Turbulence and CFD models: Theory and applications

Roadmap to Lecture 6

Part 1

1. The closure problem
2. Exact equations and solvable equations
3. Derivation rules and identities to remember
4. Derivation of the Reynolds stress transport equation
5. Derivation of the turbulent kinetic energy equation
6. Additional comments
7. Another touch to the closure problem

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The closure problem

- Let us recall the incompressible RANS equations,

Reynolds stress tensor

$$\tau^R = -\rho\left(\overline{\mathbf{u}'\mathbf{u}'}\right)$$

$$\nabla \cdot (\bar{\mathbf{u}}) = 0$$

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) = -\frac{1}{\rho}(\nabla \overline{p}) + \nu \nabla^2 \bar{\mathbf{u}} + \frac{1}{\rho} \nabla \cdot \boldsymbol{\tau}^R$$

- At this point, the problem reduces on how to compute the Reynolds stress tensor.
- In CFD we do not want to resolve the velocity fluctuations as it requires very fine meshes and small time-steps.
- That is, we do not want to solve the small scales due to the fluctuating velocities and transported quantiles.
- The RANS/URANS approach to turbulence modeling requires the Reynolds stress tensor to be appropriately modeled in terms of known quantities (mean flow).

The closure problem

- Different approaches can be used to model the Reynolds stress tensor $\boldsymbol{\tau}^R$.
    - Algebraic models.
    - Eddy viscosity models (EVM) – Boussinesq approximation.
    - Non-linear eddy viscosity models.
    - Reynolds stress transport models.
    - Algebraic Reynolds stress models.
    - Vorticity based models.

- Have in mind that the literature is very rich when it comes to turbulence models.
- We will explore the most commonly used approaches.

The closure problem

- Overview of the main turbulence modeling approaches.

MODELING APPROACH

RANS
Reynolds-**A**veraged **N**avier-**S**tokes equations

URANS
Unsteady **R**eynolds-**A**veraged **N**avier-**S**tokes equations

For the moment we will focus our attention on these models

- Many more acronyms between **RANS/URANS** and **SRS** simulations.
- Some of the acronyms are used only to differentiate approaches used in commercial solvers.

PANS, **SAS**, **RSM**, **EARSM**, **PITM**, **SBES, ELES**

DES
Detached **E**ddy **S**imulations

LES
Large **E**ddy **S**imulations

DNS
Direct **N**umerical **S**imulations

SRS
Scale-**R**esolving **S**imulations

Increasing computational cost

Increasing modelling and mathematical complexity

The closure problem

- RANS/URANS models can be classified according to the number of equations.
  - First-order closure models:
    - 0-equation, 1/2-equation, 1-equation, 2-equation, 3-equation, and so on.
  - Second-order closure models (also called second-moment closure SMC, Reynolds stress modeling RSM, or Reynolds stress transport RST):
    - Reynolds-stress transport models RSM (7-equations in 3D).
    - Algebraic Reynolds-stress models ARSM (2-equations).
  - Third-order and higher order closure models.
  - All these formulations can use linear or non-linear eddy viscosity models.
  - Just to name a few models:
    - Baldwin-Barth, Spalart-Allmaras, $k-\epsilon$, $k-\omega$ SST , $k-kl-\omega$, RSM LRR, RSM SSG, Langtry-Menter SST, V2-F, Launder-Sharma, $q-\zeta$.
  - We just mentioned a small fraction of turbulence models. As you will find, there is a plethora of turbulence models.
  - Our goal, use the less wrong model in a very critical way.

Note: a nice collection of turbulence models at this link https://turbmodels.larc.nasa.gov/

The closure problem

- Turbulence models equations cannot be derived from fundamental principles.
- All turbulence models contain some sort of empiricism.
- Some level of calibration to observed physical solutions, numerical solutions, or analytical solutions is contained in every turbulence models.
- Also, some intelligent guessing is used.
- A lot of uncertainty is involved!

> *"Remember that all models are wrong; the practical question is how wrong do they have to be to not be useful."*
>
> G. E. P. Box

> *"Models are as good as the assumptions you put into them."*
>
> A. Fauci

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Exact equations and solvable equations

- In our discussion, when we talk about **exact** equations, we refer to the governing equations that were derived without using approximations.

- Whereas, when we talk about the **solvable** equations, we refer to the governing equations derived from the **exact** equations using approximations.

- The **solvable** equations are those that we are going to solve using different approximations, *e.g.*, Boussinesq hypothesis, gradient diffusion hypothesis, and so on.

- In few words, in the **solvable** equations we are inserting approximations to avoid solving the small scales in turbulence.

Exact equations and solvable equations

- For example, the **exact** RANS equations, can be written as follows,

$$\nabla \cdot (\bar{\mathbf{u}}) = 0$$

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) = -\frac{1}{\rho}(\nabla \bar{p}) + \nu \nabla^2 \bar{\mathbf{u}} + \frac{1}{\rho} \nabla \cdot \boldsymbol{\tau}^R$$

where

$$\boldsymbol{\tau}^R = -\rho \left(\overline{\mathbf{u}'\mathbf{u}'} \right)$$

- Then, the **solvable** RANS equations (after using approximations), can be written as follows,

$$\nabla \cdot (\bar{\mathbf{u}}) = 0$$

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) = -\frac{1}{\rho}\left(\nabla \bar{p} + \frac{2}{3}\rho \nabla k\right) + \nabla \cdot \left[\frac{1}{\rho}(\mu + \mu_t)\nabla \bar{\mathbf{u}}\right]$$

- In this case, the **solvable** RANS equations were obtained after substituting the Boussinesq approximation into the **exact** RANS equations.
- The problem now reduces to computing the turbulent eddy viscosity in the momentum equation.

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Derivation rules and identities to remember

- During the derivation of the equations, we will use the product rule and a few additional vector identities to simplify the equations.
- The product rule is written as follows,

$$\frac{\partial A_i B_j}{\partial x_k} = A_i \frac{\partial B_j}{\partial x_k} + B_j \frac{\partial A_i}{\partial x_k}$$

- The product rule can also be expressed as follows,

$$A_i \frac{\partial B_j}{\partial x_k} = \frac{\partial A_i B_j}{\partial x_k} - B_j \frac{\partial A_i}{\partial x_k}$$

$$B_j \frac{\partial A_i}{\partial x_k} = \frac{\partial A_i B_j}{\partial x_k} - A_i \frac{\partial B_j}{\partial x_k}$$

- Notice that the product rule can also be used with the time derivative.

