

Residual of Momentum Equation and solution accuracy

The problem is to calculate the steady-state fully developed laminar velocity profile in a pipe for a specified pressure drop: radius = 1 cm, length = 80 cm, $\Delta P = 2.5758$ dyne/cm², $\mu = 1.8e-4$ g/cm.s, $\rho = 1.2 e-3$ g/cm³. The analytical solution gives the centerline velocity as 44.719 cm/s, and the Reynolds number is 298.

The following table gives the predicted centerline velocity for various grid refinements in the radial direction. Three divisions were used in the axial direction. Therefore, the aspect ratio of the grid is very poor. The velocity profiles at the three axial locations are identical and look parabolic. In the following tables only the centerline velocity is given, which is used for determining the solution accuracy.

Number of Radial divisions	Residual of axial momentum eq.	Number of Iterations	Centerline velocity (cm/s)
3	1.E-3	28	44.5
6	„	61	44.0
12	„	154	42.2
25	„	366	35.5
50	„	633	21.0
100	„	820	7.3
200	„	913	2.0
Analytical Solution			44.719

The residuals of other equations were very small (~1E-10). The above table shows that for a given value of the residual the prediction became worse as the grid was refined!

To ensure that the above problem does not arise from a bug in MFIX, I conducted simulations with another well-tested CFD code that uses a numerical technique similar to that in MFIX. Here are the results:

Number of Radial divisions	Residual of axial momentum eq.	Number of Iterations	Centerline velocity (cm/s)
6	1.E-3	40	44.0
50	„	231	16.0
200	„	311	1.5
Analytical Solution			44.719

(Only the residual of the axial momentum equation is given in the above table. The residual of the continuity equation in this code was high, ~1.E2. So the code did not report convergence, even when the correct solution was reached. This is perhaps because the normalization factor for the continuity equation was too small.) The above results are similar to that given by MFIX, and, hence, the anomaly appears not to arise from a bug in the code.

How does the solution change when the residual is further decreased? The following table gives the answer:

Number of Radial divisions	Residual of axial momentum eq.	Number of Iterations	Centerline velocity (cm/s)
50	1.E-3	633	21.0
„	1.E-4	2154	40.6
„	1.E-5	4085	44.275
„	1.E-6	6074	44.674
„	1.E-7	8069	44.714
Analytical Solution			44.719

Clearly as the residual decreases the solution becomes more accurate. This confirms the well-known fact that the residual by itself does not guarantee the degree of the accuracy of the solution. Only by decreasing the residual and confirming that the solution doesn't change, can we be sure of the accuracy of the solution.

To check whether the linear equation solver had any effect, I tried using GMRES with 100 inner iterations to solve the axial momentum equation (usually we use SOR with 5 inner iterations). This did not make any difference:

Number of Radial divisions	Residual of axial momentum eq.	Number of Iterations	Centerline velocity (cm/s)
50	1.E-4	2154	40.6

To check whether the numerical value of pressure drop was too small such that the results are affected by round-off errors, I changed the pressure drop, viscosity and density by three orders of magnitude. Such a change will preserve the value of centerline velocity and the Reynolds number. This change also did not make any difference.

All the above calculations were started with an initial value of zero for all the fields. As shown in the following table, I found that the initial value of the axial velocity made a 20% difference in the centerline velocity even when the residual was the same. The following calculations are for 50 radial divisions.

Initial axial (uniform) Velocity	Residual of axial momentum eq.	Number of Iterations	Centerline velocity (cm/s)
0.0	1.E-4	2154	40.6
20.0	„	1251	40.6
30.0	„	493	42.59
32.0	„	516	44.5
32.5	„	524	44.91
35.0	„	588	47.15
40.0	„	970	49.36
50.0	„	1586	49.62
89.4	„	2559	49.62
Analytical Solution			44.719

I repeated the tightening of the residual with a better initial guess to get the following results:

Initial axial (uniform) Velocity	Residual of axial momentum eq.	Number of Iterations	Centerline velocity (cm/s)
32.0	1.E-4	516	44.5
„	1.E-5	1206	45.124
„	1.E-6	3152	44.764
„	1.E-7	5149	44.723
„	1.E-8	7147	44.719
„	1.E-9	9146	44.719
„	1.E-10	11144	44.719
Analytical Solution			44.719

The above table clearly shows that reduction in the residual is surely a measure of increasing solution accuracy, but the absolute value of the residual is not an indicator of solution accuracy.

To check whether the axisymmetric cylindrical coordinate system had anything to do with the anomalous results, the calculations were repeated for a (2 cm wide) 2D slit. The convergence behavior is similar to that of the pipe flow, as shown below.

Number of x divisions	Residual of axial momentum eq.	Number of Iterations	Centerline velocity (cm/s)
3	1.E-3	56	88.166
6	„	101	86.215
12	„	199	79.174
25	„	245	57.338
50	„	108	35.857
100	„	29	32.26
200	„	8	32.019
Analytical Solution			89.4375

As the tolerance is tightened again we a get better solution.

Number of X divisions	Residual of axial momentum eq.	Number of Iterations	Centerline velocity (cm/s)
50	1.E-3	108	35.857
„	1.E-4	2402	73.62
„	1.E-5	6750	87.571
„	1.E-6	11399	89.247
„	1.E-7	16082	89.418
„	1.E-8	20773	89.436
„	1.E-9	25484	89.437
„	1.E-10	30172	89.437
Analytical Solution			89.4375

To check the influence of the aspect ratio, simulations were conducted with a cell aspect ratio of 1. The calculations were conducted for half of 2cm x 1cm slit with various grid resolutions. The pressure drop is 0.01 dyne/cm².

The grid resolution	Residual of axial momentum eq.	Number of Iterations	Centerline velocity (cm/s)
3x3	1.E-3	85	34.513
6x6	„	98	34.940
12x12	„	102	33.748
25x25	„	60	32.423
50x50	„	32	32.086
100x100	„	29	32.026
200x200	„	60	32.016
Analytical Solution			27.7778

The above table shows that the solution becomes better as the grid is further refined. In the following tables the tolerance is tightened for two different grid resolutions. As expected the solution becomes better as the tolerance is tightened. But for a given tolerance (say 1.E-6), the 50x50 grid does not necessarily give a better solution than the 6x6 grid. Furthermore, for the 50x50 grid the convergence was not monotonic with respect to the tolerance (1.e-4 solution is less accurate than the 1.e-3 solution).

The grid resolution	Residual of axial momentum eq.	Number of Iterations	Centerline velocity (cm/s)
6x6	1.E-3	98	34.940
„	1.E-4	1039	29.233
„	1.E-5	2152	27.912
„	1.E-6	3214	27.791
„	1.E-7	4271	27.779
„	1.E-8	5328	27.778
Analytical Solution			27.7778

The grid resolution	Residual of axial momentum eq.	Number of Iterations	Centerline velocity (cm/s)
50x50	1.E-3	32	32.086
„	1.E-4	1021	34.587
„	1.E-5	12393	30.183
„	1.E-6	30272	27.994
„	1.E-7	47225	27.799
„	1.E-8	64094	27.780
Analytical Solution			27.7778

Conclusion: To ensure accuracy, repeat the simulations with a tighter tolerance. For a given grid accept only that part of the solution, which did not change when the convergence tolerance is reduced by an order of magnitude. This procedure may be used to define the uncertainty in the solution.