Numerical integration of turbulence models

1 K-Epsilon turbulence model

1.1 Differential equations of the k-epsilon model

For the purpose of this paper, we will concentrate on the k-epsilon-turbulence formulation. The model equations are

$$
\begin{aligned}
\frac{d(\rho k)}{dt} &= \nabla^T\left(\left(\eta+\frac{\eta_{turb}}{\sigma_k}\right)\nabla k\right) - \rho\varepsilon + P_k + P_b \\
\frac{d(\rho\varepsilon)}{dt} &= \nabla^T\left(\left(\eta+\frac{\eta_{turb}}{\sigma_\varepsilon}\right)\nabla \varepsilon\right) - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} + C_{1\varepsilon}\frac{\varepsilon}{k}\cdot\left(P_k + P_b\right)
\end{aligned}
\tag{1.1}
$$

Here, P_k means the turbulent production rate, and it is determined by

$$
P_k = \eta_{turb}\cdot\|\mathbf{D}\|_M^2 \tag{1.2}
$$

The term $\|\mathbf{D}\|_M$ is the norm of the matrix of the velocity gradient.

A similar expression, $\mathrm{P_b}$, is dedicated to turbulent buoyancy effects.

The turbulent viscosity is a function of the turbulent quantities k and epsilon, its quantification is

$$\eta_{turb} = \rho \cdot \mathrm{C}_\eta \cdot \frac{\mathrm{k}^2}{\varepsilon} \tag{1.3}$$

The given constants are $\sigma_\mathrm{k},\ \sigma_\varepsilon,\ \mathrm{C}_{2\varepsilon},\ \mathrm{C}_{1\varepsilon},\ \mathrm{C}_\eta$.

1.2 Numerical evolution scheme and time integration of the k-epsilon model

The numerical evolution scheme is

$$\begin{aligned}
\frac{\mathrm{d}(\rho \mathrm{k})}{\mathrm{dt}} &= \tilde{\nabla}^T\left(\left(\eta+\frac{\eta_{turb}}{\sigma_\mathrm{k}}\right)\tilde{\nabla}\mathrm{k}\right) - \rho\varepsilon + \mathrm{P_k} + \mathrm{P_b} \\
\frac{\mathrm{d}(\rho \varepsilon)}{\mathrm{dt}} &= \tilde{\nabla}^T\left(\left(\eta+\frac{\eta_{turb}}{\sigma_\varepsilon}\right)\tilde{\nabla}\varepsilon\right) - \mathrm{C}_{2\varepsilon}\rho\frac{\varepsilon^2}{\mathrm{k}} + \mathrm{C}_{1\varepsilon}\frac{\varepsilon}{\mathrm{k}}\cdot\left(\mathrm{P_k} + \mathrm{P_b}\right)
\end{aligned} \tag{1.4}$$

which just arises by replacing the spatial derivatives by its FPM-MLS operators.

For better numerical analysis, we can rewrite this scheme by replacing $\mathrm{P_k}$ by its formal expression (1.2) together with (1.3) and, for simplicity, omitting the term $\mathrm{P_b}$

$$\begin{aligned}
\frac{\mathrm{d}(\mathrm{k})}{\mathrm{dt}} &= \frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}}\mathrm{k}\right) - \varepsilon + \mathrm{C}_\eta\frac{\mathrm{k}^2}{\varepsilon}\|\mathbf{D}\|_M^2 \\
\frac{\mathrm{d}(\varepsilon)}{\mathrm{dt}} &= \frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}}\varepsilon\right) - \mathrm{C}_{2\varepsilon}\frac{\varepsilon^2}{\mathrm{k}} + \mathrm{C}_{1\varepsilon}\mathrm{C}_\eta\cdot\mathrm{k}\cdot\|\mathbf{D}\|_M^2
\end{aligned} \tag{1.5}$$

From system (1.5), we derive a singularity formulation, which is either

$$\frac{\mathrm{d}}{\mathrm{dt}}\left(\frac{\mathrm{k}}{\varepsilon}\right) = \left(\mathrm{C}_{2\varepsilon}-1\right) + \mathrm{C}_\eta\left(1-\mathrm{C}_{1\varepsilon}\right)\|\mathbf{D}\|_M^2\cdot\left(\frac{\mathrm{k}}{\varepsilon}\right)^2 + \frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}}\frac{\mathrm{k}}{\varepsilon}\right) \tag{1.6}$$

or

$$\frac{\mathrm{d}}{\mathrm{dt}}\left(\frac{\varepsilon}{\mathrm{k}}\right) = \left(1-\mathrm{C}_{2\varepsilon}\right)\cdot\left(\frac{\varepsilon}{\mathrm{k}}\right)^2 + \mathrm{C}_\eta\left(\mathrm{C}_{1\varepsilon}-1\right)\|\mathbf{D}\|_M^2 + \frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}}\left(\frac{\varepsilon}{\mathrm{k}}\right)\right) \tag{1.7}$$

If not both values k and ε are zero, we can provide numerical mean values (ref. section 1.3 Analytical evaluation of the mean values of the singular terms)

$$\left.\frac{k}{\varepsilon}\right|_{mean} = \frac{1}{\Delta t}\int_0^{\Delta t}\left(\frac{k}{\varepsilon}\right)dt \tag{1.8}$$

and

$$\left.\frac{\varepsilon}{k}\right|_{mean} = \frac{1}{\Delta t}\int_0^{\Delta t}\left(\frac{\varepsilon}{k}\right)dt \tag{1.9}$$

