Chapter 2

Mathematical background and CFD

2.1 Flow Calculation

The flow is governed by the continuity equation, the energy equation and Navier-Stokes momentum equations. Transport of mass, energy and momentum occur through convective flow and diffusion of molecules and turbulent eddies. All equations are set up over a control volume where *i, j, k* = 1; 2; 3 correspond to the three dimensions [1].

2.1.1 Continuity Equation

The continuity equation describes the conservation of mass and is written as in equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_1}{\partial x_1} + \frac{\partial \rho U_2}{\partial x_2} + \frac{\partial \rho U_3}{\partial x_3} = 0 \qquad (2.1)$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_i}{\partial x_i} = 0, i = 1, 2, 3$$

Equation 2.1 defines the rate of increase of mass in a control volume as equal to the amount through its faces. Whereas, for constant density continuity equation is reduced to

$$\frac{\partial U_i}{\partial x_i} = 0, i = 1, 2, 3$$

2.1.2 Momentum Equations (Navier-Stokes Equations)

The momentum balance, also known as the Navier-Stokes equations, follows Newton's second law: The change in momentum in all directions equals the sum of forces acting in those directions. There are two different kinds of forces acting on a finite volume element, surface forces and body forces. Surface forces include pressure and viscous forces and body forces include gravity, centrifugal and electro-magnetic forces [1].

The momentum equation in tensor notation for a Newtonian fluid can be written as in equation 2.2

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \nu \frac{\partial}{\partial x_j}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) + g_i \qquad (2.2)$$

The equation 2.2 can be written in different forms for constant density and viscosity. In addition to gravity, there can be further external sources that may affect the acceleration of fluid e.g. electrical and magnetic fields. Strictly it is the momentum equations that form the Navier-Stokes equations but sometimes the continuity and momentum equations together are called

the Navier-Stokes equations. The Navier-Stokes equations are limited to macroscopic conditions [1].
The continuity equation is difficult to solve numerically. In CFD programs, the continuity equation is often combined with momentum equation to form Poisson equation 2.3. For constant density and viscosity the new equation can be written as below.

$$\frac{\partial}{\partial x_i}\left(\frac{\partial P}{\partial x_i}\right) = -\frac{\partial}{\partial x_i}\left(\frac{\partial(\rho U_i U_j)}{\partial x_j}\right) \qquad (2.3)$$

This equation has more suitable numerical properties and can be solved by proper iteration methods.

2.1.3 Energy Equation

Energy is present in many forms in flow i.e. as kinetic energy due to the mass and velocity of the fluid, as thermal energy, and as chemically bounded energy. Thus the total energy can be defined as the sum of all these energies [1].

$$h = h_m + h_T + h_C + \Phi \qquad (2.4)$$

$h_m = \frac{1}{2}\rho U_i U_i$	Kinetic energy
$h_T = \sum_n m_n \int_{T_{ref}}^{T} C_{p,n} dT$	Thermal energy
$h_C = \sum_n m_n h_n$	Chemical energy
$\Phi = g_i x_i$	Potential energy

In the above equations m_n and $C_{p,n}$ are the mass fraction and specific heat for species n. The transport equation for total energy can be written by the help of above equations. The coupling between energy equations and momentum equations is very weak for incompressible flows, thus equations for kinetic and thermal energies can be written separately. The chemical energy is not included because there was no species transport involved in this project.
The transport equation for kinetic energy can be written as under,

$$\frac{\partial(h_m)}{\partial t} = -U_j\frac{\partial(h_m)}{\partial x_j} + P\frac{\partial U_i}{\partial x_i} - \frac{\partial(PU_i)}{\partial x_i} - \frac{\partial}{\partial x_j}(\tau_{ij}U_i) - \tau_{ij}\frac{\partial U_i}{\partial x_j + \rho g U_i} \qquad (2.5)$$

The last term in the equation 2.5 is the work done by the gravity force. Similarly, a balance for heat can be formulated generally by simply adding the source terms from the kinetic energy equation.

$$\frac{\partial(\rho C_p T)}{\partial t} = -U_j\frac{\partial(\rho C_p T)}{\partial x_j} + k_{eff}\frac{\partial^2 T}{\partial x_j x_j} - P\frac{\partial U_j}{\partial x_j} + \tau_{kj}\frac{\partial U_k}{\partial x_j} \qquad (2.6)$$

The term on left side of the equation is accumulation term. The first on the right is convection term, second is the conduction, third expansion and last is dissipation term. Here the terms in the equation for transformation between thermal and kinetic energy, i.e. expansion and dissipation occur as source terms.

