Computational Fluid Dynamics (CFD) for Chemical Industries

Md Mamunur Rashid
Faculty, Bangladesh Institute of Management, Dhaka.
mamun87245@gmail.com

Abstract
Simulation is shown a demonstration of the nature or effects of an event without really experience it. The computer program can simulate the effects of location and remedy equipment problems without causing production downtime in the process. In the numerical approach a limited number of assumptions are made and a high-speed digital computer is to solve the resulting governing fluid dynamic equations for fluid flow problems both in static and rotating equipments. Thus a numerical simulation concept of chemical industries for continuous production plant has been developed. A case on non-Newtonian fluid flow, Carbopol through a circular tube by using numerical simulation technique is added here for compliance with chemical industries.

Key words: Numerical simulation; Computational Fluid dynamics, Circular pipe, Chemical Industries

1.0 Introduction
The development of the high speed digital computer has had a great impact on the preventive maintenance industries by utilizing numerical simulation technique. Maintenance engineering and management is a vital branch of mechanical engineering in respect that without proper maintenance it is difficult to derive full benefit from chemical industries [1]. This has become more so with the erection of giant size process plants worldwide where the outage cost for even an hour is huge in figure. In developing countries its importance is getting momentum slowly. In the recent past, emergence of faster digital computers together with the development of more versatile and efficient numerical solution method has led to a substantial increase in number of mathematical models of fluid flow related to technology. Designers are looking for computational investigation to seek the optimum design. This is because of experiments with either model, or full-scale prototypes are generally laborious, expensive and time consuming. A computer package program, which can run on available personal computer, will be helpful for preventive maintenance of fluid flow equipment. In the field of power generation the computer program can be used for study of various flows in gas turbine, reciprocating engines, furnaces and boilers and nuclear reactor. In chemical plants like heat exchangers, blast furnaces, packet reactors and fluidized beds provides further areas for application. Numerical simulation is one of the ways of fulfilling this requirement by detection of problem of fluid flow, while equipment is operated before major problem is developed [2-4]. It permits scheduling repairs without loss of productivity. It provides factual data that is readily interpreted. Numerical simulation requires mainly the monitoring of machine vibration, lube oil/control oil/ seal oil (quality, quantity, temperature etc), leakage, corrosion, wear debris, operating parameters and machine performances. Numerical simulation technique [5] helps maintenance engineer to identify a problem of special nature, even in the formative stage, with fairly good degree of accuracy, which is beyond the scope of
conventional trouble shooting method. Hence, numerical simulation reduces production losses and maintenance costs (reduced overtime payments for labor, spare parts and stocked inventory costs are decreased). It enhances efficiency, reliability, safety, environmental programs, availability arrangement and longevity of both in static and rotating equipments. It improves workload planning. Corrosion is occurred in chemical industries, like fertilizer factories corrosion occurs in ammonia liquid process pipeline, Benfield section; boiler feed water (BFW) for ammonia plant and blow down (BD) line etc. The thickness of pipe is reduced due to corrosion and sometimes leakage may be found in the pipeline and may be occurred plant shut down. Normally scale form in effluent disposal line and sometimes blow down line. For this reason, flow passage of process pipeline becomes smaller and factory production is hampered. In both cases, flow problem through pipeline can be predicted by numerical simulation. Then the flow problem in the pipeline can be resolved by maintenance. In this aspect CFD is needed study for chemical industries.

2.0 Governing Differential Equation

This work is concerned with steady laminar flow in concentric annuli with center body rotation. The rheological equation used in this work is well-known power law, viz.

\[ \tau_{rz} = -K\left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial z}\right)^n \]  

(1)

Where, \( \tau_{rz} \) in shear stress, \( n \) is a temperature independent exponent, and consistency index \( K \), which is also temperature independent.