It remains to provide a possibly precise numerical time integration of the scheme (1.5) where we avoid singularities by using the mean values (1.8) and (1.9). Thus, the numerical evolution scheme is

$$\begin{aligned}
\frac{d(k)}{dt} &= \frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}}k\right) - \left(\left.\frac{\varepsilon}{k}\right|_{mean}\right)\cdot k + C_\eta\cdot\left(\left.\frac{k}{\varepsilon}\right|_{mean}\right)k\left\|\mathbf{D}\right\|_M^2 \\
\frac{d(\varepsilon)}{dt} &= \frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}}\varepsilon\right) - C_{2\varepsilon}\cdot\left(\left.\frac{\varepsilon}{k}\right|_{mean}\right)\cdot\varepsilon + C_{1\varepsilon}C_\eta\cdot\left(\left.\frac{k}{\varepsilon}\right|_{mean}\right)\cdot\varepsilon\cdot\left\|\mathbf{D}\right\|_M^2
\end{aligned} \tag{1.10}$$

For the scheme (1.10), we can now apply two schemes that guaranty the positivity of the terms k and ε.

The first scheme is based on semi-implicit first order time stepping, which is

$$\begin{aligned}
\frac{k^{n+1}-k^n}{\Delta t} &= \frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}}k^n\right) - \left(\left.\frac{\varepsilon}{k}\right|_{mean}\right)\cdot k^{n+1} + C_\eta\cdot\left(\left.\frac{k}{\varepsilon}\right|_{mean}\right)\left\|\mathbf{D}\right\|_M^2\cdot k^n \\
\frac{\varepsilon^{n+1}-\varepsilon^n}{\Delta t} &= \frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}}\varepsilon^n\right) - C_{2\varepsilon}\cdot\left(\left.\frac{\varepsilon}{k}\right|_{mean}\right)\cdot\varepsilon^{n+1} + C_{1\varepsilon}C_\eta\cdot\left(\left.\frac{k}{\varepsilon}\right|_{mean}\right)\cdot\left\|\mathbf{D}\right\|_M^2\cdot\varepsilon^n
\end{aligned} \tag{1.11}$$

Which finally leads to

$$\begin{aligned}
k^{n+1} + \Delta t\cdot\left(\left.\frac{\varepsilon}{k}\right|_{mean}\right)\cdot k^{n+1} &= k^n + \Delta t\cdot C_\eta\cdot\left(\left.\frac{k}{\varepsilon}\right|_{mean}\right)\left\|\mathbf{D}\right\|_M^2\cdot k^n + \Delta t\cdot\frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}}k^n\right) \\
\varepsilon^{n+1} + \Delta t\cdot C_{2\varepsilon}\cdot\left(\left.\frac{\varepsilon}{k}\right|_{mean}\right)\cdot\varepsilon^{n+1} &= \varepsilon^n + \Delta t\cdot C_{1\varepsilon}C_\eta\cdot\left(\left.\frac{k}{\varepsilon}\right|_{mean}\right)\cdot\left\|\mathbf{D}\right\|_M^2\cdot\varepsilon^n + \Delta t\cdot\frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}}\varepsilon^n\right)
\end{aligned} \tag{1.12}$$

and more easily to

$$\begin{aligned} \mathrm{LHS}_k \cdot \mathrm{k}^{n+1} &= \mathrm{RHS}_k \\ \mathrm{LHS}_\varepsilon \cdot \varepsilon^{n+1} &= \mathrm{RHS}_\varepsilon \end{aligned} \tag{1.13}$$

where

$$\mathrm{LHS}_k \equiv 1 + \Delta t \cdot \left(\frac{\varepsilon}{k}\bigg|_{mean} \right), \qquad \mathrm{RHS}_k \equiv \left(1 + \Delta t \cdot C_\eta \cdot \left(\frac{k}{\varepsilon}\bigg|_{mean} \right) \|\mathbf{D}\|_M^2 \right) \cdot k^n + \Delta t \cdot \frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}} k^n \right)$$

$$\mathrm{LHS}_\varepsilon \equiv 1 + \Delta t \cdot C_{2\varepsilon} \cdot \left(\frac{\varepsilon}{k}\bigg|_{mean} \right), \qquad \mathrm{RHS}_\varepsilon \equiv \left(1 + \Delta t \cdot C_{1\varepsilon} C_\eta \cdot \left(\frac{k}{\varepsilon}\bigg|_{mean} \right) \cdot \|\mathbf{D}\|_M^2 \right) \cdot \varepsilon^n + \Delta t \cdot \frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}} \varepsilon^n \right)$$

The second idea is to analytically integrate the system of equations (1.10) , which can be rewritten in a simpler way as

$$\begin{aligned} \frac{d(k)}{dt} &= A_k \cdot k + B_k \\ \frac{d(\varepsilon)}{dt} &= A_\varepsilon \cdot \varepsilon + B_\varepsilon \end{aligned} \tag{1.14}$$

where

$$A_k \equiv C_\eta \cdot \left(\frac{k}{\varepsilon}\bigg|_{mean} \right) \|\mathbf{D}\|_M^2 - \left(\frac{\varepsilon}{k}\bigg|_{mean} \right), \qquad B_k \equiv \frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}} k^n \right)$$

$$A_\varepsilon \equiv + C_{1\varepsilon} C_\eta \cdot \left(\frac{k}{\varepsilon}\bigg|_{mean} \right) \cdot \|\mathbf{D}\|_M^2 - C_{2\varepsilon} \cdot \left(\frac{\varepsilon}{k}\bigg|_{mean} \right), \qquad B_\varepsilon \equiv \frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}} \varepsilon \right)$$

