**APPENDIX A**

**Table 4.1 Comparison among the different methods of nondimensionalization for different conditions in Couette flow**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Dy | 0.001  | 0.005  | 0.010  | 0.001  | 0.001  | 0.001  | 0.001  | 0.001  | 0.001  |
| h | 1.00  | 1.00  | 1.00  | 1.00  | 0.10  | 0.20  | 1.00  | 1.00  | 1.00  |
| U | 1.00  | 1.00  | 1.00  | 1.00  | 1.00  | 1.00  | 1.00  | 0.10  | 0.50  |
| $$D\_{L,anl}$$ | 8.33  | 1.67  | 0.83  | 8.33  | 0.08  | 0.33  | 8.33  | 0.08  | 2.08  |
| $$C\_{1}$$ | 125.85  | 5.69  | 1.44  | 125.85  | 1.4E-02 | 0.26  | 125.85  | 1.3E-02 | 7.87  |
| $$C\_{2}$$ | 1.59  | 0.07  | 0.02  | 1.59  | -4.3E-06 | 1.9E-03 | 1.59  | 1.6E-04 | 9.9E-02 |
| $$R\_{sq}$$ | 0.93  | 0.97  | 0.94  | 0.93  | 0.96  | 0.97  | 0.93  | 0.93  | 0.93  |
| Nondimensionalize |
| $${D\_{L}}/{D\_{L,anl}}$$ | $$C\_{1,ndim}$$ | 1.81  | 2.05  | 2.07  | 1.81  | 2.08  | 2.33  | 1.81  | 1.81  | 1.81  |
| $$Δt∙{U}/{d}$$ | $$C\_{2,ndim}$$ | 2.3E-02 | 2.5E-02 | 2.5E-02 | 2.3E-02 | -6.2E-06 | 6.8E-04 | 2.3E-02 | 2.3E+00 | 9.1E-02 |
| $${D\_{L}}/{D\_{L,anl}}$$ | $$C\_{1,ndim}$$ | 1.81  | 2.05  | 2.07  | 1.81  | 2.08  | 2.33  | 1.81  | 1.81  | 1.81  |
| $$Δt∙{D\_{L,ana}}/{d^{2}}$$ | $$C\_{2,ndim}$$ | 3.3E-04 | 8.9E-03 | 3.5E-02 | 3.3E-04 | -8.9E-06 | 2.4E-04 | 3.3E-04 | 3.3E+00 | 5.3E-03 |
| $${D\_{L}}/{D\_{L,anl}}$$ | $$C\_{1,ndim}$$ | 1.81  | 2.05  | 2.07  | 1.81  | 2.08  | 2.33  | 1.81  | 1.81  | 1.81  |
| $$Δt∙{D\_{z}}/{d^{2}}$$ | $$C\_{2,ndim}$$ | 2.3E+04 | 9.8E+02 | 2.5E+02 | 2.3E+04 | -6.2E-02 | 2.7E+01 | 2.3E+04 | 2.3E+04 | 2.3E+04 |
| $${D\_{L}}/{D\_{z}}$$ | $$C\_{1,ndim}$$ | 1.3E+08 | 2.3E+05 | 1.4E+04 | 1.3E+08 | 1.4E+04 | 2.6E+05 | 1.3E+08 | 1.3E+04 | 7.9E+06 |
| $$Δt∙{U}/{d}$$ | $$C\_{2,ndim}$$ | 1.6E+06 | 2.7E+03 | 1.7E+02 | 1.6E+06 | -4.3E-02 | 7.5E+01 | 1.6E+06 | 1.6E+04 | 4.0E+05 |
| $${D\_{L}}/{D\_{z}}$$ | $$C\_{1,ndim}$$ | 1.3E+08 | 2.3E+05 | 1.4E+04 | 1.3E+08 | 1.4E+04 | 2.6E+05 | 1.3E+08 | 1.3E+04 | 7.9E+06 |
| $$Δt∙{D\_{L,ana}}/{d^{2}}$$ | $$C\_{2,ndim}$$ | 2.3E+04 | 9.8E+02 | 2.5E+02 | 2.3E+04 | -6.2E-02 | 2.7E+01 | 2.3E+04 | 2.3E+04 | 2.3E+04 |
| $${D\_{L}}/{D\_{z}}$$ | $$C\_{1,ndim}$$ | 1.3E+08 | 2.3E+05 | 1.4E+04 | 1.3E+08 | 1.4E+04 | 2.6E+05 | 1.3E+08 | 1.3E+04 | 7.9E+06 |
| $$Δt∙{D\_{z}}/{d^{2}}$$ | $$C\_{2,ndim}$$ | 1.6E+12 | 1.1E+08 | 1.7E+06 | 1.6E+12 | -4.3E+02 | 3.0E+06 | 1.6E+12 | 1.6E+08 | 9.9E+10 |

**Table 4.2 ∆t and N sets for the study of the influence of particles numbers** $MSE\_{N}$

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| $N$(1) | 5000 | 4000 | 3500 | 3000 | 2500 | 2000 | 1900 | 1800 | 1700 |
| $Δt$ (s) | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 |
| $N$(1) | 1600 | 1500 | 1400 | 1300 | 1200 | 1100 | 1000 | 900 | 800 |
| $Δt$ (s) | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 |
| $N$(1) | 700 | 600 | 500 | 400 | 300 | 200 | 100 | - | - |
| $Δt$ (s) | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | - | - |

**Appendix B**

Open channel flow

The logarithmic flow, which is also referred as the open channel flow. The velocity profile over the vertical direction is determined by the logarithmic law, as Eq.(3.2.1). And the diffusivity profile and its gradient in the vertical direction are given as Eq.(3.2.2) and Eq.(3.2.3), respectively. The velocity profile over the vertical is determined by the logarithmic law.

 (B.1)

where u∗ is the shear velocity and set to be 0.01m/s; κ is the Karman constant, which has the value 0.41; and roughness height ks = 0.01m, so that ux is a function of the vertical location, z. The vertical view of this open channel ﬂow is as shown in Fig.5.9

Since the eddy viscosity coefficient represents the rate of turbulent mixing in fully-developed boundary layer ﬂows, such as the open channel ﬂow we studied here, it can be chosen as the description for the diffusivity, as:

 (B.2)

According to Taylor’s discussion in [76], the analytical solution of $D\_{L}$ for open channel flow is

 (B.3)

**Table 5.1 Flow condition of the example logarithmic flow**

|  |  |
| --- | --- |
| $$u\_{\*} (m/s)$$ | 0.01 |
| $$d (m)$$ | 1 |
| $$D\_{z,avg} (m^{2}/s)$$ | 6.83E-04 |
| $$D\_{L,ana} (m^{2}/s)$$ | 5.86E-02 |

With the velocity profile and the diffusivity profile available, the random walk method can be applied and the dispersion coefficient $D\_{L}$ can be calculated through Eq.4. By applying different sizes of time step while keeping the particles number the same, $D\_{L}$ is calculated for the flow defined in Table.5.1.