Turbulence and CFD models: Theory and applications

Roadmap to Lecture 5

- 1. Governing equations of fluid dynamics
- 2. RANS equations Reynolds averaging
- 3. The Boussinesq hypothesis
- 4. The gradient diffusion hypothesis
- 5. Sample turbulence models
- 6. Quick review of solution methods for the governing equations of fluid dynamics
- 7. What is Ansys Fluent? Executive summary

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"That we have written an equation does not remove from the flow of fluids its charm or mystery or its surprise."

Richard Feynman

Governing equations of fluid dynamics

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \tau + \mathbf{S}_{\mathbf{u}}$$
Source terms
$$\frac{\partial (\rho e_t)}{\partial t} + \nabla \cdot (\rho e_t \mathbf{u}) = -\nabla \cdot q - \nabla \cdot (p \mathbf{u}) + \boldsymbol{\tau} : \nabla \mathbf{u} + \mathbf{S}_{e_t}$$

$$+$$

Additional equations to close the system

Relationships between two or more thermodynamics variables (p, ρ, T, e_t) Additionally, relationships to relate the transport properties (μ, k)

In the absent of models (turbulence, multiphase, mass transfer, combustion, particles interaction, chemical reactions, acoustics, and so on), this set of equations will resolve all scales in space and time.

Governing equations of fluid dynamics

I like to write the governing equations in matrix-vector form,

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{e}_i}{\partial x} + \frac{\partial \mathbf{f}_i}{\partial y} + \frac{\partial \mathbf{g}_i}{\partial z} = \frac{\partial \mathbf{e}_v}{\partial x} + \frac{\partial \mathbf{f}_v}{\partial y} + \frac{\partial \mathbf{g}_v}{\partial z}$$

Where q is the vector of the conserved flow variables,

$$\mathbf{q} = egin{bmatrix}
ho & & \leftarrow & \text{CE} \
ho u \
ho v \
ho w \
ho e_t \end{bmatrix} lacksquare$$

Governing equations of fluid dynamics

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The vectors e_i, f_i, and g_i contain the inviscid fluxes (or convective fluxes) in the x, y, and z directions,

$$\mathbf{e}_{i} = \begin{bmatrix} \rho u \\ \rho u^{2} + p \\ \rho u v \\ \rho u w \\ (\rho e_{t} + p) u \end{bmatrix}, \qquad \mathbf{f}_{i} = \begin{bmatrix} \rho v \\ \rho v u \\ \rho v v \\ \rho v w \\ (\rho e_{t} + p) v \end{bmatrix}, \qquad \mathbf{g}_{i} = \begin{bmatrix} \rho w \\ \rho w u \\ \rho w v \\ \rho w^{2} + p \\ (\rho e_{t} + p) w \end{bmatrix}$$

Governing equations of fluid dynamics

I like to write the governing equations in matrix-vector form.

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{e}_i}{\partial x} + \frac{\partial \mathbf{f}_i}{\partial y} + \frac{\partial \mathbf{g}_i}{\partial z} = \frac{\partial \mathbf{e}_v}{\partial x} + \frac{\partial \mathbf{f}_v}{\partial y} + \frac{\partial \mathbf{g}_v}{\partial z}$$

• The vectors $\mathbf{e_v}$, $\mathbf{f_v}$, and $\mathbf{g_v}$ contain the viscous fluxes (or diffusive fluxes) in the x, y, and z directions,

$$\mathbf{e}_{\boldsymbol{v}} = \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ \tau_{xz}u\tau_{xx} + v\tau_{xy} + w\tau_{xz} - q_x \end{bmatrix}, \ \mathbf{f}_{\boldsymbol{v}} \ = \begin{bmatrix} 0 \\ \tau_{yx} \\ \tau_{yy} \\ \tau_{yz} \\ u\tau_{yx} + v\tau_{yy} + w\tau_{yz} - q_y \end{bmatrix}, \ \mathbf{g}_{\boldsymbol{v}} = \begin{bmatrix} 0 \\ \tau_{zx} \\ \tau_{zy} \\ \tau_{zz} \\ u\tau_{zx} + v\tau_{zy} + w\tau_{zz} - q_z \end{bmatrix}$$