The analytical solution of (1.14) is given by

$$\begin{aligned} k &= \left(k_0 + \frac{B_k}{A_k} \right) \cdot \exp\left(A_k \left(t - t_0 \right) \right) - \frac{B_k}{A_k} \\ \varepsilon &= \left(\varepsilon_0 + \frac{B_\varepsilon}{A_\varepsilon} \right) \cdot \exp\left(A_\varepsilon \left(t - t_0 \right) \right) - \frac{B_\varepsilon}{A_\varepsilon} \end{aligned} \tag{1.15}$$

This integration scheme is not yet implemented, however the scheme (1.13) is implemented in FLIQUID_KEPSILON_explicit.F

1.3 Analytical evaluation of the mean values of the singular terms

The singular terms $\left.\frac{k}{\varepsilon}\right|_{mean} = \frac{1}{\Delta t}\int_0^{\Delta t}\left(\frac{k}{\varepsilon}\right)dt$ and $\left.\frac{\varepsilon}{k}\right|_{mean} = \frac{1}{\Delta t}\int_0^{\Delta t}\left(\frac{\varepsilon}{k}\right)dt$ need to be evaluated analytically if we assume negligibility of the diffusion term $\frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}}\left(\frac{\varepsilon}{k}\right)\right)$ in the equation (1.6). This equation then reduces to

$$\frac{d}{dt}\left(\frac{k}{\varepsilon}\right) = \left(C_{2\varepsilon} - 1\right) + C_{\eta}\left(1 - C_{1\varepsilon}\right)\|\mathbf{D}\|_M^2 \cdot \left(\frac{k}{\varepsilon}\right)^2 \tag{1.16}$$

and a bit more simple

$$\frac{d}{dt}x = A - B\cdot x^2 \tag{1.17}$$

where $x = \frac{\varepsilon}{k}$, $A = \left(C_{2\varepsilon} - 1\right)$, and $B = C_{\eta}\left(C_{1\varepsilon} - 1\right)\|\mathbf{D}\|_M^2$

The analytical solution to the differential equation (1.17) is

$$\left.\left(\frac{1}{\sqrt{AB}}\cdot arc\tanh\left(\sqrt{\frac{B}{A}}x\right)\right)\right|_{x_0}^{x} = t - t_0 \tag{1.18}$$

In the same fashion,

$$\left.\left(\frac{1}{\sqrt{AB}}\cdot arc\coth\left(\sqrt{\frac{B}{A}}x\right)\right)\right|_{x_0}^{x} = t - t_0 \tag{1.19}$$

is also a solution to the same differential equation. Thus the time evolution of x is given by solving (1.18) and (1.19) for the variable x, i.e.

$$x = \sqrt{\frac{A}{B}}\tanh\left(\sqrt{AB}\left(t - t_0\right) + arc\tanh\left(\sqrt{\frac{B}{A}}x_0\right)\right) \tag{1.20}$$

as well as

$$x = \sqrt{\frac{A}{B}}\coth\left(\sqrt{AB}\left(t - t_0\right) + arc\coth\left(\sqrt{\frac{B}{A}}x_0\right)\right) \tag{1.21}$$

The arctanh is defined between -1 and 1, the arccoth is defined from 1 to infinity and -1 to -infinity. Hence, if

$$\sqrt{\frac{B}{A}}x_0 > 1 \;\Rightarrow\; x_0 > \sqrt{\frac{A}{B}} \tag{1.22}$$

then equation (1.21) has to be used, if

$$\sqrt{\frac{B}{A}}x_0 < 1 \;\Rightarrow\; x_0 < \sqrt{\frac{A}{B}} \tag{1.23}$$

then equation (1.20) has to be used, and finally if

$$\sqrt{\frac{B}{A}}x_0 = 1 \tag{1.24}$$

then the limit of the differential equation is reached and hence

$$x = \sqrt{\frac{A}{B}} \tag{1.25}$$

1.4 Boundary conditions for solid walls

The solid walls particles in FPM can be treated like interior particles, with one exception: the wall particles are assumed to be shifted to the interior of the flow domain by a small value $\alpha \cdot h$. The value of α is called the wall layer thickness (stored in ind_WallLayer or in the common-variable WallLayer). Thus, in the model (1.10) , the term $\frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}}\mathrm{k}\right)$ needs to have an additional contribution, namely the contribution that comes from the fact that the velocity drops to zero exactly at the wall. So, we have the enhanced model

$$\begin{aligned}
\frac{\mathrm{d}(\mathrm{k})}{\mathrm{dt}} &= \frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}}\mathrm{k}\right) - \left(\frac{\varepsilon}{\mathrm{k}}\bigg|_{mean}\right)\cdot \mathrm{k} + \mathrm{C}_{\eta}\cdot\left(\frac{\mathrm{k}}{\varepsilon}\bigg|_{mean}\right)\mathrm{k}\left\|\mathbf{D}\right\|_M^2 + \frac{\hat{\eta}}{\rho}\cdot\left(\frac{\partial \mathrm{k}}{\partial \mathrm{n}} - \frac{\mathrm{k}}{\alpha\cdot h}\right)\cdot\frac{1}{\frac{1}{2}\left(\alpha\cdot h+\frac{1}{2}h\right)} \\
\frac{\mathrm{d}(\varepsilon)}{\mathrm{dt}} &= \frac{1}{\rho}\left(\tilde{\Delta}_{\hat{\eta}}\varepsilon\right) - \mathrm{C}_{2\varepsilon}\cdot\left(\frac{\varepsilon}{\mathrm{k}}\bigg|_{mean}\right)\cdot\varepsilon + \mathrm{C}_{1\varepsilon}\mathrm{C}_{\eta}\cdot\left(\frac{\mathrm{k}}{\varepsilon}\bigg|_{mean}\right)\cdot\varepsilon\cdot\left\|\mathbf{D}\right\|_M^2 + \frac{\hat{\eta}}{\rho}\cdot\left(\frac{\partial \varepsilon}{\partial \mathrm{n}} - \frac{\varepsilon}{\alpha\cdot h}\right)\cdot\frac{1}{\frac{1}{2}\left(\alpha\cdot h+\frac{1}{2}h\right)}
\end{aligned} \tag{1.26}$$