Derivation rules and identities to remember

- We can also use the product rule with the Laplacian operator as follows,

$$\underbrace{A_i}_{A}\frac{\partial}{\partial x_j}\underbrace{\frac{\partial A_i}{\partial x_j}}_{B}=\underbrace{\frac{\partial}{\partial x_j}\left(\underbrace{A_i}_{A}\underbrace{\frac{\partial A_i}{\partial x_j}}_{B}\right)}_{\frac{\partial\frac{1}{2}A_iA_i}{\partial x_j}=A_i\frac{\partial A_i}{\partial x_j}}-\underbrace{\frac{\partial A_i}{\partial x_j}}_{B}\frac{\partial\overbrace{A_i}^{A}}{\partial x_j}$$

- The previous relation was derived using the product rule as follows,

$$A_i\frac{\partial B_j}{\partial x_k}=\frac{\partial A_iB_j}{\partial x_k}-B_j\frac{\partial A_i}{\partial x_k}$$

Derivation rules and identities to remember

- Using the product rule, we can write the following relation,

$$\frac{\partial A_i A_i}{\partial x_j} = A_i \frac{\partial A_i}{\partial x_j} + A_i \frac{\partial A_i}{\partial x_j} = 2A_i \frac{\partial A_i}{\partial x_j}$$

- Which is equivalent to,

$$\frac{\partial \frac{1}{2} A_i A_i}{\partial x_j} = A_i \frac{\partial A_i}{\partial x_j}$$

- Always have these relations at hand as we are going to use them very often to simplify (or complicate) the equations.
- Anytime that we use the product rule, you will find the following legend next to the term,

Product rule

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Derivation of the Reynolds stress transport equation

- To derive the **exact** Reynolds stress transport equation, we can proceed as follows,
  - Starting from the Navier-Stokes equations with no models (or the exact NSE or laminar NSE equations), we apply a first order moment to the equations (in analogy to statistical moments).
  - That is, we multiply the NSE by the fluctuating velocities u_i' and u_j', so we obtain the operator $u_i' u_j$, a second order tensor.
  - Then, the instantaneous velocity and pressure are replaced with the respective Reynolds decomposition expression.
  - At this point, we proceed to time average the equations.
  - Finally, we do a lot of algebra to simplify the resulting equations.
  - We also use the same averaging rules and vector identities used when deriving the RANS equations.
  - Plus, some additional differentiation rules.

- Probably, the Reynolds stress model (RSM) is the most physically sound RANS model as it avoids the use of hypothesis/assumptions to model the Reynolds stress tensor.
- But this does not necessarily mean that this method is better that the others.

Each method has different capabilities and limitations.

Derivation of the Reynolds stress transport equation

- After doing a lot algebra, the **exact** Reynolds stress transport equations are written as follows,

$$\underbrace{\frac{\partial \tau_{ij}^{R}}{\partial t}}_{1} + \underbrace{\bar{u}_k \frac{\partial \tau_{ij}^{R}}{x_k}}_{2} = \underbrace{-\left(\tau_{ik}^{R}\frac{\partial \bar{u}_j}{\partial x_k} + \tau_{jk}^{R}\frac{\partial \bar{u}_i}{\partial x_k}\right)}_{3} + \underbrace{2\nu\overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_j'}{\partial x_k}}}_{4} + \dots$$

$$\dots + \underbrace{\frac{1}{\rho}\left(\overline{u_i'\frac{\partial p'}{\partial x_j}} + \overline{u_j'\frac{\partial p'}{\partial x_i}}\right)}_{5} + \underbrace{\frac{\partial}{\partial x_k}\left(\nu\frac{\partial \tau_{ij}^{R}}{\partial x_k}\right)}_{6} + \underbrace{\frac{\partial}{\partial x_k}\left(\overline{u_i'u_j'u_k'}\right)}_{7}$$

1. Transient stress rate of change term.
2. Convective term.
3. Production term.
4. Dissipation term.
5. Turbulent stress transport related to the velocity and pressure fluctuations (redistribution).
6. Viscous stress diffusion (molecular).
7. Diffusive stress transport resulting from the triple correlation of velocity fluctuations.

We get 6 new equations, but we also generate 22 new unknowns.

$$\overline{u_i'u_j'u_k'} \quad \rightarrow \quad \text{10 unknowns}$$

$$2\nu\overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_j'}{\partial x_k}} \quad \rightarrow \quad \text{6 unknowns}$$

$$\frac{1}{\rho}\left(\overline{u_i'\frac{\partial p'}{\partial x_j}} + \overline{u_j'\frac{\partial p'}{\partial x_i}}\right) \quad \rightarrow \quad \text{6 unknowns}$$

Derivation of the Reynolds stress transport equation

- Let us derive the **exact** Reynolds stress transport equation.
- Let $\mathcal{N}(u_i)$ denote the Navier-Stokes operator,

$$\mathcal{N}(u_i) = \rho \frac{\partial u_i}{\partial t} + \rho u_k \frac{\partial u_i}{\partial x_k} + \frac{\partial p}{\partial x_i} - \mu \frac{\partial^2 u_i}{\partial x_k x_k} = 0$$

- To derive the **exact** Reynolds stress transport equation, we form the following time average,

$$\overline{u_i' \mathcal{N}(u_j) + u_j' \mathcal{N}(u_i)} = 0$$

- Then, the instantaneous velocity and pressure variables are replaced with the respective Reynolds decomposition.
- Finally, we do a lot of algebra in order to simplify the equations.

Derivation of the Reynolds stress transport equation

- Basically, we are multiplying the exact momentum equations by the velocity fluctuations in order to obtain governing equations for $\tau_{ij} = -\overline{u'_i u'_j}$.
- In doing so, we are increasing the order of closure of the equations, from first-order moment closure to second-order moment closure (in analogy to statistical moments).
- In theory, we can continue increasing the order of the moment closure up to infinite.
- However, as we keep increasing the moment, higher order correlations will keep appearing in the equations.
- For example, in the **exact** Reynolds stress transport equations, which are second-order moment closure equations, a triple correlation appears, namely,

$$\overline{u'_i u'_j u'_k}$$

- We could derive a set of governing equations for this triple correlation, but the resulting equations will contain quadruple correlations.
- Therefore, it is easier to model this term.
- It is worth noting that third-order moment closure models do exist, but they are not widely diffused, and they do not guarantee better results.
- Let us derive the **exact** Reynolds stress transport equation term-by-term.

Derivation of the Reynolds stress transport equation

- Unsteady term,

$$
\begin{aligned}
\overline{u_i'(\rho u_j)_{,t} + u_j'(\rho u_i)_{,t}} &= \overline{\rho u_i'(\bar{u}_j + u_j')_{,t}} + \overline{\rho u_j'(\bar{u}_i + u_i')_{,t}} \\
&= \overline{\rho u_i' \bar{u}_{j,t}} + \overline{\rho u_i' u'_{j,t}} + \overline{\rho u_j' \bar{u}_{i,t}} + \overline{\rho u_j' u'_{i,t}} \\
&= \overline{\rho u_i' u'_{j,t}} + \overline{\rho u_j' u'_{i,t}} \\
&= \overline{\rho (u_i' u_j')_{,t}} \\
&= -\rho \frac{\partial \tau_{ij}}{\partial t}
\end{aligned}
$$

Product rule

Derivation of the Reynolds stress transport equation

- Convective term,

$$\overline{\rho u_i' u_k u_{j,k} + \rho u_j' u_k u_{i,k}} = \overline{\rho u_i'(\bar{u}_k + u_k')(\bar{u}_j + u_j')_{,k}} + \overline{\rho u_j'(\bar{u}_k + u_k')(\bar{u}_i + u_i')_{,k}}$$

Product rule

$$= \overline{\rho u_i' \bar{u}_k u'_{j,k}} + \overline{\rho u_i' u_k'(\bar{u}_j + u_j')_{,k}} + \overline{\rho u_j' \bar{u}_k u'_{i,k}} + \overline{\rho u_j' u_k'(\bar{u}_i + u_i')_{,k}}$$

Product rule

$$= \rho \bar{u}_k \overline{(u_i' u_j')_{,k}} + \overline{\rho u_i' u_k'}\,\bar{u}_{j,k} + \overline{\rho u_j' u_k'}\,\bar{u}_{i,k} + \overline{\rho u_k (u_i' u_j')_{,k}}$$

$$= -\rho \bar{u}_k \frac{\partial \tau_{ij}}{\partial x_k} - \rho \tau_{ik} \frac{\partial \bar{u}_j}{\partial x_k} - \rho \tau_{jk} \frac{\partial \bar{u}_i}{\partial x_k} + \rho \frac{\partial}{\partial x_k} \overline{(u_i' u_j' u_k')}$$