Governing equations of fluid dynamics

The heat fluxes \mathbf{q} in the vectors $\mathbf{e_v}$, $\mathbf{f_v}$, and $\mathbf{g_v}$ can be computed using Fourier's law of heat conduction as follows,

$$q_x = -k \frac{\partial T}{\partial x}, \qquad q_y = -k \frac{\partial T}{\partial y}, \qquad q_z = -k \frac{\partial T}{\partial z}$$

Where *k* is the thermal conductivity

 If we assume that the fluid behaves as a Newtonian fluid (a fluid where the shear stresses are proportional to the velocity gradients), the viscous stresses can be computed as follows,

$$\tau_{xx} = \lambda \left(\nabla \cdot \mathbf{u} \right) + 2\mu \frac{\partial u}{\partial x} = \frac{2}{3}\mu \left(2\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} - \frac{\partial w}{\partial z} \right) \qquad \tau_{xy} = \tau_{yx} = \mu \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)$$

$$\tau_{yy} = \lambda \left(\nabla \cdot \mathbf{u} \right) + 2\mu \frac{\partial v}{\partial y} = \frac{2}{3}\mu \left(2\frac{\partial v}{\partial y} - \frac{\partial u}{\partial x} - \frac{\partial w}{\partial z} \right) \qquad \tau_{xz} = \tau_{zx} = \mu \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right)$$

$$\tau_{zz} = \lambda \left(\nabla \cdot \mathbf{u} \right) + 2\mu \frac{\partial w}{\partial z} = \frac{2}{3}\mu \left(2\frac{\partial w}{\partial z} - \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right) \qquad \tau_{yz} = \tau_{zy} = \mu \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right)$$

Governing equations of fluid dynamics

- In virtually all practical aerodynamic problems, the working fluid can be assumed to be Newtonian.
- In the normal viscous stresses $\tau_{xx}, \tau_{yy}, \tau_{zz}$, the variable λ is known as the second viscosity coefficient (or bulk viscosity).
- If we use Stokes hypothesis, the second viscosity coefficient can be approximated as follows,

$$\lambda = -\frac{2}{3}\mu$$

- Except for extremely high temperature or pressure, there is so far no experimental evidence that Stokes hypothesis does not hold.
- For gases and incompressible flows, Stokes hypothesis is a good approximation.

Governing equations of fluid dynamics

By using Stokes hypothesis and assuming a Newtonian flow, the viscous stresses can be expressed as follows,

$$\tau_{xx} = \frac{2}{3}\mu \left(2\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} - \frac{\partial w}{\partial z} \right), \qquad \tau_{xy} = \tau_{yx} = \mu \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)$$

$$\tau_{yy} = \frac{2}{3}\mu \left(2\frac{\partial v}{\partial y} - \frac{\partial u}{\partial x} - \frac{\partial w}{\partial z} \right), \qquad \tau_{xz} = \tau_{zx} = \mu \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right)$$

$$\tau_{zz} = \frac{2}{3}\mu \left(2\frac{\partial w}{\partial z} - \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right) \qquad \tau_{yz} = \tau_{zy} = \mu \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right)$$

- In our discussion, it is also necessary to relate the transported fluid properties (μ,k) to the thermodynamic variables (temperature and pressure).
- We will discuss this later.

Governing equations of fluid dynamics

 If you examine closely the equations we have seen so far, you will notice that we have five equations and seven variables.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \tau + \mathbf{S}_{\mathbf{u}}$$
Source terms
$$\frac{\partial (\rho e_t)}{\partial t} + \nabla \cdot (\rho e_t \mathbf{u}) = -\nabla \cdot q - \nabla \cdot (p \mathbf{u}) + \boldsymbol{\tau} : \nabla \mathbf{u} + \mathbf{S}_{e_t}$$

To close the system, we need to find two more equations by determining the relationship that exist between the thermodynamics variables (p, ρ, T, e_t) .

Governing equations of fluid dynamics

• Choosing the internal energy e_i and the density ρ as the two independent thermodynamic variables, we can find equations of state of the form,

$$p = p(e_i, \rho)$$
 $T = T(e_i, \rho)$

 Assuming that the working fluid is a gas, that behaves as a perfect gas and is also a calorically perfect gas, the following relations for pressure p and temperature T can be used,

$$p = (\gamma - 1) \rho e_i, \qquad T = \frac{p}{\rho R_g} = \frac{(\gamma - 1) e_i}{R_g}$$

- Now our system of equations is closed.
- That is, seven equations and seven variables.