In reference to the FPM-code, we call

$$\left.\frac{\mathrm{d}(\mathrm{k})}{\mathrm{dt}}\right|_{\mathrm{add}} = \frac{\hat{\eta}}{\rho}\left(\frac{\partial \mathrm{k}}{\partial \mathrm{n}} - \frac{\mathrm{k}}{\alpha \cdot h}\right) \cdot \frac{1}{\frac{1}{2}\left(\alpha \cdot h + \frac{1}{2} h\right)}$$

$$\left.\frac{\mathrm{d}(\varepsilon)}{\mathrm{dt}}\right|_{\mathrm{add}} = \frac{\hat{\eta}}{\rho}\left(\frac{\partial \varepsilon}{\partial \mathrm{n}} - \frac{\varepsilon}{\alpha \cdot h}\right) \cdot \frac{1}{\frac{1}{2}\left(\alpha \cdot h + \frac{1}{2} h\right)} \tag{1.27}$$

Moreover, also the production rate P_k has to be extended by a term, which is in the order of magnitude of

$$\hat{\eta} \cdot \left(\frac{\left\| \left(\mathbf{v} - \mathbf{v}_p\right) - \left(\left(\mathbf{v} - \mathbf{v}_p\right)^T \cdot \mathbf{n}\right) \cdot \mathbf{n} \right\|}{\alpha h} \right)^2 \tag{1.28}$$

where $\mathbf{v}$ = velocity, $\mathbf{v}_p$ =velocity of the wall movement, $\mathbf{n}$ = boundary normal

1.5 Incorporation of turbulent wall tension into the velocity boundary conditions

The turbulent wall stress is computed by the following set of equations:

$$U^* = \frac{1}{\kappa} \cdot \ln\left(E \cdot y^*\right) \tag{1.29}$$

where the definitions are given by

$$U^* \equiv \frac{U_p \cdot c_\mu^{1/4} \cdot k_p^{1/2}}{\tau_W / \rho} \tag{1.30}$$

$$y^* \equiv \frac{\rho \cdot c_\mu^{1/4} \cdot k_p^{1/2} \cdot y_p}{\eta} \tag{1.31}$$

U_p, $k_p^{1/2}$ are the measured values of the tangential velocity and the turbulent kinetic energy at some location with the distance y_p to the wall. We assume this value to be governed by the non-dimensionalized parameter α (see equations (1.26) ff.). In fact we define

$$y_p \equiv \alpha \cdot h \tag{1.32}$$

with h being the smoothing length. α is also referred to as "wall layer".

With the known values of $\eta,\ \rho$ (Viscosity, density) we are able to resolve for the turbulent boundary tension τ_W. The boundary tension finally will be part of the momentum and energy balance of the sliding wall particles. That is done in the following sense: If $\mathbf{t} = \dfrac{\mathbf{v} - \left(\mathbf{v}^T \cdot \mathbf{n}\right) \cdot \mathbf{n}}{\left\| \mathbf{v} - \left(\mathbf{v}^T \cdot \mathbf{n}\right) \cdot \mathbf{n} \right\|}$ is the direction of the velocity along the wall, then we can write down the momentum balance in this direction by

$$\mathbf{t}^T \cdot \dot{\mathbf{v}} + \frac{1}{\rho} \mathbf{t}^T \cdot \nabla p = \frac{1}{\rho} \nabla^T \left(\hat{\eta} \cdot \nabla \left(\mathbf{t}^T \cdot \mathbf{v} \right) \right) + \mathbf{t}^T \cdot \mathbf{g} \tag{1.33}$$

where the viscous term $\nabla^T \left(\hat{\eta} \cdot \nabla \left(\mathbf{t}^T \cdot \mathbf{v} \right) \right)$ is comprised of the physical and turbulent viscosity. The discretization of equation (1.33), based on a control element of the thickness of the wall layer αh, is straight forward in the sense:

$$\frac{\mathbf{t}^T \cdot \mathbf{v}^{n+1} - \mathbf{t}^T \cdot \mathbf{v}^n}{\Delta t} + \frac{1}{\rho} \mathbf{t}^T \cdot \tilde{\nabla} p = \frac{1}{\rho} \frac{\hat{\eta} \cdot \tilde{\nabla} \left(\mathbf{t}^T \cdot \mathbf{v}^{n+1} \right) \cdot \mathbf{n}^T - \tau_W}{\alpha h} + \mathbf{t}^T \cdot \mathbf{g} \tag{1.34}$$

or equivalently

$$\frac{\mathbf{t}^T \cdot \mathbf{v}^{n+1} - \mathbf{t}^T \cdot \mathbf{v}^n}{\Delta t} + \frac{1}{\rho} \mathbf{t}^T \cdot \tilde{\nabla} p = \frac{1}{\rho} \frac{\hat{\eta} \cdot \frac{\tilde{\partial}}{\tilde{\partial} n} \left(\mathbf{t}^T \cdot \mathbf{v}^{n+1} \right) - \tau_W}{\alpha h} + \mathbf{t}^T \cdot \mathbf{g} \tag{1.35}$$