Derivation of the Reynolds stress transport equation

- Pressure gradient term,

$$
\begin{aligned}
\overline{u'_i p_{,j} + u'_j p_{,i}} &= \overline{u'_i (\bar{p} + p')_{,j}} + \overline{u'_j (\bar{p} + p')_{,i}} \\
&= \overline{u'_i p'_{,j} + u'_j p'_{,i}} \\
&= \overline{u'_i \frac{\partial p'}{\partial x_j}} + \overline{u'_j \frac{\partial p'}{\partial x_i}}
\end{aligned}
$$

Derivation of the Reynolds stress transport equation

- Viscous term,

$$
\begin{aligned}
\mu\overline{(u_i' u_{j,kk} + u_j' u_{i,kk})} &= \mu\overline{u_i'(\bar{u}_j + u_j')_{,kk}} + \mu\overline{u_j'(\bar{u}_i + u_i')_{,kk}} \\
&= \mu\overline{u_i' u'_{j,kk}} + \mu\overline{u_j' u'_{i,kk}} \\
&= \mu\overline{(u_i' u'_{j,k})_{,k}} + \mu\overline{(u_j' u'_{i,k})_{,k}} - 2\mu\overline{u'_{i,k} u'_{j,k}} \\
&= \mu\overline{(u_i' u_j')_{,kk}} - 2\mu\overline{u'_{i,k} u'_{j,k}} \\
&= -\mu\frac{\partial^2 \tau_{ij}}{\partial x_k \partial x_k} - 2\mu\overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_j'}{\partial x_k}}
\end{aligned}
$$

Product rule

Derivation of the Reynolds stress transport equation

- Collecting terms, we arrive at the transport equation for the Reynolds stress tensor,

$$
\begin{aligned}
\frac{\partial \tau_{ij}}{\partial t} + \bar{u}_k \frac{\partial \tau_{ij}}{\partial x_k} = -\tau_{ik}\frac{\partial \bar{u}_j}{\partial x_k} - \tau_{jk}\frac{\partial \bar{u}_i}{\partial x_k} + \\
2\nu \overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_j'}{\partial x_k}} + \overline{\frac{u_i'}{\rho}\frac{\partial p'}{\partial x_j}} + \overline{\frac{u_j'}{\rho}\frac{\partial p'}{\partial x_i}} + \\
\frac{\partial}{\partial x_k}\left[\nu \frac{\partial \tau_{ij}}{\partial x_k} + \overline{u_i' u_j' u_k'}\right]
\end{aligned}
$$

Derivation of the Reynolds stress transport equation

- The previous equation can be further simplified as follows,

$$\frac{\partial \tau_{ij}}{\partial t} + \bar{u}_k \frac{\partial \tau_{ij}}{\partial x_k} = -\tau_{ik}\frac{\partial \bar{u}_j}{\partial x_k} - \tau_{jk}\frac{\partial \bar{u}_i}{\partial x_k} + \epsilon_{ij} - \Pi_{ij} + \frac{\partial}{\partial x_k}\left[\nu \frac{\partial \tau_{ij}}{\partial x_k} + C_{ijk}\right]$$

- In the previous equation, we can group terms as follows,

$$\epsilon_{ij} = 2\nu \overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_j'}{\partial x_k}}$$

Dissipation term

$$P = \tau_{ik}\frac{\partial \bar{u}_j}{\partial x_k} + \tau_{jk}\frac{\partial \bar{u}_i}{\partial x_k}$$

Production term

$$\Pi_{ij} = \overline{\frac{p'}{\rho}\left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i}\right)}$$

Pressure strain term

$$\rho C_{ijk} = \rho\overline{u_i'u_j'u_k'} + \overline{p'u_i'}\delta_{jk} + \overline{p'u_j'}\delta_{ik}$$

Turbulent transport term

- These are the **exact** Reynolds stress transport equations.
- To derive the **solvable** equations, we need to use approximations in place of the terms that contain the velocity and pressure fluctuations (ϵ_{ij}, Π_{ij}, ρC_{ijk}, P).

Derivation of the Reynolds stress transport equation

- At this point, we can group the different terms in the **exact** Reynolds stress transport equations RSM as follows.

$$\underbrace{\frac{\partial \tau_{ij}}{\partial t} + \bar{u}_k \frac{\partial \tau_{ij}}{\partial x_k}}_{\text{Material derivative}} = \underbrace{-\tau_{ik}\frac{\partial \bar{u}_j}{\partial x_k} - \tau_{jk}\frac{\partial \bar{u}_i}{\partial x_k}}_{\text{Production term}} + \overbrace{\epsilon_{ij}}^{\text{Dissipation term}} \underbrace{- \Pi_{ij} + \frac{\partial}{\partial x_k}\left[\nu \frac{\partial \tau_{ij}}{\partial x_k} + C_{ijk}\right]}_{\text{Turbulent diffusion and redistribution term}}$$

- Or in more compact form,

$$\underbrace{\nabla_t \boldsymbol{\tau}^R}_{\text{Transient}} + \underbrace{\nabla \cdot \bar{\mathbf{u}}\boldsymbol{\tau}^R}_{\text{Convection}} = \underbrace{P^{\tau}}_{\text{Production}} + \underbrace{\epsilon^{\tau}}_{\text{Dissipation}} + \underbrace{D^{\tau}}_{\text{Diffusion}} + \underbrace{S^{\tau}}_{\text{Source terms}}$$

- These equations have, a production term (eddy factory), a dissipation or destruction term (where eddies are destroyed or the eddy graveyard), and a turbulence diffusion term (transport, diffusion, and redistribution due to turbulence).

Derivation of the Reynolds stress transport equation

- At this point, we can group the different terms in the **exact** Reynolds stress transport equations RSM as follows.

$$\underbrace{\nabla_t \boldsymbol{\tau}^R}_{\text{Transient}} + \underbrace{\nabla \cdot \bar{\mathbf{u}} \boldsymbol{\tau}^R}_{\text{Convection}} = \underbrace{P^\tau}_{\text{Production}} + \underbrace{\epsilon^\tau}_{\text{Dissipation}} + \underbrace{D^\tau}_{\text{Diffusion}} + \underbrace{S^\tau}_{\text{Source terms}}$$

- Remember, the Reynolds stress tensor is a symmetric tensor.
- Therefore, it has six components. Henceforth, we derive one equation for each component.
- These equations have,
    - A transient term.
    - A convective term.
    - A production term.
    - A dissipation term.
    - A turbulence diffusion term (transport, diffusion, and redistribution due to turbulence).