2.2 Turbulence Modeling

Definition of Turbulence

Turbulent flows have some characteristic properties which distinct them from laminar flows [1].

• The motions of the fluid in a turbulent flow are irregular and chaotic due to random movements by the fluid. The flow has a wide range of length, velocity and time scales.

• Turbulence is a three dimensional diffusive transport of mass, momentum and energy through the turbulent eddies that result in faster mixing rates.

• Energy has to be constantly supplied or the turbulent eddies will decay and the flow will become laminar, the kinetic energy becomes internal energy.

Turbulence arises due to the instability in the flow. This happens when the viscous dampening of the velocity fluctuations is slower than the convective transport, i.e. the fluid element can rotate before it comes in contact with wall that stops the rotation. For high Reynolds numbers the velocity fluctuations cannot be dampened by the viscous forces and the flow becomes turbulent.

Turbulent flows contain a wide range of length, velocity and time scales and solving all of them makes the costs of simulations large. Therefore, several turbulence models have been developed with different degrees of resolution. All turbulence models have made approximations simplifying the Navier-Stokes equations. There are several turbulence models available in CFD-softwares including the Large Eddy Simulation (LES) and Reynolds Average NavierStokes (RANS). There are several RANS models available depending on the characteristic of flow, e.g., Standard k − ε model, k − ε RNG model, Realizable k − ε, k –ω and RSM (Reynolds Stress Model) models.

2.2.1 Turbulence Model

The RANS models assume that the variables can be divided into a mean and fluctuating part. The pressure and velocity are then expressed as

$$U_i = \langle U_i \rangle + u_i$$

$$P_i = \langle P_i \rangle + p_i$$

where the average velocity is defined as

$$\langle U_i \rangle = \frac{1}{2T} \int_{-T}^{T} U_i dt$$

The decomposition of velocity and pressure inserted into Navier-Stokes equations gives

$$\frac{\partial \langle U_i \rangle}{\partial t} + \langle U_i \rangle \frac{\partial \langle U_i \rangle}{\partial x_j} = -\frac{1}{\rho} \frac{\partial}{\partial x_j} \left\{ \langle P \rangle \delta_{ij} + \mu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \rho \langle u_i u_j \rangle \right\} \qquad (2.7)$$

The Reynolds averaged stress models use the Boussinesq approximation which is based on the assumption that the Reynolds stresses are proportional to mean velocity gradient. The Boussinesq approximation assumes that the eddies behave like the molecules, that the

turbulence is isotropic and that the stress and strain are in local equilibrium. These assumptions cannot be made for certain flows, e.g., the highly swirling flows having a large degree of anisotropic turbulence and then inaccurate results are obtained. The Boussinesq approximation allows the Reynolds stresses to be modeled using a turbulent viscosity which is analogous to the molecular viscosity [1]. Thus above equation becomes,

$$\frac{\partial\langle U_i\rangle}{\partial t}+\langle U_i\rangle\frac{\partial\langle U_i\rangle}{\partial x_j}=-\frac{1}{\rho}\frac{\partial\langle P\rangle}{\partial x_i}-\frac{2}{3}\frac{\partial k}{\partial x_i}+\frac{\partial}{\partial x_j}\left[(\nu+\nu_T)\left(\frac{\partial U_i}{\partial x_j}+\frac{\partial U_j}{\partial x_i}\right)\right] \qquad (2.8)$$

The use of RANS models requires that two additional transport equations, for the turbulence kinetic energy, k, and the turbulence dissipation rate, ε, or the specific dissipation rate, ω, are solved.

2.2.2 Two-Equations Models

Different turbulence models can be classified on the basis of number of extra equations used to close the set of equations. There are zero, one and two equations models which are commonly employed for turbulence modeling. Zero equation model makes a simple assumption of constant viscosity (Prandtl's mixing length model). Whereas one equation model assumes that viscosity is related to history effects of turbulence by relating to time average kinetic energy. Similarly, two equation model uses two equations to close the set of equations. These two equations can model turbulent velocity or turbulent length scales. There are many variables which can be modeled for example vortices scale, frequency scale, and time scale and dissipation rate. Among these variables, dissipation rate ε is the most commonly used variable. This model is named with respect to the variables being modeled. For example k − ε model, as it models k (Turbulent kinetic energy) and k − ε (Turbulent energy dissipation rate). Another, important turbulence model is k − ω model. It models k (Turbulent kinetic energy) and ω (Specific dissipation rate). These models have become now common in industrial use. These provide significant amount of reliability as they use two variables to close the set of equations [2].