which is, in other words, a momentum balance on a control element of the thickness $y_p \equiv \alpha \cdot h$ in the direction of $\mathbf{t}$. The term $\hat{\eta} \cdot \frac{\tilde{\partial}}{\tilde{\partial} n} \left(\mathbf{t}^T \cdot \mathbf{v} \right)$ are the viscous stresses on the free-flow-side and τ_W are the viscous stresses at the wall side of the layer-control element. In order to provide a numerically stable formulation, we employ a trick such that τ_W acts as a viscous force that counteracts the velocity, that is

$$\frac{\mathbf{t}^T \cdot \mathbf{v}^{n+1} - \mathbf{t}^T \cdot \mathbf{v}^n}{\Delta t} + \frac{1}{\rho} \mathbf{t}^T \cdot \tilde{\nabla} p = \frac{1}{\rho} \frac{\hat{\eta} \cdot \frac{\tilde{\partial}}{\tilde{\partial} n} \left(\mathbf{t}^T \cdot \mathbf{v}^{n+1} \right)}{\alpha h} + \mathbf{t}^T \cdot \mathbf{g} - \frac{1}{\alpha h} \frac{1}{\rho} \frac{\tau_W}{\left\| \mathbf{t}^T \cdot \mathbf{v}^* \right\|} \mathbf{t}^T \cdot \mathbf{v}^{n+1}$$

The representative velocity $\mathbf{v}^*$ would most preferably have to be $\mathbf{v}^{n+1}$, however then the equation becomes nonlinear and difficult to solve numerically. Actually, we choose $\mathbf{v}^* = \mathbf{v}^n$. Finally, the whole solution of the boundary velocity can be rewritten as

$$\left(\frac{1}{\Delta t}+\frac{1}{\alpha h}\frac{1}{\rho}\frac{\tau_W}{\left\|\mathbf{t}^T\cdot\mathbf{v}^*\right\|}\right)\mathbf{t}^T\cdot\mathbf{v}^{n+1}-\frac{1}{\rho}\frac{\hat{\eta}\cdot\frac{\tilde{\partial}}{\tilde{\partial}n}\left(\mathbf{t}^T\cdot\mathbf{v}^{n+1}\right)}{\alpha h}=\frac{\mathbf{t}^T\cdot\mathbf{v}^n}{\Delta t}-\frac{1}{\rho}\mathbf{t}^T\cdot\tilde{\nabla}p+\mathbf{t}^T\cdot\mathbf{g}$$

2 Further analytical considerations of the k-epsilon model

The following small analysis of the k epsilon model is based on simply the production and dissipation rates of the model, however we neglect the diffusion terms. This is a simplification that signifies a homogeneous turbulence distribution, for instance in a mixing unit without big gradients in the turbulent quantities.

2.1 Reduced model without diffusion

$$\begin{aligned}\dot{\mathrm{k}} &= c_\mu\cdot\frac{\mathrm{k}^2}{\varepsilon}\cdot\mathrm{G}-\varepsilon\\ \dot{\varepsilon} &= \mathrm{C}_{1\varepsilon}\cdot c_\mu\cdot\mathrm{k}\cdot\mathrm{G}-\mathrm{C}_{2\varepsilon}\frac{\varepsilon^2}{\mathrm{k}}\end{aligned}\tag{2.1}$$

Here, $\mathrm{G}=\left\|\mathbf{D}\right\|_M^2$. The consideration of the k-epsilon system without viscous terms seems to be useful as we can always imagine cases where k and epsilon are evenly distributed, for instance a liquid in a turbulent mixing unit.

2.2 Limit of the relation k and epsilon

The time derivative of the term $\frac{\mathrm{k}}{\varepsilon}$ is given by the scheme above

$$\begin{aligned}\dot{\mathrm{k}}\cdot\varepsilon &= c_\mu\cdot\mathrm{k}^2\cdot\mathrm{G}-\varepsilon^2\\ \mathrm{k}\cdot\dot{\varepsilon} &= \mathrm{C}_{1\varepsilon}\cdot c_\mu\cdot\mathrm{k}^2\cdot\mathrm{G}-\mathrm{C}_{2\varepsilon}\cdot\varepsilon^2\end{aligned}\tag{2.2}$$

$$
\begin{aligned}
\frac{d}{dt}\left(\frac{\mathrm{k}}{\varepsilon}\right) &= \frac{\dot{\mathrm{k}}\cdot\varepsilon - \mathrm{k}\cdot\dot{\varepsilon}}{\varepsilon^2} \\
&= \frac{c_\mu\cdot\mathrm{k}^2\cdot\mathrm{G} - \varepsilon^2 - \mathrm{C}_{1\varepsilon}\cdot c_\mu\cdot\mathrm{k}^2\cdot\mathrm{G} + \mathrm{C}_{2\varepsilon}\cdot\varepsilon^2}{\varepsilon^2} \\
&= \frac{c_\mu\cdot\left(1-\mathrm{C}_{1\varepsilon}\right)\cdot\mathrm{k}^2\cdot\mathrm{G} + \left(\mathrm{C}_{2\varepsilon}-1\right)\cdot\varepsilon^2}{\varepsilon^2} \\
&= c_\mu\cdot\left(1-\mathrm{C}_{1\varepsilon}\right)\cdot\frac{\mathrm{k}^2}{\varepsilon^2}\cdot\mathrm{G} + \left(\mathrm{C}_{2\varepsilon}-1\right)
\end{aligned}
\tag{2.3}
$$