Derivation of the Reynolds stress transport equation

- Finally, recall that the Reynolds stress tensor τ_{ij} or τ_{ij}^R, is defined as follows,

$$\boldsymbol{\tau}^R = \tau_{ij}^R = -\rho\left(\overline{u_i' u_j'}\right) = -\begin{pmatrix} \rho\overline{u'u'} & \rho\overline{u'v'} & \rho\overline{u'w'} \\ \rho\overline{v'u'} & \rho\overline{v'v'} & \rho\overline{v'w'} \\ \rho\overline{w'u'} & \rho\overline{w'v'} & \rho\overline{w'w'} \end{pmatrix}$$

- The Reynolds stress tensor is rather important in turbulence modeling.
- It represents the transfer of momentum due to turbulent fluctuations.
- The Reynolds stress tensor is symmetric. Therefore, it has six components.
  - The diagonal components represents normal stresses.

$$\rho\overline{u'u'} \qquad \rho\overline{v'v'} \qquad \rho\overline{w'w'}$$

  - The off-diagonal components represents the shear stresses.

$$\rho\overline{u'v'} = \rho\overline{v'u'} \qquad \rho\overline{u'w'} = \rho\overline{w'u'} \qquad \rho\overline{v'w'} = \rho\overline{w'v'}$$

Derivation of the Reynolds stress transport equation

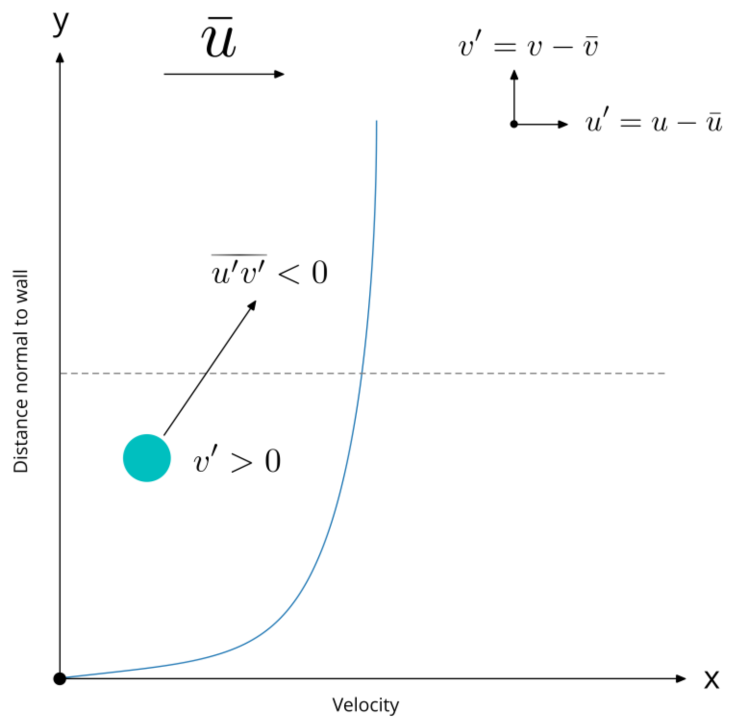
- Finally, recall that the Reynolds stress tensor τ_{ij} or τ_{ij}^R, is defined as follows,

$$\boldsymbol{\tau}^R = \tau_{ij}^R = -\rho\left(\overline{u_i' u_j'}\right) = -\begin{pmatrix} \rho\overline{u'u'} & \rho\overline{u'v'} & \rho\overline{u'w'} \\ \rho\overline{v'u'} & \rho\overline{v'v'} & \rho\overline{v'w'} \\ \rho\overline{w'u'} & \rho\overline{w'v'} & \rho\overline{w'w'} \end{pmatrix}$$

- By using a second-order moment closure method, we are deriving governing equations for each component of the second-rank tensor (six equations as the tensor is symmetric).
  - Therefore, there is no need to use the Boussinesq hypothesis.
  - However, we still need to introduce approximations to model the fluctuating quantities.
- Notice that the Reynolds stress tensor is not actually a stress, it must be multiplied by density in order to have dimensions corresponding to stresses.
- It is not compulsory to multiply this definition by the density.
- But if you do so, you need to divide by the density as well the term in the equation where you added this definition.

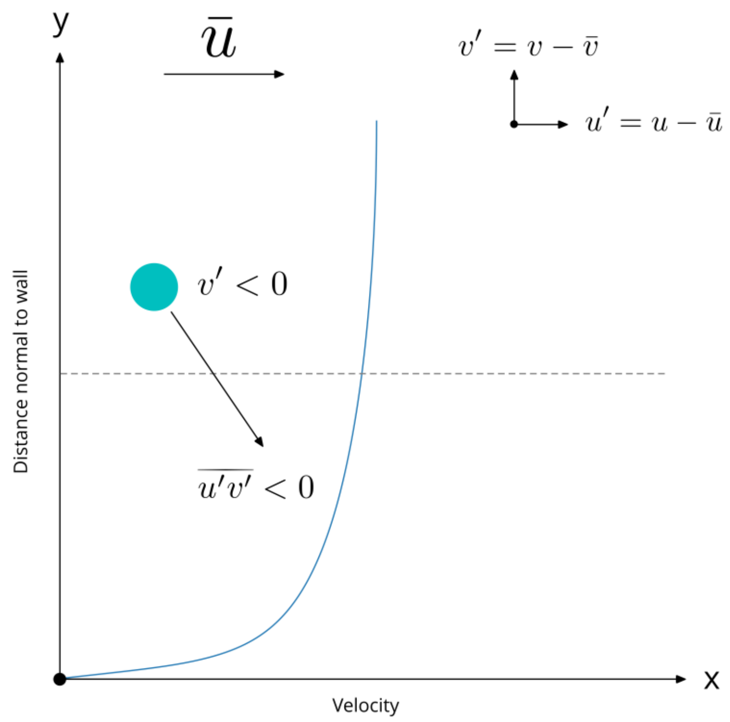
Derivation of the Reynolds stress transport equation

- Let us establish a physical interpretation to the Reynolds stress tensor.
- Imagine a fluid parcel in a boundary layer with a velocity gradient $\partial \bar{u} / \partial y > 0$.
- Now imagine the same fluid parcel crossing the dashed line in the figure (from bottom-to-top).
- A positive velocity fluctuation will imply that a slow-moving fluid parcel is transported into a faster moving flow stream.
- This slow-moving fluid parcel will generate a momentum deficit in the fast-moving flow stream.
- That is, a negative velocity correlation.



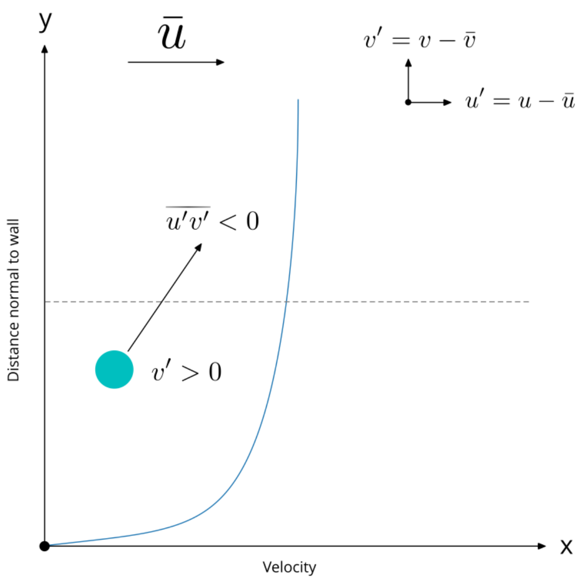
Derivation of the Reynolds stress transport equation

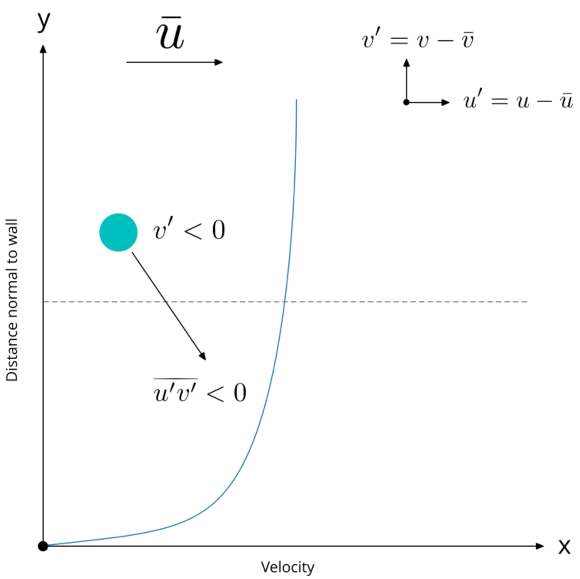
- Let us establish a physical interpretation to the Reynolds stress tensor.
- Imagine a fluid parcel in a boundary layer with a velocity gradient $\partial \bar{u} / \partial y > 0$.
- Now imagine the same fluid parcel crossing the dashed line in the figure (from top-to-bottom).
- Similarly, a negative velocity fluctuation will imply that a fast-moving fluid parcel is transported into a slower moving flow stream.
- This fast-moving fluid parcel will generate a momentum excess in the slow-moving flow stream.
- That is, a positive velocity correlation.



