smaller than that of GS method after 300 iterations. Additionally, we notice that GS method satisfies the continuity condition only when the residual of pressure system is very small, 100 times smaller than that of PCG method.

Another interesting observation is that in contrast with monotonicity on residual of GS method, the residual of PCG method always fluctuates, even with some obvious increase. This can be explained by the property of residual, that while the A-norm of the error has to decrease monotonically at each step,
the residual norm oscillated and might even increase in each but the last step\cite{5}\cite{6}. An example of this behavior was even used in\cite{7}.

4. Gas-liquid Flow Simulation

First of all, some previous heat power melting experiments have been reiterated on sinusoidal cyclical movement. Then the outcomes show that the sloshing condition actually influences the melting process of Adblue, therefore a gas-liquid flow simulation basing on the three-dimensional VOF method (Figure 7) is implanted for the phase change simulation coupling sloshing condition. The mark function is volume fraction of Adblue \( C_{i,j,k}^n \). The basic verification of this model has been realized and showed that it worked. Moreover, an in-depth test would be done in the future.

![Figure 7. Schema of Volume of Fluid method.](image)

Where, the LSF method is a calibration of the normal \( m \) based on the ‘preliminary reconstruction’ plane calculated by the MYC method in the whole domain, where the \( \alpha \) is also estimated everywhere \cite{8}.

Referring to the book \cite{9}, I developed the 2D method into 3D method for Continuous surface force (CSF) method for surface tension and Combine LE-EI method for interface advection.

Finally, the simplifying expression of the procedure for the time step \( n+1 \), \( C_{i,j,k}^{n+1} \), by combining LE and EI method, can be illustrated by

\[
C_{i,j,k}^{n+1} = T_{x1}^I T_{y1}^I T_{x2}^E T_{y2}^E T_{x3}^I T_{y3}^E
\]

To minimize the asymmetries, the procedure of the next time step \( n+2 \), is alternated by

\[
C_{i,j,k}^{n+2} = T_{y1}^I T_{x1}^I T_{Z2}^E T_{Z2}^E T_{Z3}^I T_{y3}^E
\]

Besides, some other issues have been taken into account. Since our program approximates the category of a component by the percentage of its grid, so that no grid is cut by two different regions, therefore it’s not necessary to use a immersed boundary method in general. Moreover, due to the enthalpy formulation for solid-liquid phase boundary, the velocity of a phase changing grid is negligible for interface advection. Hence, for all solid boundaries, the fluid velocity is equal to the wall velocity, and the current thermal boundary condition is remained.

In our Stephan problem, there is no mass transfer on the gas-liquid interface, therefore no extra source term is added to the former heat transfer modeling. However, thermal conductivity and density of interface is approximated by the arithmetic means and viscosity is approximated by the harmonic means owing to its large difference between Adblue and air.

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