From equation (2.3) we learn that the limit of the value $\frac{\mathrm{k}}{\varepsilon}$ as time goes to infinity is

$$
\begin{aligned}
&0 = c_\mu\cdot\left(1-\mathrm{C}_{1\varepsilon}\right)\cdot\frac{\mathrm{k}^2}{\varepsilon^2}\cdot\mathrm{G} + \left(\mathrm{C}_{2\varepsilon}-1\right) \\
&\left(1-\mathrm{C}_{2\varepsilon}\right) = c_\mu\cdot\left(1-\mathrm{C}_{1\varepsilon}\right)\cdot\frac{\mathrm{k}^2}{\varepsilon^2}\cdot\mathrm{G} \\
&\frac{\left(1-\mathrm{C}_{2\varepsilon}\right)}{\left(1-\mathrm{C}_{1\varepsilon}\right)}\cdot\frac{1}{c_\mu\cdot\mathrm{G}} = \frac{\mathrm{k}^2}{\varepsilon^2} \\
&\frac{\mathrm{k}}{\varepsilon} = \sqrt{\frac{\left(1-\mathrm{C}_{2\varepsilon}\right)}{\left(1-\mathrm{C}_{1\varepsilon}\right)}}\cdot\sqrt{\frac{1}{c_\mu\cdot\mathrm{G}}}
\end{aligned}
\tag{2.4}
$$

2.3 Relation of time change of diffusion

The turbulent diffusion is given by

$$
\nu = \mathrm{c}_\mu\cdot\frac{\mathrm{k}^2}{\varepsilon} \tag{2.5}
$$

The time change rate is

$$
\begin{aligned}
\dot{\nu} &= c_\mu \cdot \frac{d}{dt}\left(k^2 \cdot \varepsilon^{-1}\right) \\
&= c_\mu \cdot \left(2k \cdot \dot{k} \cdot \varepsilon^{-1} - k^2 \cdot \varepsilon^{-2} \cdot \dot{\varepsilon}\right) \\
&= c_\mu \cdot \left(2k \cdot \varepsilon^{-1} \cdot \left(c_\mu \cdot \frac{k^2}{\varepsilon} \cdot G \; - \; \varepsilon \right) - k^2 \cdot \varepsilon^{-2} \cdot \left(C_{1\varepsilon} \cdot c_\mu \cdot k \cdot G \; - \; C_{2\varepsilon} \frac{\varepsilon^2}{k} \right) \right) \\
&= c_\mu \cdot \left(\left(2c_\mu \cdot \frac{k^3}{\varepsilon^2} \cdot G \; - \; 2k \right) - \left(C_{1\varepsilon} \cdot c_\mu \cdot \frac{k^3}{\varepsilon^2} \cdot G \; - \; C_{2\varepsilon} \cdot k \right) \right) \\
&= c_\mu \cdot \left(\left(2 - C_{1\varepsilon}\right) c_\mu \cdot \frac{k^3}{\varepsilon^2} \cdot G + \left(C_{2\varepsilon} - 2\right) \cdot k \right)
\end{aligned}
\tag{2.6}
$$

And finally

$$
\begin{aligned}
\frac{\dot{\nu}}{\nu} &= \frac{c_\mu \cdot \left(\left(2 - C_{1\varepsilon}\right) c_\mu \cdot \frac{k^3}{\varepsilon^2} \cdot G + \left(C_{2\varepsilon} - 2\right) \cdot k \right)}{c_\mu \cdot \frac{k^2}{\varepsilon}} \\
\frac{\dot{\nu}}{\nu} &= \left(\left(2 - C_{1\varepsilon}\right) \cdot c_\mu \cdot \frac{k}{\varepsilon} \cdot G + \left(C_{2\varepsilon} - 2\right) \cdot \frac{\varepsilon}{k} \right)
\end{aligned}
\tag{2.7}
$$

So, of course we can also determine the change rate of the turbulent viscosity at infinite time:

$$
\begin{aligned}
\frac{\dot{\nu}}{\nu} &= \left(\left(2 - C_{1\varepsilon}\right) \cdot \sqrt{\frac{\left(1 - C_{2\varepsilon}\right)}{\left(1 - C_{1\varepsilon}\right)}} \cdot \sqrt{c_\mu \cdot G} + \left(C_{2\varepsilon} - 2\right) \cdot \sqrt{\frac{\left(1 - C_{1\varepsilon}\right)}{\left(1 - C_{2\varepsilon}\right)}} \cdot \sqrt{c_\mu \cdot G} \right) \\
\frac{\dot{\nu}}{\nu} &= \left(\left(2 - C_{1\varepsilon}\right) \cdot \sqrt{\frac{\left(1 - C_{2\varepsilon}\right)}{\left(1 - C_{1\varepsilon}\right)}} + \left(C_{2\varepsilon} - 2\right) \cdot \sqrt{\frac{\left(1 - C_{1\varepsilon}\right)}{\left(1 - C_{2\varepsilon}\right)}} \right) \cdot \sqrt{c_\mu \cdot G}
\end{aligned}
\tag{2.8}
$$

We can now also ask for a dedicated change of the turbulent viscosity during a given time step, i.e.

$$
\alpha = \frac{\dot{\nu} \cdot \Delta t}{\nu} = \left(\left(2 - C_{1\varepsilon}\right) \cdot c_\mu \cdot \frac{k}{\varepsilon} \cdot G + \left(C_{2\varepsilon} - 2\right) \cdot \frac{\varepsilon}{k} \right) \cdot \Delta t
\tag{2.9}
$$