k − ε Models

The first transported variable is turbulent kinetic energy, k. The second transported variable in this case is the turbulent dissipation, ε. Their respective modeled transport equations are as under,
For k,

$$\frac{\partial k}{\partial t}+\langle U_j\rangle\frac{\partial k}{\partial x_j}=\nu_T\left[\left(\frac{\partial\langle U_i\rangle}{\partial x_j}+\frac{\partial\langle U_j\rangle}{\partial x_i}\right)\frac{\partial\langle U_i\rangle}{\partial x_j}\right]-\varepsilon+\frac{\partial}{\partial x_j}\left[\left(\nu+\frac{\nu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]$$

And for ε

$$\underset{1}{\frac{\partial\varepsilon}{\partial t}}+\underset{2}{\langle U_j\rangle\frac{\partial\varepsilon}{\partial x_j}}=\underset{3}{C_{\varepsilon1}\nu_T\frac{\varepsilon}{k}\left[\left(\frac{\partial\langle U_i\rangle}{\partial x_j}+\frac{\partial\langle U_j\rangle}{\partial x_i}\right)\frac{\partial\langle U_i\rangle}{\partial x_j}\right]}+\underset{4}{C_{\varepsilon2}\frac{\varepsilon^2}{k}}+\underset{5}{\frac{\partial}{\partial x_j}\left[\left(\nu+\frac{\nu_T}{\sigma_\varepsilon}\right)\frac{\partial\varepsilon}{\partial x_j}\right]}$$

The physical interpretation of the ε equation is,
1. Accumulation of ε
2. Convection of ε by the mean velocity
3. Production of ε

4. Dissipation of ε
5. Diffusion of ε

The time constant for turbulence is calculated from the turbulent kinetic energy and dissipation rate of turbulent kinetic energy.

$$\tau = \frac{k}{\varepsilon}$$

Note that the source term in ε equation is same as in the k-equation divided by the time constant τ and the rates of dissipation ε is proportional to

$$\frac{\varepsilon}{\tau} = \frac{\varepsilon^2}{k}.$$

The turbulent viscosity must be calculated to close the k− ε model. As the turbulent viscosity is given as the product between characteristic length and velocity scales, $\nu_T \propto ul$. This means that,

$$\nu_T = C_\mu \frac{k^2}{\varepsilon}.$$

Finally five closure coefficients are considered to be constant for all flows, though they can change a little from one flow to the other [1].The values for these closure coefficients are given in the Table below.

Table 2.1: Closure Coefficients for $k - \varepsilon$ Model

Constant	Value
C_μ	0.09
$C_{\varepsilon 1}$	1.44
$C_{\varepsilon 2}$	1.92
σ_k	1.00
σ_ε	1.30

The standard k − ε model does not always give good results. There are some flows which cannot be predicted accurately, such as streamline curvature, swirling flows and axis-symmetrical jets. The inaccuracies stem from underlying Boussinesq hypothesis which imposes isotropy and the way it models the dissipation equation. This model was derived and tuned for high Reynolds numbers. This implies that it is suited for flows where the turbulence is nearly isotropic and to flows where energy cascade proceeds in local equilibrium with respect to generation.

Furthermore, the model parameters in k − ε model are a compromise to give a best performance for wide range of different flows. Due to these weaknesses in k − ε model, several variants are derived for overcoming some of its short comings. Realizable k − ε model is one of them and is described here.