The continuity and momentum equations for an incompressible fluid in cylinder co-ordinate \((r, \theta, z)\) system are:

Continuity:

\[ \frac{\partial v_r}{\partial r} + \frac{\partial v_z}{\partial z} + \frac{V_r}{r} = 0 \]  

(2)

Momentum:

\[ V_r \frac{\partial \sigma_{rr}}{\partial r} + V_z \frac{\partial \sigma_{r\theta}}{\partial z} = \frac{\partial \sigma_{rr}}{\partial r} + \frac{\partial \sigma_{r\theta}}{\partial z} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} \]

\[ V_r \frac{\partial \sigma_{r\theta}}{\partial r} + V_z \frac{\partial \sigma_{\theta\theta}}{\partial z} = \frac{\partial \sigma_{r\theta}}{\partial r} + \frac{\partial \sigma_{\theta\theta}}{\partial z} + \frac{2\sigma_{r\theta}}{r} \]

3.0 A case for numerical simulation technique in circular tube or pipe

For an example, non-Newtonian fluid flow problem can be studied through a circular tube using numerical simulation technique. The presented study was deal with the computational analysis of the flow characteristics of non-Newtonian fluid. The analysis is concerned with the radial velocity profile for Carbopol, a non-Newtonian, flowing through a circular tube having the same temperature profiles for the same fluid flowing through the same tube but in this case at a higher temperature than that of the fluid. This analysis is also concerned with the comparison of obtained results with that obtained by F. Popovska and W.L Wilkinson [1976].
3.1 Sequence of investigation

A general computer program “TEACH-T” [6] has been modified for this purpose. The program was used after sufficient justification. The computer program was used for the prediction of the no heat transfer condition using flat velocity profile and heating condition using fully developed parabolic by solving the modified Navier-Stokes equations. For numerical simulation, considering a tube where fluid was pumped and heated. Also considering, tube wall temperature was higher than fluid temperature. Thus, fluid was heated by means of tube. The tube for the flow of test fluid, which was Carbopol, a non-Newtonian fluid, was 17.4 mm in diameter and different lengths were chosen for the two different conditions. For no heat transfer condition the length taken was 435 [25 times of dia.] and heating condition the length taken was 65.25 mm [3.75 times of dia.]. The wall of the tube was maintained at a constant temperature. The simulation was started with the assumption that the flow is uniform. The inlet velocity was 0.018993 m/s, the inlet temperature of the fluid was 40 °C and the wall temperature was 112.93 °C. Although at the entry the velocity profile was a flat one, the test section in such way that for no heat transfer condition, the flow is fully developed at the exit and the heating condition at the entry of the test section the velocity profile was parabolic and fully developed. At the test section velocity, temperature, viscosity and pressure were measured at different locations. From the results obtained from the numerical simulation is now ready for comparison with that obtained by F. Popovska and W.L Wilkinson.

3.2 No heat transfer condition using flat velocity profile

For this analysis flat profile of Carbopol was chosen and the length of the tube is taken 25 times of diameter of the tube is taken 25 times of diameter of the tube and grid is taken 220 X 20. At 2.5 times of diameter the flow becomes fully developed. While carrying out this numerical simulation both the temperature of the wall of the tube and temperature of the Carbopol at inlet is 40 °C. At the end of the tube the velocity profile that was obtained from the equation of fully developed velocity profile for non-Newtonian fluid. The data for no heat transfer condition and flat velocity profile is shown in table 1. The result for fully developed velocity profile is shown in figure 1.

<table>
<thead>
<tr>
<th>Inlet velocity in m/s</th>
<th>Mass flow rate in Kg/s</th>
<th>Inlet fluid temperature °C</th>
<th>Reynolds number, Re</th>
<th>Prandtl number , Pr</th>
<th>Fluid density in Kg/m³</th>
<th>Laminar viscosity in N·s/m²</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.496875 X 10⁻⁵</td>
<td>2.5524399 X 10⁻⁵</td>
<td>40</td>
<td>21.62</td>
<td>72.5</td>
<td>1130</td>
<td>1.420 X10⁶</td>
</tr>
</tbody>
</table>
3.3 Heating condition using fully developed profile