Governing equations of fluid dynamics

To derive the thermodynamics relations for pressure p and temperature T, the following equations where used,

$$p = \rho R_g T$$

Equation of state

Recall that R_a is the specific gas constant

$$e_i = c_v T,$$

$$\gamma = \frac{c_p}{c_v},$$

 $e_i = c_v T, \qquad h = c_p T, \qquad \gamma = \frac{c_p}{c_v}, \qquad c_v = \frac{R_g}{\gamma - 1}, \qquad c_p = \frac{\gamma R_g}{\gamma - 1}$

$$c_p = \frac{\gamma R_g}{\gamma - 1}$$

Internal energy

Enthalpy

Ratio of specific heats

Specific heat at constant volume

Specific heat at constant pressure

$$e_t = e_i + \frac{1}{2} (u^2 + v^2 + w^2)$$

Total energy

Governing equations of fluid dynamics

- In our discussion, it is also necessary to relate the transported fluid properties (μ,k) to the thermodynamic variables.
- The molecular viscosity (or laminar viscosity) can be computed using Sutherland's formula with two coefficients (one of the many models available),

$$\mu = \frac{C_1 T^{\frac{3}{2}}}{(T + C_2)}$$

The thermal conductivity k can be computed as follows,

$$k = \frac{c_p \mu}{Pr}$$
 Prandtl number of the working fluid

Governing equations of fluid dynamics

- If you are working with high-speed compressible flows, it is useful to introduce the Mach number.
- The Mach number is a non-dimensional parameter that measures the speed of the gas motion in relation to the speed of sound a,

$$a = \left[\left(\frac{\partial p}{\partial \rho} \right)_S \right]^{\frac{1}{2}} = \sqrt{\gamma \frac{p}{\rho}} = \sqrt{\gamma R_g T}$$

• Then, the Mach number M can be computed as follows,

$$M_{\infty} = \frac{U_{\infty}}{a} = \frac{U_{\infty}}{\sqrt{\gamma(p/\rho)}} = \frac{U_{\infty}}{\sqrt{\gamma R_g T}}$$

And never forget the definition of the Reynolds number,

$$Re_L = \frac{\rho UL}{\mu} = \frac{UL}{\nu}$$

Governing equations of fluid dynamics

- The previous equations, together with appropriate equations of state, boundary conditions, and initial conditions, govern the unsteady three-dimensional motion of a viscous Newtonian compressible fluid.
- These equations solve all the scales in space and time.
 - Therefore, we need to use very fine meshes and very small time-steps.
- Notice that besides the thermodynamics models (or constitutive equations) and a few assumptions (Newtonian fluid and Stokes hypothesis), we did not use any other model.
- Our goal now is to add turbulence models to these equations in order to avoid solving all scales.
- This will allow us use coarse meshes and larger time-steps.
 - Therefore, we will be able to get fast outcomes (with good accuracy?).
- We can also use steady solvers.
- Before deriving the RANS equations, let us add a few simplifications to this beautiful set of equations.

Simplifications of the governing equations of fluid dynamics

- In many applications the fluid density can be assumed to be constant.
- If the flow is also isothermal, the viscosity is also constant.
- This is true not only for liquids, but also for gases if the Mach number is below 0.3.
- Such flows are known as incompressible flows.
- If the fluid is also Newtonian, the governing equations written in compact conservation differential form and in primitive variable formulation (u, v, w, p) reduce to the following set of equations,

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

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

Simplifications of the governing equations of fluid dynamics

 In expanded three-dimensional Cartesian coordinates, the simplified governing equations can be written as follows,

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

$$\frac{\partial u}{\partial t} + \frac{\partial uu}{\partial x} + \frac{\partial uv}{\partial y} + \frac{\partial uw}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right)$$

$$\frac{\partial v}{\partial t} + \frac{\partial uv}{\partial x} + \frac{\partial vv}{\partial y} + \frac{\partial vw}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \nu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right)$$

$$\frac{\partial w}{\partial t} + \frac{\partial uw}{\partial x} + \frac{\partial vw}{\partial y} + \frac{\partial ww}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial z} + \nu \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right)$$

- It is worth noting that the simplifications added do not make the equations easier to solve.
- The mathematical complexity is the same. We just eliminated a few variables, so from the computational point of few, it means less storage.
- Also, the convergence rate is not necessarily faster.