2.3 Wall Treatment Methods

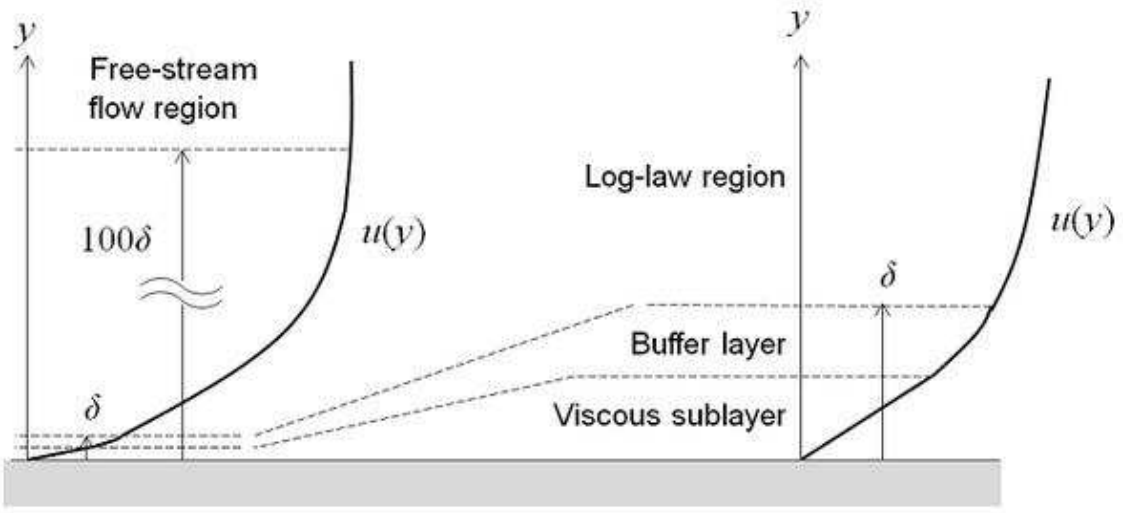
The near-wall modeling considerably effects the reliability of numerical solutions, because walls are the major cause of mean vorticity and turbulence. Near the wall, gradients of variable such as velocity and pressure are high and other scalar variables also undergo sudden increase or decrease. So, precise estimation of flow variables in these regions is of major concern, which will lead to good predictions of turbulence as well [3].

It is known that the region near wall can be divided into three sub sections. The section/layer next to the wall is named as viscous sub-layer. The flow in this layer is entirely laminar and molecular viscosity is major factor in calculating the heat and momentum transfer. In this region turbulent viscosity assumption is not valid at all. While, the section farthest from the

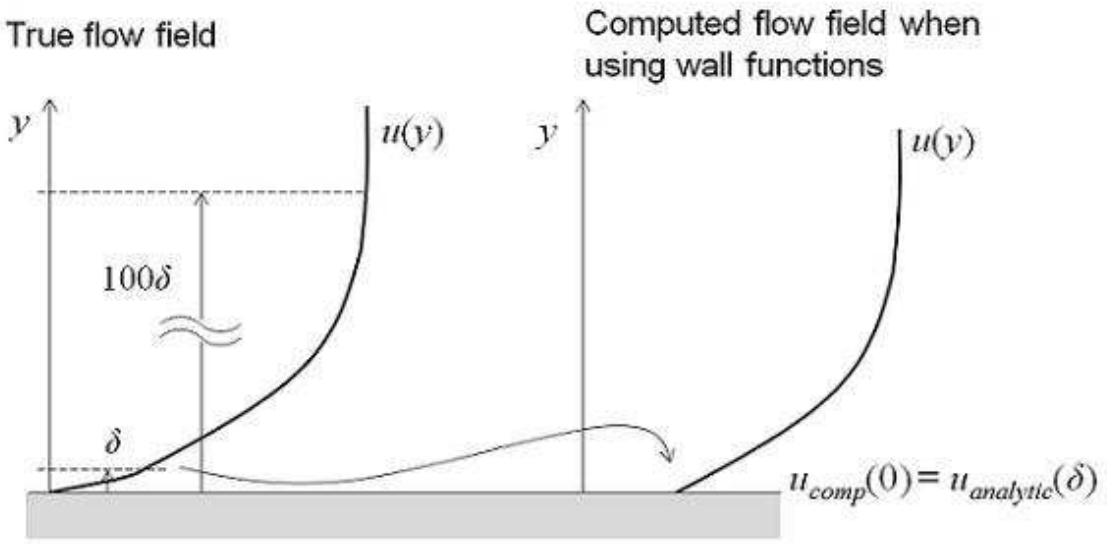
wall inside the near wall region, is called the fully turbulent layer. Here the assumption of turbulent viscosity is valid and turbulence has a major effect over the heat and momentum transport. Then there is a transition region in between these two sections called buffer layer. In this layer, both molecular and turbulent viscosity is important [3].
Modeling of the near wall region can be achieved by fully resolving the region all the way to the wall. This approach may need very fine mesh near the wall and would definitely need huge computational resources to solve. There is another approach, in which near wall region is not resolved completely and empirical formulas are used to guess the variables at the wall. These empirical formulas are called the wall functions. Wall functions are applied on a point away from the wall outside the viscous sub layer. These wall functions are used to connect the turbulent regions with the viscous sub layer [3]. Graphical representation of these both methods can be seen in the Figure 2.1.

