

Governing Equations for Fully Compressible Flow

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Continuity equation:

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

i.e. in scalar form:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0$$

Momentum equation (Navier-Stokes equation):

Conservation form

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

where $\boldsymbol{\tau} = \mu[\nabla \mathbf{V} + (\nabla \mathbf{V})^T] - \frac{2}{3}\mu(\nabla \cdot \mathbf{V})\mathbf{I}$,

$$\boldsymbol{\tau} = \mu \begin{bmatrix} 2\frac{\partial u}{\partial x} - \frac{2}{3}(\nabla \cdot \mathbf{V}) & \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} & \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \\ \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} & 2\frac{\partial v}{\partial y} - \frac{2}{3}(\nabla \cdot \mathbf{V}) & \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \\ \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} & \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} & 2\frac{\partial w}{\partial z} - \frac{2}{3}(\nabla \cdot \mathbf{V}) \end{bmatrix}$$

$$\tau_x = \mu \left[2\frac{\partial u}{\partial x} - \frac{2}{3}(\nabla \cdot \mathbf{V}), \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}, \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right]$$

$$\tau_y = \mu \left[\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}, 2\frac{\partial v}{\partial y} - \frac{2}{3}(\nabla \cdot \mathbf{V}), \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right]$$

$$\tau_z = \mu \left[\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}, \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}, 2\frac{\partial w}{\partial z} - \frac{2}{3}(\nabla \cdot \mathbf{V}) \right]$$

The $\nabla \cdot (\rho \mathbf{V} \otimes \mathbf{V})$ term:

x-component, $\nabla \cdot (\rho u \mathbf{V})$

y-component, $\nabla \cdot (\rho v \mathbf{V})$

z-component, $\nabla \cdot (\rho w \mathbf{V})$

The $\nabla \cdot \boldsymbol{\tau}$ term:

x-component,

$$\nabla \cdot \boldsymbol{\tau}_x = \left[\frac{\partial}{\partial x} \left(\mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left(\mu \frac{\partial u}{\partial z} \right) \right] + \left[\frac{\partial}{\partial x} \left(\mu \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial z} \left(\mu \frac{\partial v}{\partial z} \right) \right] - \frac{2}{3} \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)$$

$$\nabla \cdot \boldsymbol{\tau}_x = \nabla \cdot (\mu \nabla u) + \left\{ \left[\frac{\partial}{\partial x} \left(\mu \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial z} \left(\mu \frac{\partial v}{\partial z} \right) \right] - \frac{2}{3} \mu \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right\}$$

$$\nabla \cdot \boldsymbol{\tau}_x = \nabla \cdot (\mu \nabla u) + S_{Mx}$$

where $S_{Mx} = \left[\frac{\partial}{\partial x} \left(\mu \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial z} \left(\mu \frac{\partial v}{\partial z} \right) \right] - \frac{2}{3} \mu \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)$

Assume constant viscosity μ

$$\nabla \cdot \boldsymbol{\tau}_x = \mu \nabla^2 u + \mu \left[\frac{\partial}{\partial x} \left(\frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial z} \left(\frac{\partial v}{\partial z} \right) - \frac{2}{3} \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right]$$

$$\nabla \cdot \boldsymbol{\tau}_x = \mu \nabla^2 u + \mu \left[\frac{\partial}{\partial x} \left(\frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial z} \left(\frac{\partial v}{\partial z} \right) - \frac{2}{3} \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right]$$

$$\nabla \cdot \boldsymbol{\tau}_x = \mu \nabla^2 u + \mu \left[\frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) - \frac{2}{3} \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right]$$

$$\nabla \cdot \boldsymbol{\tau}_x = \mu \nabla^2 u + \frac{\mu}{3} \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)$$

$$\nabla \cdot \boldsymbol{\tau}_x = \mu \nabla^2 u + \frac{\mu}{3} \frac{\partial}{\partial x} (\nabla \cdot \mathbf{V})$$

Therefore,

x-component, $\nabla \cdot \boldsymbol{\tau}_x = \nabla \cdot (\mu \nabla u) + S_{Mx}$, or constant μ , $\nabla \cdot \boldsymbol{\tau}_x = \mu \nabla^2 u + \frac{\mu}{3} \frac{\partial}{\partial x} (\nabla \cdot \mathbf{V})$

y-component, $\nabla \cdot \boldsymbol{\tau}_y = \nabla \cdot (\mu \nabla v) + S_{My}$, or constant μ , $\nabla \cdot \boldsymbol{\tau}_y = \mu \nabla^2 v + \frac{\mu}{3} \frac{\partial}{\partial y} (\nabla \cdot \mathbf{V})$

z-component, $\nabla \cdot \boldsymbol{\tau}_z = \nabla \cdot (\mu \nabla w) + S_{Mz}$, or constant μ , $\nabla \cdot \boldsymbol{\tau}_z = \mu \nabla^2 w + \frac{\mu}{3} \frac{\partial}{\partial z} (\nabla \cdot \mathbf{V})$