Derivation of the Reynolds stress transport equation

- From this rather simply explanation, we can see that the Reynolds stress tensor is responsible for the momentum exchange.
- The same reasoning can be applied to all directions or other flows, such as, jets with a negative mean velocity gradient or three-dimensional boundary layer.
- At this point, I hope it is clear why the velocity fluctuations have a negative correlation in the Reynolds stress tensor.
  - The negative correlation means that if one fluctuating component is positive, the Reynolds stress will be negative, and vice versa.
  - Therefore, there will be a momentum exchange.





Derivation of the Reynolds stress transport equation

- Both, the normal Reynolds stresses and the shear Reynolds stresses are responsible for momentum exchange.
- The normal Reynolds stresses denote the turbulent transport of momentum in the respective directions.
  - They can be interpreted as the intensity of the fluctuations.
- The shear Reynolds stresses denote the turbulent transport of momentum from one direction to the one in its perpendicular direction.
  - For example, from the x-direction to y-direction in the component τ_{xy}.
- The shear Reynolds stresses drastically enhance the transport phenomenon.
- The Reynolds stresses are a direct consequence of the velocity fluctuations.
  - They arise from the non-linear terms in the momentum equations.
- Without velocity fluctuations, there is no turbulence.
  - That is why it is so important to understand the behavior of these fluctuations in order to construct accurate turbulence models.
- Remember, the Reynolds stresses are much larger than the viscous stresses.
- Finally, the Reynolds stress not only transport momentum, it also transport scalar quantities (e.g., pressure, temperature, concentration, and so on).

Roadmap to Lecture 6

Part 1

1. ~~The closure problem~~
2. ~~Exact equations and solvable equations~~
3. ~~Derivation rules and identities to remember~~
4. ~~Derivation of the Reynolds stress transport equation~~
5. **Derivation of the turbulent kinetic energy equation**
6. Additional comments
7. Another touch to the closure problem

Derivation of the turbulent kinetic energy equation

- The transport equation for the turbulent kinetic energy can be derived by just taking the trace of the Reynolds stress transport equation.
- Let us recall that,

$$k = \frac{1}{2}\overline{u_i' u_i'} = \frac{1}{2}\left(\overline{u'^2} + \overline{v'^2} + \overline{w'^2}\right)$$

$$-(\overline{\mathbf{u}'\mathbf{u}'})^{\mathrm{tr}} = -(\overline{u_i' u_i'}) = \tau_{ii} = -2k$$

- By taking the trace ($i = j$) of the Reynolds stress equation we obtain,

$$\underbrace{\frac{\partial \tau_{ii}}{\partial t}}_{1} + \underbrace{\bar{u}_k \frac{\partial \tau_{ii}}{\partial x_k}}_{2} = \underbrace{2\tau_{ij}\frac{\partial \bar{u}_i}{\partial x_j}}_{3} + \underbrace{\epsilon_{ii}}_{4} + \underbrace{\frac{\partial}{\partial x_k}\left(\nu \frac{\partial \tau_{ii}}{\partial x_k}\right)}_{5} + \underbrace{\frac{2}{\rho}\left(\overline{u_i' \frac{\partial p'}{\partial x_i}}\right)}_{6} + \underbrace{\frac{\partial}{\partial x_k}(\overline{u_i' u_i' u_k'})}_{7}$$

1. Transient rate of change term.
2. Convective term.
3. Production term arising from the product of the Reynolds stress and the velocity gradient.
4. Dissipation term.
5. Rate of viscous stress diffusion (molecular).
6. Turbulent transport associated with the eddy pressure and velocity fluctuations.
7. Diffusive turbulent transport resulting from the triple correlation of velocity fluctuations.

Derivation of the turbulent kinetic energy equation

- We can now substitute $\tau_{ii} = -2k$ and simplify to obtain the following equation,

$$\frac{\partial k}{\partial t} + \bar{u}_j \frac{\partial k}{\partial x_j} = \tau_{ij} \frac{\partial \bar{u}_i}{\partial x_j} - \epsilon + \frac{\partial}{\partial x_j} \left[\nu \frac{\partial k}{\partial x_j} - \frac{1}{2} \overline{u_i' u_i' u_j'} - \frac{1}{\rho} \overline{p' u_j'} \right]$$

- Where ϵ is the dissipation rate (per unit mass) as is given by the following relation,

$$\frac{\epsilon_{ii}}{2} = \epsilon = \nu \overline{\frac{\partial u_i'}{\partial x_j} \frac{\partial u_i'}{\partial x_j}}$$

- This is the **exact** turbulent kinetic energy transport equation.
- To derive the **solvable** equation, we need to use approximations in place of the terms that contain velocity fluctuations.
- The Reynolds stresses can be modeled using the Boussinesq approximation.

Derivation of the turbulent kinetic energy equation

- The division of the total energy between kinetic and internal energies has a parallel in turbulent flows.
- In turbulent flows, we can split the total mean kinetic energy (per unit mass) into the sum of the kinetic energy of the mean field $\bar{K}$ and the kinetic energy of the fluctuating field k, as follows,

$$\underbrace{\frac{1}{2}\overline{UU}}_{\bar{K}_{\text{Total}}} = \underbrace{\frac{1}{2}\bar{U}\bar{U}}_{\bar{K}} + \underbrace{\frac{1}{2}\overline{u'u'}}_{k}$$

- To derive this relation, we proceed in a similar way as for the RANS equations.
    - Use the Reynolds decomposition.
    - Time average the equations.
    - Apply averaging rules.
    - Do some algebra.

Derivation of the turbulent kinetic energy equation

- We just derived a transport equation for the turbulent kinetic energy k.
- Let us derive a transport equation for the mean kinetic energy field $\bar{K}$, which is defined as follows,

$$\bar{K} = \frac{1}{2}\bar{U}\bar{U} \qquad \bar{K} = \frac{1}{2}\bar{u}_i\bar{u}_i$$

- To derive this transport equation, we multiply the **exact** RANS/URANS equation by $\bar{u}_i$.

$$\bar{u}_i \left(\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} + \frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} - \nu \frac{\partial^2 \bar{u}_i}{\partial x_j x_j} + \frac{\partial \overline{u_i' u_j'}}{\partial x_j} \right) = 0$$

- And we do some algebra.
- By the way, remember the differentiation rules defined in section 3 of this lecture.
- Notice that we multiply the **exact** RANS/URANS equation by $\bar{u}_i$, to create the group $\bar{u}_i\bar{u}_i$.
- Similar to what we did when deriving the **exact** Reynolds stress equation.