2.3.1 Wall Functions

The turbulent flow near a flat wall can be divided up into four regimes. At the wall, the fluid velocity is zero, and for a thin layer above this, the flow velocity is linear with distance from the wall. This region is called the viscous sub layer, or laminar sub layer. Further away from the wall is a region called the buffer layer. In the buffer region, the flow begins to transition to turbulent and it eventually transitions to a region where the flow is fully turbulent and the average flow velocity is related to the log of the distance to the wall. This is known as the log-law region. Even further away from the wall, the flow transitions to the free-stream region. The viscous and buffer layers are very thin, and if the distance to the end of the buffer layer is δ , then the log-law region will extend about 100δ away from the wall.



It is possible to use a RANS model to compute the flow field in all four of these regimes. However, since the thickness of the buffer layer is so small, it can be advantageous to use an approximation in this region. Wall functions ignore the flow field in the buffer region and analytically compute a nonzero fluid velocity at the wall. By using a wall function formulation, you assume an analytic solution for the flow in the viscous layer, and the resultant models will have significantly lower computational requirements. This is a very useful approach for many practical engineering applications.



Wall functions are a set of empirical formulas which connects the different variables such as velocity, temperature and pressure at the wall to the near wall region (Turbulence boundary layer).
Wall functions are applied by using the law of wall for the variables near the wall region. Then they formulate the turbulence variables such as turbulent kinetic energy and turbulent dissipation energy. These formulations depend upon the respective turbulence model. There are following types of wall functions mostly used.

- Standard Wall Functions
- Non-Equilibrium Wall Functions
- Enhanced Wall Functions

Standard Wall Functions

Wall functions basically do not resolve the boundary layer. Thus in their true sense, these are not exact solution to any problem. Wall functions make it possible to calculate the boundary condition away from the wall. Use of wall functions permit the solution at a point where wall functions are suitable, rather than on the wall itself. The boundary conditions are then used at this point and wall functions compute the rapid variation of the flow variables which arise in close proximity to the wall region to be accounted for without resolving the viscous layer next to wall region. Furthermore, wall functions preclude the need to modify the turbulence model to explain for viscosity layer near the wall region. The average velocity in the interior region of the boundary layer can be devised on the general form in Equation 2.12.

$$\langle U \rangle^+ = f(y^+) \tag{2.12}$$

Assuming that the total stress is constant and the turbulent part of the total stress tensor is negligible in the viscous sub layer

$$\frac{\tau_w}{\rho} = v\frac{d\langle U_x \rangle}{dy} \tag{2.13}$$

Integrating with respect to y and applying the no slip boundary conditions gives

$$\langle U_x \rangle = \frac{\tau_w y}{\rho v} = \frac{u_w^2 y}{v} \tag{2.14}$$

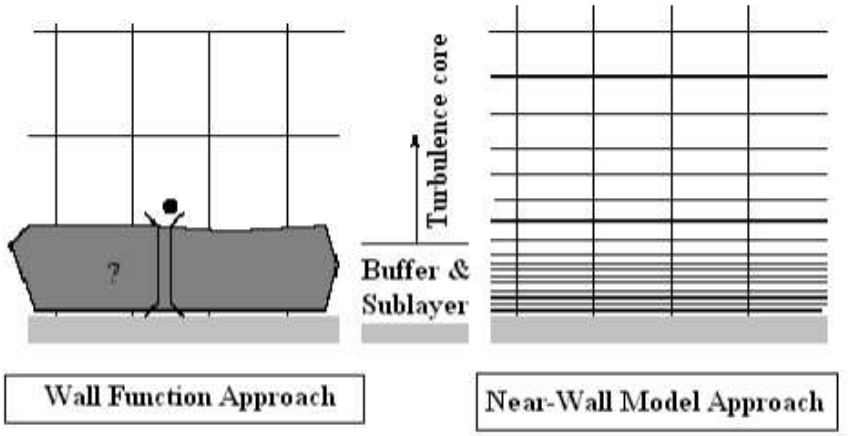


Figure 2.1: Wall Functions and Near Wall Treatment (Adopted from "Computational Fluid Dynamics for Chemical Engineers")

or in the dimensionless form

$$\langle U_x \rangle^+ = y^+ \tag{2.15}$$

In the completely turbulent layer, the total stress tensor shrinks to $\tau_{xy} = -(u_x u_y)$. As the shear stress is almost constant over the inner region of the boundary layer and is approximately equal to τ, we obtain

$$\tau_w = -\rho \langle u_x u_y \rangle \tag{2.16}$$

By introducing Prandtle's mixing length model and the relation, $l = Ky$, we obtain

$$\frac{\tau_w}{\rho} = -\langle u_x u_y \rangle = l^2 [\frac{d\langle U_x \rangle}{dy}]^2 = K^2 y^2 [\frac{d\langle U_x \rangle}{dy}]^2 \tag{2.17}$$

As the characteristic velocity scale for the sub-layers is given by
$u_* = \sqrt{\tau_w/\rho}$.