Simplifications of the governing equations of fluid dynamics

We can also write the simplified governing equations in matrix-vector form.

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{e}_i}{\partial x} + \frac{\partial \mathbf{f}_i}{\partial y} + \frac{\partial \mathbf{g}_i}{\partial z} = \frac{\partial \mathbf{e}_v}{\partial x} + \frac{\partial \mathbf{f}_v}{\partial y} + \frac{\partial \mathbf{g}_v}{\partial z}$$

$$\mathbf{q} = \begin{bmatrix} 0 \\ u \\ v \\ w \end{bmatrix} \qquad \mathbf{e}_{i} = \begin{bmatrix} u \\ u^{2} + p \\ uv \\ uw \end{bmatrix}, \qquad \mathbf{f}_{i} = \begin{bmatrix} v \\ vu \\ v^{2} + p \\ vw \end{bmatrix}, \qquad \mathbf{g}_{i} = \begin{bmatrix} w \\ wu \\ wv \\ w^{2} + p \end{bmatrix}$$

$$\mathbf{e}_{m{v}} = egin{bmatrix} 0 \ au_{xx} \ au_{xy} \ au_{xz} \end{bmatrix}, \qquad \mathbf{f}_{m{v}} = egin{bmatrix} 0 \ au_{yx} \ au_{yy} \ au_{yz} \end{bmatrix}, \qquad \mathbf{g}_{m{v}} = egin{bmatrix} 0 \ au_{zx} \ au_{zy} \ au_{zz} \end{bmatrix}$$

Simplifications of the governing equations of fluid dynamics

• Recall that the viscous stresses tensor au can be written as follows,

$$oldsymbol{ au} = egin{bmatrix} au_{xx} & au_{xy} & au_{xz} \ au_{yx} & au_{yy} & au_{yz} \ au_{zx} & au_{zy} & au_{zz} \end{bmatrix}$$

 By using Stokes hypothesis and assuming a Newtonian flow, the viscous stresses can be expressed as follows,

$$\tau_{xx} = 2\mu \frac{\partial u}{\partial x} \qquad \tau_{xy} = \tau_{yx} = \mu \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)$$

$$\tau_{yy} = 2\mu \frac{\partial v}{\partial y} \qquad \tau_{xz} = \tau_{zx} = \mu \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right)$$

$$\tau_{zz} = 2\mu \frac{\partial w}{\partial z} \qquad \tau_{yz} = \tau_{zy} = \mu \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right)$$

Simplifications of the governing equations of fluid dynamics

The viscous stress tensor can be written in compact vector form as follows,

$$\tau = 2\mu \mathbf{S}$$

Where S represents the strain-rate tensor and is given by the following relationship,

$$\mathbf{S} = \frac{1}{2} \left[\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}} \right]$$

 Additionally, the gradient tensor can be decomposed in symmetric and skew parts as follows,

$$\nabla \mathbf{u} = [\mathbf{S} + \Omega]$$

• Where Ω represents the spin tensor (vorticity), and is given by,

$$\Omega = \frac{1}{2} \left[\nabla \mathbf{u} - \nabla \mathbf{u}^{\mathrm{T}} \right]$$

Simplifications of the governing equations of fluid dynamics

- In the previous definitions, **S** represent the symmetric part of the gradient tensor and Ω represents the skew (or anti-symmetric) part of the gradient tensor.
- This decomposition is based on the fact that every second rank tensor A (e.g., the
 gradient of a vector), can be decomposed into symmetric and skew parts, as follows,

$$\mathbf{A} = \underbrace{\frac{1}{2} \left[\mathbf{A} + \mathbf{A}^{\mathrm{T}} \right]}_{\text{Symmetric part}} + \underbrace{\frac{1}{2} \left[\mathbf{A} - \mathbf{A}^{\mathrm{T}} \right]}_{\text{Skew part}} = \operatorname{symm} \mathbf{A} + \operatorname{skew} \mathbf{A}$$

- A short note regarding the notation,
 - We used **S** to denote the strain-rate tensor and Ω to denote the spin or vorticity tensor. This is the notation that we will consistently use.
 - In the literature, some authors use **D** to denote the strain-rate tensor and **S** to denote the spin tensor.