Derivation of the turbulent kinetic energy equation

- After some algebra, we obtain the following transport equation for the mean kinetic energy.

$$\underbrace{\frac{\partial \bar{K}}{\partial t} + \bar{u}_j \frac{\partial \bar{K}}{\partial x_j}}_{\text{Material derivative}} = -\overbrace{\tau_{ij} \frac{\partial \bar{u}_i}{\partial x_j}}^{\text{Production term}} - \underbrace{\nu \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_i}{\partial x_j}}_{\text{Dissipation term}} + \frac{\partial}{\partial x_j} \underbrace{\left[\left(\nu \frac{\partial \bar{K}}{\partial x_j} \right) - \left(\overline{u'_i u'_j} \bar{u}_i \right) - \left(\frac{1}{\rho} \bar{p} \bar{u}_j \right) \right]}_{\text{Turbulent diffusion and redistribution term}}$$

- And recall that,

$$\bar{K} = \frac{1}{2} \bar{u}_i \bar{u}_i \qquad \qquad \tau_{ij} = -\overline{u'_i u'_j}$$

- This is the **exact** mean kinetic energy transport equation.
- Notice that the terms appearing in this equation are very similar to those appearing in the turbulent kinetic energy transport equations.

Derivation of the turbulent kinetic energy equation

- The transport equation of the mean kinetic energy (large scales), is defined as follows,

$$\underbrace{\frac{\partial \bar{K}}{\partial t} + \bar{u}_j \frac{\partial \bar{K}}{\partial x_j}}_{\text{Material derivative}} = \overbrace{-\tau_{ij}\frac{\partial \bar{u}_i}{\partial x_j}}^{\text{Production term}} - \underbrace{\nu \frac{\partial \bar{u}_i}{\partial x_j}\frac{\partial \bar{u}_i}{\partial x_j}}_{\text{Dissipation term}} + \frac{\partial}{\partial x_j}\underbrace{\left[\left(\nu\frac{\partial \bar{K}}{\partial x_j}\right) - \left(\overline{u_i'u_j'}\bar{u}_i\right) - \left(\frac{1}{\rho}\bar{p}\bar{u}_j\right)\right]}_{\text{Turbulent diffusion and redistribution term}}$$

$$\bar{K} = \frac{1}{2}\bar{u}_i\bar{u}_i$$

- The transport equation of the turbulent kinetic energy (velocity fluctuations), is defined as follows,

$$\underbrace{\frac{\partial k}{\partial t} + \bar{u}_j \frac{\partial k}{\partial x_j}}_{\text{Material derivative}} = \overbrace{\tau_{ij}\frac{\partial \bar{u}_i}{\partial x_j}}^{\text{Production term}} - \underbrace{\nu \overline{\frac{\partial u_i'}{\partial x_j}\frac{\partial u_i'}{\partial x_j}}}_{\text{Dissipation term}} + \frac{\partial}{\partial x_j}\underbrace{\left[\left(\nu\frac{\partial k}{\partial x_j}\right) - \left(\frac{1}{2}\overline{u_i'u_i'u_j'}\right) - \left(\frac{1}{\rho}\overline{p'u_j'}\right)\right]}_{\text{Turbulent diffusion and redistribution term}}$$

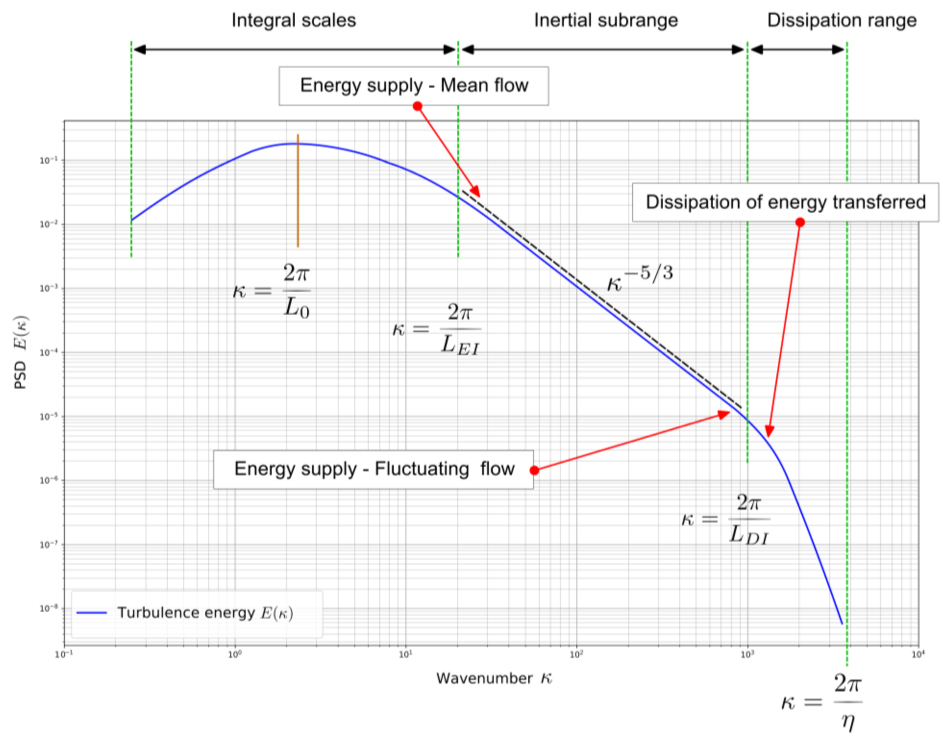
$$k = \frac{1}{2}\overline{u_i'u_i'}$$

- Notice that these equations are very similar, the main difference is the sign of the production term.
- In the mean kinetic energy equation is negative (loss of energy) and in the turbulent kinetic energy equation is positive (gain of energy). This was briefly outlined during Lecture 3.

Derivation of the turbulent kinetic energy equation

Supply of mean kinetic energy and turbulent kinetic energy in the energy cascade

- In Lecture 3, we addressed the energy cascade, and we briefly outlined the transport equations for the mean kinetic energy and for the turbulent kinetic energy.
- In this Lecture, we just derived the Reynolds stress equations, the mean kinetic energy equation, and the turbulent kinetic energy equation.
- We also gave an interpretation to each term appearing in these equations.
- So, at this point I hope all these concepts are clearer.
- Summarizing the energy cascade process:
  - Large scales (mean flow), are very energetic. They supply energy to the flow. Therefore, large scales loss energy.
  - This energy is transferred at a constant rate in the inertial subrange.
  - The energy loss of the mean flow is an energy gain of the turbulent kinetic energy.
  - At the end of the inertial subrange, the turbulent kinetic energy is dissipated.
  - Let us take a look at the transport equations of the kinetic energy.



Derivation of the turbulent kinetic energy equation

Budget of turbulent kinetic energy

- The turbulence kinetic energy and Reynolds stress budgets provide valuable guidelines for model developers, model testing, and model validation.
- These budgets can be obtained from experimental measurements or numerical simulations.
- As it can be seen, the buffer layer is very energetic.