Equation 2.17 can now be written as

$$u_*^2 = K^2 y^2 [\frac{d\langle U_x \rangle}{dy}]^2 \tag{2.18}$$

Taking the square root of the both sides and integrating with respect to y we obtain the logarithmic velocity profile, which in dimensionless form reads

$$\langle U_x \rangle^+ = \frac{1}{K} ln(y^+) + B \tag{2.19}$$

where $k \approx 0{:}42$ and $B \approx 5{:}0$ (K is Von Karman constant). Equation 2.19 is referred to as logarithmic law of wall or simply the log law. Thus in the viscous sub-layer velocity varies linearly with *y+*, whereas it approaches the log law in the buffer sub-layer.

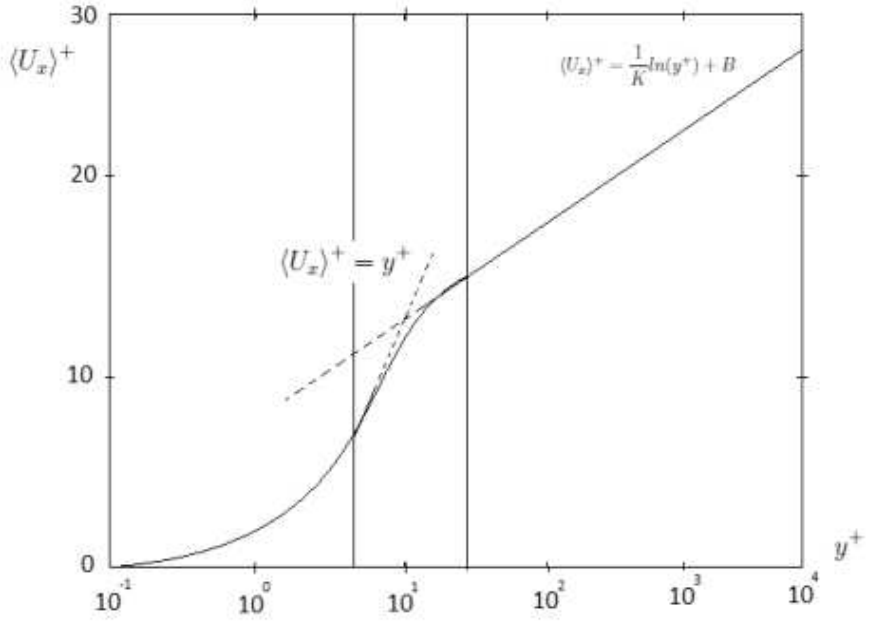


Figure 2.2: The Law of Wall (Adopted from "Computational Fluid Dynamics for Chemical Engineers")

In addition of the logarithmic profile for the average velocity, the wall functions also consists of equation for the near wall turbulent quantities. There is no transport of ***k*** to the wall while ε often has the maximum at the wall. In the derivation of boundary conditions for the turbulent quantities, it is assumed that flow is in local equilibrium which means that production equals dissipation. The boundary condition for ***k*** is given by Equation 2.20.

$$k = \frac{u_*^2}{C_\mu^{1/2}} \tag{2.20}$$

and for ε by,

$$\varepsilon = \frac{u_*^3}{ky} \tag{2.21}$$

The use of wall functions requires that the first grid point adjacent to the wall is within the logarithmic region. In dimensionless distance, that is $30 < y+ < 100$. Upper limit of *y+* can be as high as 300 but it should not exceed 300. Thus it can be said that use of standard wall functions requires *y+* values between 30 and 300. The log-law has proven very useful as a universal for the inner region of the flat plate turbulent boundary layer and has been experimentally verified in numerous studies. However, wall functions are not as valid under the conditions of strong pressure gradients, separated and impinging flows. In these situations standard wall functions are not appropriate choice [3].

References:

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[2] H. K. Versteeg and M. W., An Introduction to Computational Fluid Dynamics, The Finite Volume Method. Pearson Education Limited, 2007.
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