For given k, we can ask what should be epsilon, ergo

$$
\begin{aligned}
\alpha\cdot k\cdot\varepsilon &= \left(2-C_{1\varepsilon}\right)\cdot c_\mu\cdot k^2\cdot G\cdot\Delta t+\left(C_{2\varepsilon}-2\right)\cdot\Delta t\cdot\varepsilon^2\\
0 &= \left(2-C_{1\varepsilon}\right)\cdot c_\mu\cdot k^2\cdot G\cdot\Delta t-\alpha\cdot k\cdot\varepsilon+\left(C_{2\varepsilon}-2\right)\cdot\Delta t\cdot\varepsilon^2\\
0 &= \frac{\left(2-C_{1\varepsilon}\right)\cdot c_\mu\cdot k^2\cdot G}{\left(C_{2\varepsilon}-2\right)}-2\frac{\alpha\cdot k}{2\cdot\left(C_{2\varepsilon}-2\right)\cdot\Delta t}\cdot\varepsilon+\varepsilon^2\\
0 &= \frac{\left(2-C_{1\varepsilon}\right)\cdot c_\mu\cdot k^2\cdot G}{\left(C_{2\varepsilon}-2\right)}-\left(\frac{\alpha\cdot k}{2\cdot\left(C_{2\varepsilon}-2\right)\cdot\Delta t}\right)^2+\left(\varepsilon-\frac{\alpha\cdot k}{2\cdot\left(C_{2\varepsilon}-2\right)\cdot\Delta t}\right)^2\\
0 &= \frac{4\cdot\left(2-C_{1\varepsilon}\right)\cdot\left(C_{2\varepsilon}-2\right)\cdot c_\mu\cdot k^2\cdot\Delta t^2\cdot G}{\left(2\cdot\left(C_{2\varepsilon}-2\right)\cdot\Delta t\right)^2}-\left(\frac{\alpha\cdot k}{2\cdot\left(C_{2\varepsilon}-2\right)\cdot\Delta t}\right)^2+\left(\varepsilon-\frac{\alpha\cdot k}{2\cdot\left(C_{2\varepsilon}-2\right)\cdot\Delta t}\right)^2\\
&\frac{\alpha^2\cdot k^2-4\cdot\left(2-C_{1\varepsilon}\right)\cdot\left(C_{2\varepsilon}-2\right)\cdot c_\mu\cdot k^2\cdot\Delta t^2\cdot G}{\left(2\cdot\left(C_{2\varepsilon}-2\right)\cdot\Delta t\right)^2}=\left(\varepsilon-\frac{\alpha\cdot k}{2\cdot\left(C_{2\varepsilon}-2\right)\cdot\Delta t}\right)^2\\
\varepsilon &= \frac{\alpha\cdot k}{2\cdot\left(C_{2\varepsilon}-2\right)\cdot\Delta t}+\sqrt{\frac{\alpha^2-4\cdot\left(2-C_{1\varepsilon}\right)\cdot\left(C_{2\varepsilon}-2\right)\cdot c_\mu\cdot\Delta t^2\cdot G}{\left(2\cdot\left(C_{2\varepsilon}-2\right)\cdot\Delta t\right)^2}}\cdot k
\end{aligned}
\tag{2.10}
$$

2.4 Paradoxon of the characteristic turbulent length scale

We remember, from literature, that the turbulent length scale is defined as

$$L=\frac{k^{3/2}}{\varepsilon} \tag{2.11}$$

The time change rate is now easily derived by

$$\dot{L}=\frac{3}{2}k^{1/2}\cdot\varepsilon^{-1}\cdot\dot{k}-k^{3/2}\cdot\varepsilon^{-2}\cdot\dot{\varepsilon} \tag{2.12}$$

Replacing the time derivatives of k and epsilon yield

$$
\begin{aligned}
\dot{L}&=\frac{3}{2}k^{1/2}\cdot\varepsilon^{-1}\cdot\left(c_\mu\cdot\frac{k^2}{\varepsilon}\cdot G-\varepsilon\right)-k^{3/2}\cdot\varepsilon^{-2}\cdot\left(C_{1\varepsilon}\cdot c_\mu\cdot k\cdot G-C_{2\varepsilon}\frac{\varepsilon^2}{k}\right)\\
\dot{L}&=\left(\frac{3}{2}-C_{1\varepsilon}\right)\cdot c_\mu\cdot\frac{k^{5/2}}{\varepsilon^2}\cdot G+\left(C_{2\varepsilon}-\frac{3}{2}\right)\cdot k^{1/2}
\end{aligned}
\tag{2.13}
$$

Division by the length scale itself gives

$$\frac{\dot{L}}{L}=\left(\frac{3}{2}-C_{1\varepsilon}\right)\cdot c_\mu\cdot\frac{k}{\varepsilon}\cdot G+\left(C_{2\varepsilon}-\frac{3}{2}\right)\cdot\frac{\varepsilon}{k} \tag{2.14}$$

Therefore, for the nondimensionalized change rate of the turbulent length scale, we also find a limit as time goes to infinity:

$$
\begin{aligned}
\frac{\dot{\mathrm{L}}}{\mathrm{L}} &= \left(\frac{3}{2}-\mathrm{C}_{1\varepsilon}\right)\cdot\sqrt{\frac{\left(1-\mathrm{C}_{2\varepsilon}\right)}{\left(1-\mathrm{C}_{1\varepsilon}\right)}}\cdot\sqrt{c_\mu\cdot\mathrm{G}}+\left(\mathrm{C}_{2\varepsilon}-\frac{3}{2}\right)\cdot\sqrt{\frac{\left(1-\mathrm{C}_{1\varepsilon}\right)}{\left(1-\mathrm{C}_{2\varepsilon}\right)}}\cdot\sqrt{c_\mu\cdot\mathrm{G}} \\
\frac{\dot{\mathrm{L}}}{\mathrm{L}} &= \left(\left(\frac{3}{2}-\mathrm{C}_{1\varepsilon}\right)\cdot\sqrt{\frac{\left(1-\mathrm{C}_{2\varepsilon}\right)}{\left(1-\mathrm{C}_{1\varepsilon}\right)}}+\left(\mathrm{C}_{2\varepsilon}-\frac{3}{2}\right)\cdot\sqrt{\frac{\left(1-\mathrm{C}_{1\varepsilon}\right)}{\left(1-\mathrm{C}_{2\varepsilon}\right)}}\right)\cdot\sqrt{c_\mu\cdot\mathrm{G}}
\end{aligned}
\tag{2.15}
$$

Equation (2.14) reveals a paradoxon as the term $\frac{\dot{\mathrm{L}}}{\mathrm{L}}$ is strictly positive for all G ($\mathrm{C}_{1\varepsilon}=1.44,\ \ \mathrm{C}_{2\varepsilon}=1.92$). This means that the turbulent length scale rises even under high shear deformation of the fluid, which is not consistent in itself. We would expect a shrinkage of this quantity under high shear rates.