Comment on non-Newtonian flows

- For some non-Newtonian flows (e.g., polymers, blood, honey, chocolate), the non-Newtonian viscosity η can be written in terms of the strain-rate tensor $\eta(S)$.
- In general, the non-Newtonian viscosity depends on the shear rate magnitude (or the norm),

$$\gamma = \sqrt{2 \mathbf{S} : \mathbf{S}}$$
 This is the scalar product of two second rank tensors. $\mathbf{A} : \mathbf{B}$ $A_{ij}B_{ij}$

- There are many models to compute the viscous stress tensor in non-Newtonian flows.
- For example, using the power law model, the non-Newtonian viscosity is computed as follows,

$$\eta = k\gamma^{n-1}$$

- Where *k* (consistency index) and n (power-law index) are input parameters of the model.
- Notice that if you set *n* and *k* equal to 1, you get the Newtonian formulation.
- Therefore, the viscous stress tensor can be approximated as follows,

Non-Newtonian flow
$$au=\eta(\mathbf{S})\mathbf{S}$$
 where $\mathbf{S}=rac{1}{2}\left[
abla\mathbf{u}+
abla\mathbf{u}^{\mathrm{T}}
ight]$

Simplifications of the governing equations of fluid dynamics

 From now on, and only to reduce the amount of algebra, we will use the incompressible, isothermal, Newtonian, governing equations.

$$\nabla \cdot (\mathbf{u}) = 0$$
$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) = \frac{-\nabla p}{\rho} + \nu \nabla^2 \mathbf{u}$$

Conservative vs. non-conservative form of the governing equations

- We presented the governing equations in their conservative form, that is, the vector of conservative variables is inside the derivatives.
- From a mathematical point of view, the conservative and non-conservative form of the governing equations are the same.
- But from a numerical point of view, the conservative form is preferred in CFD. Specially if we are using the finite volume method (FVM).
- The conservative form enforces local conservation as we are computing fluxes across the faces
 of a control volume.
- The conservative form use flux variables as dependent variables, and the non-conservative form uses the primitive variables as dependent variables.

$$\frac{\partial \left(\rho \mathbf{u}\right)}{\partial t} + \nabla \cdot \left(\rho \mathbf{u} \mathbf{u}\right) = -\nabla p + \nabla \cdot \boldsymbol{\tau}$$

Conservative form

 $\rho \left(\frac{\partial \left(\mathbf{u} \right)}{\partial t} + \mathbf{u} \cdot \nabla \left(\mathbf{u} \right) \right) = -\nabla p + \nabla \cdot \boldsymbol{\tau}$

Non-conservative form

- If you integrate this equation in a control volume, fluxes across the faces will arise.
- The FVM method is based on integrating the governing equations in every control volume.

Conservative vs. non-conservative form of the governing equations

Let us recall the following identity,

$$\nabla \cdot (\mathbf{u}\mathbf{u}) = \mathbf{u} \cdot \nabla \mathbf{u} + \mathbf{u}(\nabla \cdot \mathbf{u})$$

• From the divergence-free constraint $abla\cdot {f u}=0$ it follows that ${f u}(
abla\cdot {f u})$ is equal to zero. Therefore,

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

 Henceforth, the non-conservative form of the momentum equation (also known as the advective or convective form) is equal to

$$\rho \left(\frac{\partial (\mathbf{u})}{\partial t} + \mathbf{u} \cdot \nabla (\mathbf{u}) \right) = -\nabla p + \nabla \cdot \boldsymbol{\tau}$$

And is equivalent to the conservative form of the momentum equation (also known as the divergence form),

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau}$$

Incompressible Navier-Stokes using index notation

The incompressible Navier-Stokes equations can also be written using index notation as follows,

$$\frac{\partial u_i}{\partial x_i} = 0$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j x_j}$$

$$i = 1, 2, 3$$

$$j = 1, 2, 3$$

Incompressible Navier-Stokes using index notation

 Dust your notes on index notation* as from time to time I will change from vector notation to index notation.

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

$$\frac{\partial \mathbf{u}_i}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) = \frac{-\nabla p}{\rho} + \nu \nabla^2 \mathbf{u} \qquad \longleftrightarrow \qquad \frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{x_i} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_i x_i}$$