The fully developed velocity profile obtained from the no heat transfer condition into the test section. The test section was 3.75 times of diameter in length and the wall of the tube at a temperature at 112.93 °C and that of Carbopol at inlet was 40 °C. For this analysis the grid is taken as 60 X 20. The data obtained for heating Carbopol is shown in table 2 and the velocity and temperature profiles are shown respectively in figures 2 and 3. In the first case the flow characteristics of Carbopol is found expected. The temperature of both the wall of the fluid is maintained identical. Thus the effect of temperature on viscosity is not so dominant. A uniform flat profile at the inlet starts developing gradually. At the beginning section of the tube the flow could not be developed due to entrance effect. A short axial distance from the entry that was 2.5 times of diameter in length the flow becomes fully developed. Thus velocity profile remains unchanged up to 25 times of diameter in length. This behavior was similar to that of Newtonian fluid.

<table>
<thead>
<tr>
<th>M in Kg/s</th>
<th>Inlet velocity in m/s</th>
<th>Re</th>
<th>Pr</th>
<th>Gr</th>
<th>Fluid density in Kg/m³</th>
<th>Laminar viscosity in N-s/m²</th>
<th>Q in m³/s</th>
<th>X in m</th>
<th>Tube wall temp in °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5524399 x 10⁻⁰²</td>
<td>1.899 x 10⁻⁰²</td>
<td>54.47</td>
<td>28.83</td>
<td>3337.8</td>
<td>1130</td>
<td>5.65 x 10⁻⁰³</td>
<td>2.556 x 10⁻⁰³</td>
<td>1.233</td>
<td>112.93</td>
</tr>
</tbody>
</table>

Figure 1. A velocity profile of Carbopol for no heat transfer condition.
4.0 Discussion

The main reason for this similarity is that the viscosity of the fluid remains constant due to the constancy of temperature of the tube wall and the fluid. As soon as the fully developed velocity profile is introduced into heated tube the velocity is distorted from the developing condition due to great influence of temperature on viscosity of Carbopol [7]. As the axial distance increases this distorted velocity profile again tends to be organized and at a distance of nearly almost infinity where the temperature of the tube and fluid is the same, the velocity profile may again be fully developed. The experiment performed by F. Popovska and W.L Wilkinson [8] was for Reynolds number of a remarkably wide range (2-700). The results obtained from this experiment were made by them. Here all other parameters could be properly selected except the Reynolds number, because it was such a wide range. The Reynolds number here is the only function of the length of the tube because all other parameters in the expression of Reynolds number remain constant. By choosing the proper Reynolds
number by changing the proper the suitable length of observed section the actual result obtained by F. Popovska and W.L. Wilkinson would have been found.

The results of this numerical simulation do not agree to those prediction made by F. Popovska and W.L Wilkinson. Accurate results could have been obtained by further investigation by changing the Reynolds number. The same investigation can be carried out in an annular tube. The same prediction can be carried out for the turbulent cases by incorporating the turbulent transport equations and giving the inner body rotation with vibration. Similar study can be made for eccentric annular with center body rotation and for different fluid different cooling or heating condition, size, length, diameter and rotational speed. Higher order schemes (e.g. LUDS, Quick Scheme) [5, 6, 9] can be used to have better accuracy in this type of prediction.

5.0 Conclusion

In continuous chemical process plants, like urea fertilizer factories produce ammonia and carbon-di-oxide for the production of urea. Ammonia and carbon-di-oxide are extremely hazardous. Therefore, in any problem of both static and rotating equipments, it is possible to prevent accidents and shut down of plants by utilizing numerical simulation technique.

References

[6] Gosman AD, and Idierials FJK, TEACH-T: A general computer program for two dimensional turbulent re-circulating flows, Department of Mechanical Engineering, Imperial College, London, SW7,1976

Nomenclature and list of symbols

m                      Mass flow rate , Kg/sec
θ                      Non-dimensional temperature profiles
r                      radical location in or tube
R                      Half diameter of the pipe or tube
u                      Mean axial velocity component, m/s
μ                      Laminar viscosity, N-S/m²
Q                      Volumetric flow rate, m³/s
Gz                      Graetz number
Pr                      Prandtl number
U                      Bulk axial velocity
σ                      Fluid density, Kg/m³
X                      Axial distance, m
Re                      Reynolds number