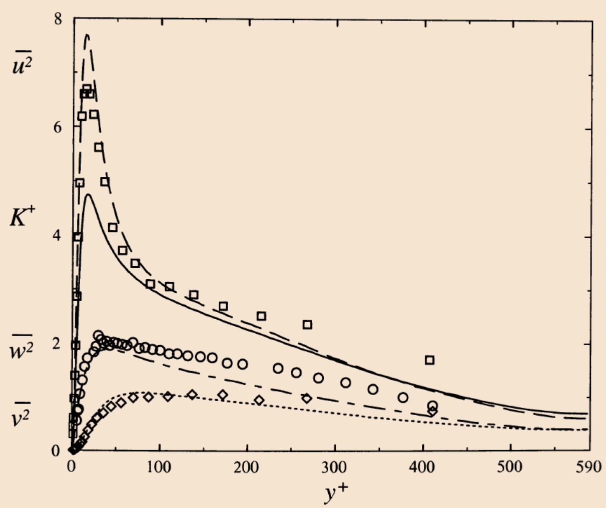


Fig. 4.7 Kinetic energy and normal stresses. Channel flow DNS [49], boundary layer measurements [33]. — —and □, $\overline{u^2}^+$; · · · and ◇, $\overline{v^2}^+$; — · —and ○, $\overline{w^2}^+$; —, K^+.

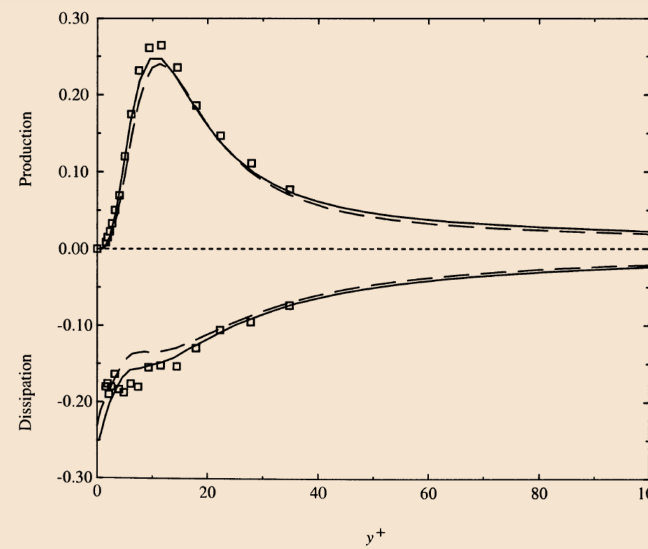


Fig. 4.11 Comparison of turbulent boundary layer and channel flow production and dissipation rates scaled with ν and u_τ. □, boundary layer measurements at $R_\tau = 1050$ [33]; —, DNS boundary layer at $R_\tau = 650$ [60]; — —, DNS channel flow $R_\tau = 590$ [49].

Left: kinetic energy and normal stresses. Right: turbulent kinetic energy budget (production and dissipation). Comparison using experimental and numerical data. Images reproduced from reference [1].

[1] P. Bernard, J. Wallace. Turbulent Flow. Analysis, Measurement and Prediction. 2002.

Roadmap to Lecture 6

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6. **Additional comments**
7. Another touch to the closure problem

Additional comments

- We just derived the **exact** form of the Reynolds stress transport equation and the **exact** form of the transport equation for the turbulent kinetic energy.
- The **exact** form of the turbulent kinetic energy was derived from the Reynolds stress transport equation; therefore, they share some similarities.
- Namely,
    - A production term or the eddy factory.
    - A dissipation or destruction term, where eddies are destroyed (the eddy graveyard).
    - A turbulence diffusion term that is responsible for the transport, diffusion, and redistribution due to turbulence.
    - Plus, any additional source term, such as buoyancy or gravity forces.
- In general, all equations used in turbulence modeling share the same similarities.

Additional comments

- For the example, the RSM equations can be grouped as follows,

$$\underbrace{\nabla_t \boldsymbol{\tau}^R}_{\text{Transient}} + \underbrace{\nabla \cdot \bar{\mathbf{u}} \boldsymbol{\tau}^R}_{\text{Convection}} = \underbrace{P^{\tau}}_{\text{Production}} + \underbrace{\epsilon^{\tau}}_{\text{Dissipation}} + \underbrace{D^{\tau}}_{\text{Diffusion}} + \underbrace{S^{\tau}}_{\text{Source terms}}$$

- And the turbulent kinetic energy can be grouped as follows,

$$\underbrace{\nabla_t k}_{\text{Transient term}} + \underbrace{\nabla \cdot \bar{\mathbf{u}} k}_{\text{Convection}} = \underbrace{P^{k}}_{\text{Production}} + \underbrace{\epsilon^{k}}_{\text{Dissipation}} + \underbrace{D^{k}}_{\text{Diffusion}} + \underbrace{S^{k}}_{\text{Source terms}}$$

- It is easy to see that any other derived turbulent quantity ϕ can be expressed in the same way,

$$\underbrace{\nabla_t \phi}_{\text{Transient term}} + \underbrace{\nabla \cdot \bar{\mathbf{u}} \phi}_{\text{Convection}} = \underbrace{P^{\phi}}_{\text{Production}} + \underbrace{\epsilon^{\phi}}_{\text{Dissipation}} + \underbrace{D^{\phi}}_{\text{Diffusion}} + \underbrace{S^{\phi}}_{\text{Source terms}}$$

Additional comments

- It is worth mentioning that the production term appearing in the turbulence equations, it always shows a similar structure.
- That is, it is the product of the Reynolds stress tensor times the mean velocity gradient, times some proportionality constant.
- Using index notation, the production term can be written as follows,

$$\mathrm{Constant} \times \tau_{ij} \frac{\partial \bar{u}_i}{\partial x_j}$$

- This operation represents the scalar product of two second-rank tensors.
- Using vector notation, the production term is written as follows,

$$\mathrm{Constant} \times \boldsymbol{\tau} : \nabla \bar{\mathbf{u}}$$

- Where the semicolons (**:**) represents the double dot product or the scalar product of two second-rank tensors.
- And to some extension the same can be said for the dissipation and diffusion terms.

Additional comments

- For example, the production term in the Reynolds stress equation it is written as follows,

$$-\tau_{ik}\frac{\partial \bar{u}_j}{\partial x_k} - \tau_{jk}\frac{\partial \bar{u}_i}{\partial x_k}$$

- And in the turbulent kinetic energy equation, the production term is written as follows,

$$\tau_{ij}\frac{\partial \bar{u}_i}{\partial x_j}$$

- Whereas, in the turbulent dissipation equation, the production term is written as follows,

$$C_{\epsilon 1}\frac{\epsilon}{k}\tau_{ij}\frac{\partial \bar{u}_i}{\partial x_j}$$

- And in the specific turbulent dissipation equation, the production term is written as follows,

$$\alpha\frac{\omega}{k}\tau_{ij}\frac{\partial \bar{u}_i}{\partial x_j}$$

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7. **Another touch to the closure problem**

Another touch to the closure problem

- From the **solvable** RANS equations, our problem reduces to computing the turbulent viscosity.

$$\nabla \cdot (\bar{\mathbf{u}}) = 0$$

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) = -\frac{1}{\rho}\left(\nabla \bar{p} + \frac{2}{3}\rho \nabla k\right) + \nabla \cdot \left[\frac{1}{\rho}\left(\mu + \mu_t\right)\nabla \bar{\mathbf{u}}\right]$$

Turbulent viscosity

- As we have seen, a relationship for the turbulent viscosity can be derived by using dimensional analysis.
- We just need to find a combination of variables that results in the same units of the molecular viscosity,

$$\mu_t = f(k, \epsilon, \omega, l, t, v, \ldots)$$

- We should also be careful that we do not introduce more variables than equations.

