# 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 of the Reynolds stress transport equation
4. Derivation of the turbulent kinetic energy equation
5. Another touch to the closure problem

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# Closure problem

- Let us recall the incompressible RANS equations,

Reynolds stress tensor

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

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

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

- 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).

# Closure problem

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

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

# Closure problem

- Overview of the main turbulence modeling approaches.

## MODELING APPROACH

**RANS**
**R**eynolds-**A**veraged **N**avier-**S**tokes equations

**URANS**
**U**nsteady **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**
**D**etached **E**ddy **S**imulations

**LES**
**L**arge **E**ddy **S**imulations

**DNS**
**D**irect **N**umerical **S**imulations

**SRS**
**S**cale-**R**esolving **S**imulations

Increasing computational cost

Increasing modelling and mathematical complexity

# Closure problem

- At the same time, RANS/URANS models can be classified according to the number of equations.
  - First-order closure models:
    - 0-equation, ½-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).
    - Algebraic Reynolds-stress models ARSM (2-equations).
  - 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, $k-kl-\omega$, LRR, SSG, Langtry-Menter SST, V2-F, Launder-Sharma, $q-\zeta$.
  - We only listed 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/

# 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.

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

# Exact equations and solvable equations

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

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

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) = -\frac{1}{\rho}(\nabla p) + \nu \nabla^2 \bar{\mathbf{u}} + \frac{1}{\rho}\nabla \cdot \boldsymbol{\tau}^R \qquad \text{where} \qquad \boldsymbol{\tau}^R = -\rho \left(\overline{\mathbf{u}'\mathbf{u}'}\right)$$

- 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 of the Reynolds stress transport equation

- To derive the Reynolds stress transport equation, we can proceed as follows,
  - Starting from the Navier-Stokes equations with no models (often known as the laminar NSE equations), we apply a first order moment to the equations.
  - That is, we multiply the NSE by the fluctuating velocities $u_i'$ and $u_j'$, so we obtain a second order tensor.
  - Then, the instantaneous velocity and pressure are replaced with the respective Reynolds decomposition expression.
  - At this point, we 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.

# Derivation of the Reynolds stress transport equation

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    - Starting from the Navier-Stokes equations with no models (often known as the laminar NSE equations), we apply a first order moment to the equations.
    - That is, we multiply the NSE by the fluctuating velocities $u'_i$ and $u'_j$ .
    - Then, the instantaneous velocity and pressure are replaced with the respective Reynolds decomposition expression.
    - At this point, we time average the equations.
    - Finally, we do a lot of algebra to simplify the resulting equations.

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

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

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

# Derivation of the Reynolds stress transport equation

- Let us derive the Reynolds stress transport equation.
- Let $\mathcal{N}(u_i)$ denote the Naiver-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 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.
- Let us work in a term by term basis.

# Derivation of the Reynolds stress transport equation

- Unsteady term,

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

# Derivation of the Reynolds stress transport equation

- Convective term,

$$
\begin{aligned}
\overline{\rho u_i' u_k u_{j,k} + \rho u_j' u_k u_{i,k}} &= \overline{\rho u_i' (\bar{u}_k + u_k')(\bar{u}_j + u_j')_{,k}} + \overline{\rho u_j' (\bar{u}_k + u_k')(\bar{u}_i + u_i')_{,k}} \\
&= \overline{\rho u_i' \bar{u}_k u_{j,k}'} + \overline{\rho u_i' u_k' (\bar{u}_j + u_i')_{,k}} + \overline{\rho u_j' \bar{u}_k u_{i,k}'} + \overline{\rho u_j' u_k' (\bar{u}_i + u_i')_{,k}} \\
&= \rho \bar{u}_k \overline{(u_i' u_j')_{,k}} + \rho \overline{u_i' u_k'} \bar{u}_{j,k} + \rho \overline{u_j' u_k'} \bar{u}_{i,k} + \rho \overline{u_k (u_i' u_j')_{,k}} \\
&= -\rho \bar{u}_k \frac{\partial \tau_{ij}}{\partial x_k} - \rho \tau_{ik} \frac{\partial \bar{u}_j}{\partial x_k} - \rho \tau_{jk} \frac{\partial \bar{u}_i}{\partial x_k} + \rho \frac{\partial}{\partial x_k} \overline{(u_i' u_j' u_k')}
\end{aligned}
$$

# 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,

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

# Derivation of the Reynolds stress transport equation

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

$$\frac{\partial \tau_{ij}}{\partial t} + \bar{u}_k \frac{\partial \tau_{ij}}{\partial x_k} = -\tau_{ik} \frac{\partial \bar{u}_j}{\partial x_k} - \tau_{jk} \frac{\partial \bar{u}_i}{\partial x_k} +$$

$$2\nu \overline{\frac{\partial u_i'}{\partial x_k} \frac{\partial u_j'}{\partial x_k}} + \overline{\frac{u_i'}{\rho} \frac{\partial p'}{\partial x_j}} + \overline{\frac{u_j'}{\rho} \frac{\partial p'}{\partial x_i}} +$$

$$\frac{\partial}{\partial x_k} \left[ \nu \frac{\partial \tau_{ij}}{\partial x_k} + \overline{u_i' u_j' u_k'} \right]$$

# Derivation of the Reynolds stress transport equation

- These equations can be further simplified as follows,

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

- Where,

$$\epsilon_{ij} = 2\nu \overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_j'}{\partial x_k}} \qquad \Pi_{ij} = \overline{\frac{p'}{\rho}\left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i}\right)}$$

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

- 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 velocity fluctuations ($\epsilon_{ij}$, $\Pi_{ij}$, $\rho C_{ijk}$).
- The Reynolds stresses can be modeled using the Boussinesq approximation.

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# 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 rate.
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 $\epsilon$ is the dissipation rate (per unit mass) as is given by the following relation,

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

- 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.

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# Another touch to the closure problem

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

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

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

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

# 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 $\epsilon$ or $\omega$.
- 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 this is our problem (with closure using the $k - \epsilon$ turbulence model),

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

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

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

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

- 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 closure relationships,

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

- And as this is an IVBP problem, you need to assign boundary and initial conditions to all variables.

# Another touch to the closure problem

- Summarizing:
  - By using the Reynolds decomposition and time-averaging the governing 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 $\mu_t$.
  - To compute the turbulent viscosity $\mu_t$ 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 $\epsilon$.
  - 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.
  - Remember, 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.