Momentum equation in scalar form:

x-component,

$$\begin{aligned}\frac{\partial(\rho u)}{\partial t} + \nabla \cdot (\rho u \mathbf{V}) &= \rho g_x - \frac{\partial p}{\partial x} + \nabla \cdot (\mu \nabla u) + S_{Mx} \\ \frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho uu)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial(\rho uw)}{\partial z} \\ &= \rho g_x - \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left(\mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left(\mu \frac{\partial u}{\partial z} \right) + S_{Mx}\end{aligned}$$

y-component,

$$\begin{aligned}\frac{\partial(\rho v)}{\partial t} + \nabla \cdot (\rho v \mathbf{V}) &= \rho g_y - \frac{\partial p}{\partial y} + \nabla \cdot (\mu \nabla v) + S_{My} \\ \frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho vu)}{\partial x} + \frac{\partial(\rho vv)}{\partial y} + \frac{\partial(\rho vw)}{\partial z} \\ &= \rho g_y - \frac{\partial p}{\partial y} + \frac{\partial}{\partial x} \left(\mu \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial z} \left(\mu \frac{\partial v}{\partial z} \right) + S_{My}\end{aligned}$$

z-component,

$$\begin{aligned}\frac{\partial(\rho w)}{\partial t} + \nabla \cdot (\rho w \mathbf{V}) &= \rho g_z - \frac{\partial p}{\partial z} + \nabla \cdot (\mu \nabla w) + S_{Mz} \\ \frac{\partial(\rho w)}{\partial t} + \frac{\partial(\rho wu)}{\partial x} + \frac{\partial(\rho wv)}{\partial y} + \frac{\partial(\rho ww)}{\partial z} \\ &= \rho g_z - \frac{\partial p}{\partial z} + \frac{\partial}{\partial x} \left(\mu \frac{\partial w}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu \frac{\partial w}{\partial y} \right) + \frac{\partial}{\partial z} \left(\mu \frac{\partial w}{\partial z} \right) + S_{Mz}\end{aligned}$$

Momentum equation in scalar form (constant viscosity μ):

x-component,

$$\begin{aligned}\frac{\partial(\rho u)}{\partial t} + \nabla \cdot (\rho u \mathbf{V}) &= \rho g_x - \frac{\partial p}{\partial x} + \mu \nabla^2 u + \frac{\mu}{3} \frac{\partial}{\partial x} (\nabla \cdot \mathbf{V}) \\ \frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u u)}{\partial x} + \frac{\partial(\rho u v)}{\partial y} + \frac{\partial(\rho u w)}{\partial z} \\ &= \rho g_x - \frac{\partial p}{\partial x} + \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + \frac{\mu}{3} \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)\end{aligned}$$

y-component,

$$\begin{aligned}\frac{\partial(\rho v)}{\partial t} + \nabla \cdot (\rho v \mathbf{V}) &= \rho g_y - \frac{\partial p}{\partial y} + \mu \nabla^2 v + \frac{\mu}{3} \frac{\partial}{\partial y} (\nabla \cdot \mathbf{V}) \\ \frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho v u)}{\partial x} + \frac{\partial(\rho v v)}{\partial y} + \frac{\partial(\rho v w)}{\partial z} \\ &= \rho g_y - \frac{\partial p}{\partial y} + \mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) + \frac{\mu}{3} \frac{\partial}{\partial y} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)\end{aligned}$$

z-component,

$$\begin{aligned}\frac{\partial(\rho w)}{\partial t} + \nabla \cdot (\rho w \mathbf{V}) &= \rho g_z - \frac{\partial p}{\partial z} + \mu \nabla^2 w + \frac{\mu}{3} \frac{\partial}{\partial z} (\nabla \cdot \mathbf{V}) \\ \frac{\partial(\rho w)}{\partial t} + \frac{\partial(\rho w u)}{\partial x} + \frac{\partial(\rho w v)}{\partial y} + \frac{\partial(\rho w w)}{\partial z} \\ &= \rho g_z - \frac{\partial p}{\partial z} + \mu \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) + \frac{\mu}{3} \frac{\partial}{\partial z} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)\end{aligned}$$

Species equation:

$$\frac{\partial(\rho Y_k)}{\partial t} + \nabla \cdot (\rho \mathbf{V} Y_k) = -\nabla \cdot (\rho Y_k \mathbf{V}_k) + \dot{\omega}_k$$