Another touch to the closure problem

- We just derived an equation for the turbulent kinetic energy.
- So, using the turbulent kinetic energy, we can compute the turbulent kinematic viscosity as follows,

$$\nu_t = \frac{C_\mu k^2}{\epsilon} \qquad\qquad \nu_t = \frac{k}{\omega}$$

- Now we need to derive an additional turbulent transport equation to properly close the system (our closure problem).
- In this case, we need an equation for ϵ or ω.
- These are two equations models, which are probably the most widely used models.
- Remember, there are many models.
- Have in mind that at the end of the day all equations must be rewritten in terms of mean quantities.

Another touch to the closure problem

- At the end of the day, the **solvable equations** used in the standard $k - \epsilon$ turbulence model are the following ones,

$$\nabla \cdot (\bar{\mathbf{u}}) = 0$$

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) = -\frac{1}{\rho}\left(\nabla \bar{p} + \frac{2}{3}\rho \nabla k\right) + \nabla \cdot \left[\frac{1}{\rho}\left(\mu + \mu_t\right)\nabla \bar{\mathbf{u}}\right]$$

$$\nabla_t k + \nabla \cdot (\bar{\mathbf{u}} k) = \tau^R : \nabla \bar{\mathbf{u}} - \epsilon + \nabla \cdot \left[\left(\nu + \frac{\nu_t}{\sigma_k}\right)\nabla k\right]$$

$$\nabla_t \epsilon + \nabla \cdot (\bar{\mathbf{u}} \epsilon) = C_{\epsilon_1}\frac{\epsilon}{k}\tau^R : \nabla \bar{\mathbf{u}} - C_{\epsilon_2}\frac{\epsilon^2}{k} + \nabla \cdot \left[\left(\nu + \frac{\nu_t}{\sigma_\epsilon}\right)\nabla \epsilon\right]$$

Another touch to the closure problem

- The **solvable equations** of the standard $k-\epsilon$ turbulence model are solved together with the following closure coefficients,

$$C_{\epsilon_1} = 1.44 \qquad C_{\epsilon_2} = 1.92 \qquad C_\mu = 0.09 \qquad \sigma_k = 1.0 \qquad \sigma_\epsilon = 1.3$$

- And the following closure relationships,

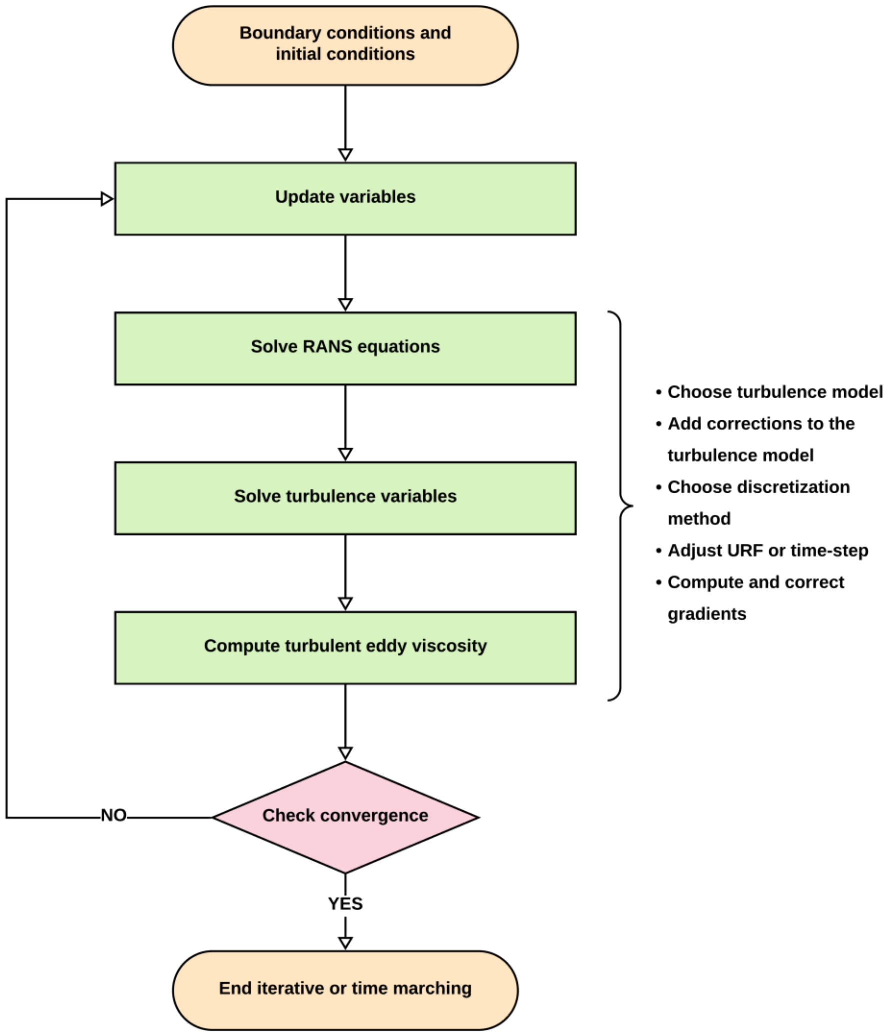
$$\nu_t = \frac{C_\mu k^2}{\epsilon} \qquad\qquad l = \frac{C_\mu k^{3/2}}{\epsilon}$$

- No need to mention that different turbulent models will have different closure coefficients and different closure relationships.
- Later, we will give a few remarks on the calibration of the closure coefficients.
- And as we studied during Lecture 2-4, the closure relationships are derived using dimensional analysis.
- Remember, as this is an IVBP problem, you need to assign boundary and initial conditions to all variables.

Another touch to the closure problem

A naïve CFD loop for turbulence modeling

- The first step consist in defining the boundary and initial conditions of all variables. Including the variables related to the turbulence model.
- The loop will solve first the RANS/URANS equations.
- Then, it will move to the next step, where it solves the equations of the turbulence model using the mean values of the RANS/URANS equations.
- It will then compute the turbulent eddy viscosity.
- At this point, it will check the convergence.
- If it is necessary, it will update the variables and it will do another sweep.
- To solve this problem, you can use any of the different numerical methods that we covered in Lecture 5.
- Generally speaking, it is better to use pressure-based methods.
- If you are conducting RANS simulations (steady simulations) we recommend to use coupled methods.
- If coupled methods are not available, you can use any segregated method (SIMPLE or SIMPLEC).
- Instead, if you are conducting URANS simulations (unsteady simulations), we recommend to use the PISO method or the fractional step method.



Another touch to the closure problem

- Summarizing:
  - By using the Reynolds decomposition and time-averaging the exact Navier-Stokes equations, we obtain the RANS/URANS equations.
  - The Reynolds stress tensor $\boldsymbol{\tau}^R$ appearing in the RANS/URANS equations needs to be modeled.
    - The most widely used approach is the Boussinesq approximation.
  - From the Boussinesq approximation a new variable emerges, namely, the turbulent viscosity μ_t.
  - To compute the turbulent viscosity μ_t, we need to use additional closure equations.
    - We just illustrated the $k - \epsilon$ model, which solves two additional equations. One for the turbulent kinetic energy k and one for the turbulent dissipation rate ϵ.
  - All equations used must be expressed in terms of mean flow quantities. That is, we need to remove the instantaneous fluctuations from the equations by using proper engineering approximations.
  - This is our closure problem.
  - The derivation of the equation for the turbulent viscosity is based on dimensional analysis.
  - Which does not tell much about the underlying physics of the relationships used, so we need to be very critical when using turbulence models.