2.5 Strategies of initializing k and epsilon at high shear rates

Due to the paradoxon described in the section above, and also due to the fact that small starting values of k and epsilon might lead to extremely long times until reaching significant k and epsilon, we might want to initialize the values of k and epsilon at high shear rates.

2.5.1 Strategy 1:

Assume the infinity ratio of k and epsilon and assume an initial turbulent viscosity equal to physical viscosity. I.e.

$$
\frac{\mathrm{k}_{init}}{\varepsilon_{init}}=\sqrt{\frac{\left(1-\mathrm{C}_{2\varepsilon}\right)}{\left(1-\mathrm{C}_{1\varepsilon}\right)}}\cdot\sqrt{\frac{1}{c_\mu\cdot\mathrm{G}}}
\tag{2.16}
$$

And

$$
\begin{aligned}
\nu=\nu_{phys}&=\mathrm{c}_\mu\cdot\frac{\mathrm{k}_{init}}{\varepsilon_{init}}\cdot\mathrm{k}_{init}=\mathrm{c}_\mu\cdot\sqrt{\frac{\left(1-\mathrm{C}_{2\varepsilon}\right)}{\left(1-\mathrm{C}_{1\varepsilon}\right)}}\cdot\sqrt{\frac{1}{c_\mu\cdot\mathrm{G}}}\cdot\mathrm{k}_{init} \\
\mathrm{k}_{init}&=\frac{\nu_{phys}}{\mathrm{c}_\mu\cdot\sqrt{\frac{\left(1-\mathrm{C}_{2\varepsilon}\right)}{\left(1-\mathrm{C}_{1\varepsilon}\right)}}\cdot\sqrt{\frac{1}{c_\mu\cdot\mathrm{G}}}}=\frac{\sqrt{\left(1-\mathrm{C}_{1\varepsilon}\right)}\cdot\sqrt{\mathrm{G}}}{\sqrt{c_\mu\cdot\left(1-\mathrm{C}_{2\varepsilon}\right)}}\cdot\nu_{phys}
\end{aligned}
\tag{2.17}
$$

With the so computed initial value of k and equation (2.16) we are able to compute the initial value of epsilon.

2.5.2 Strategy 2:

We can also assume a certain initial value for k by

$$k_{init} = \alpha \cdot h^2 \cdot G \tag{2.18}$$

With values for $\alpha = 0.001 ... 0.1$, then we can find the initial value for epsilon by either the well known relation (2.16) or by forcing the initial turbulent viscosity again to physical viscosity, i.e.

$$\nu = \nu_{phys} = c_\mu \cdot \frac{k_{init}^2}{\varepsilon_{init}} \tag{2.19}$$

If we force equation (2.16), then we can compute the initialized viscosity by

$$\begin{aligned} \nu_t &= c_\mu \cdot \frac{k_{init}}{\varepsilon_{init}} \cdot k_{init} = c_\mu \cdot \sqrt{\frac{(1 - C_{2\varepsilon})}{(1 - C_{1\varepsilon})}} \cdot \sqrt{\frac{1}{c_\mu \cdot G}} \cdot \alpha \cdot h^2 \cdot G \\ &= \sqrt{c_\mu} \cdot \sqrt{\frac{(1 - C_{2\varepsilon})}{(1 - C_{1\varepsilon})}} \cdot \alpha \cdot h^2 \cdot \sqrt{G} \end{aligned} \tag{2.20}$$

Plugging in the values of the constants we have

$$\nu_t = 0.4338 \cdot \alpha \cdot h^2 \cdot \sqrt{G} \tag{2.21}$$

If we choose $\alpha = 0.2305 \ ... \ 0.4610$ the we find

$$\nu_t = (0.1 ... 0.2) \cdot h^2 \cdot \sqrt{G} \tag{2.22}$$

which is exactly the turbulent viscosity proposed be the Smagorinsky-Turbulence model. In this way, for turbulent production, Smagorinsky and k-epsilon are similar. The are different in the decay of the turbulences.

The turbulent length scale produced by this is

$$L_{init}=\frac{k_{init}^{3/2}}{\varepsilon_{init}}=\frac{k_{init}}{\varepsilon_{init}}\cdot k_{init}^{1/2}=\sqrt{\frac{\left(1-C_{2\varepsilon}\right)}{\left(1-C_{1\varepsilon}\right)}}\cdot\sqrt{\frac{1}{c_{\mu}\cdot G}}\cdot\sqrt{\alpha\cdot h^{2}\cdot G}=\sqrt{\frac{\left(1-C_{2\varepsilon}\right)}{\left(1-C_{1\varepsilon}\right)}}\cdot\sqrt{\frac{\alpha}{c_{\mu}}}\cdot h \qquad (2.23)$$

That means by choosing alpha we have the freedom to either influence the turbulent viscosity or the turbulent length scale to a desired value.

Strategy 2 is, bw the way, the one implemented right now in FPM.