In scalar form,

$$\begin{aligned} \frac{\partial(\rho Y_k)}{\partial t} + \left[\frac{\partial(\rho u Y_k)}{\partial x} + \frac{\partial(\rho v Y_k)}{\partial y} + \frac{\partial(\rho w Y_k)}{\partial z} \right] \\ = - \left[\frac{\partial(\rho Y_k V_{k,x})}{\partial x} + \frac{\partial(\rho Y_k V_{k,y})}{\partial y} + \frac{\partial(\rho Y_k V_{k,z})}{\partial z} \right] + \dot{\omega}_k \end{aligned}$$

Energy equation:

$$\rho c_p \frac{DT}{Dt} = - \sum_{k=1}^{KK} \dot{\omega}_k h_k - \nabla \cdot \mathbf{q} + \frac{Dp}{Dt} + \boldsymbol{\tau} : \nabla \mathbf{V} + \text{body force work}$$

$$\mathbf{q} = -\lambda \nabla T + \sum_{k=1}^{KK} (h_k Y_k \mathbf{V}_k) + \text{Dufour effects} + \text{radiation}$$

By neglecting Dufour effects, radiation and body force work,

$$\rho c_p \frac{DT}{Dt} = - \sum_{k=1}^{KK} \dot{\omega}_k h_k + \nabla \cdot (\lambda \nabla T) - \rho \sum_{k=1}^{KK} (c_{p,k} Y_k \mathbf{V}_k) \cdot \nabla T + \frac{Dp}{Dt} + \boldsymbol{\tau} : \nabla \mathbf{V}$$

Further neglect viscous dissipation $\boldsymbol{\tau} : \nabla \mathbf{V}$ and $\frac{Dp}{Dt}$

$$c_p \left[\frac{\partial(\rho T)}{\partial t} + \nabla \cdot (\rho \mathbf{V} T) \right] = - \sum_{k=1}^{KK} \dot{\omega}_k h_k + \nabla \cdot (\lambda \nabla T) - \rho \sum_{k=1}^{KK} (c_{p,k} Y_k \mathbf{V}_k) \cdot \nabla T$$

In scalar form,

$$\begin{aligned} c_p \left[\frac{\partial(\rho T)}{\partial t} + \frac{\partial(\rho u T)}{\partial x} + \frac{\partial(\rho v T)}{\partial y} + \frac{\partial(\rho w T)}{\partial z} \right] \\ = - \sum_{k=1}^{KK} \dot{\omega}_k h_k + \left[\frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(\lambda \frac{\partial T}{\partial z} \right) \right] \\ - \left\{ \rho \sum_{k=1}^{KK} (c_{p,k} Y_k V_{k,x}) \frac{\partial T}{\partial x} + \rho \sum_{k=1}^{KK} (c_{p,k} Y_k V_{k,y}) \frac{\partial T}{\partial y} + \rho \sum_{k=1}^{KK} (c_{p,k} Y_k V_{k,z}) \frac{\partial T}{\partial z} \right\} \end{aligned}$$

If assuming all the species have the same specific heat capacity $c_{p,k}$, then the mass diffusion term is zero.

Some details for diffusion velocity V_k :

V_k is the diffusion velocity of species k in the x - y - z -direction, by neglecting Soret effect, body-force, pressure gradient induced barodiffusion,

$$V_k = V'_k + V_c = -\frac{D_k}{X_k} \nabla X_k + V_c$$

$$V_c = \frac{1}{W} \sum_{k=1}^{KK} D_k W_k \nabla X_k \text{ or } V_c = -\sum_{k=1}^{KK} Y_k V'_k$$

If the last species is solved by $Y_{KK} = 1 - \sum_{k=1}^{KK-1} Y_k$, since $\sum Y_k V_k = 0$. The correction velocity V_c is not used, i.e. $V_k = V'_k$. The last species absorbs all the inconsistencies, typically N_2 .

For mixture-averaged model, with Curtiss-Hirschfelder approximation,

$$D_k = D_k^{mix} = \frac{1 - Y_k}{\sum_{j \neq k}^{KK} X_j / D_{kj}}$$

where D_{kj} is the binary diffusion coefficient between species k and j .

In mass fraction form,

$$X_k = Y_k W / W_k, W = \sum X_k W_k = \left(\sum \frac{Y_j}{W_j} \right)^{-1}, \nabla W = \sum_{j=1}^{KK} W_j \nabla X_j = -W^2 \sum_{j=1}^{KK} \frac{\nabla Y_j}{W_j}$$

Then, we transform V_k to the mass fraction form,

$$\begin{aligned} \nabla X_k &= \frac{W}{W_k} \nabla Y_k + \frac{Y_k}{W_k} \nabla W = \left(\nabla Y_k + \frac{Y_k}{W} \nabla W \right) \frac{W}{W_k} = \left(\nabla Y_k + \frac{Y_k}{W} \nabla W \right) \frac{X_k}{Y_k} \\ -\frac{D_{km}}{X_k} \nabla X_k &= -\frac{D_k}{Y_k} \left(\nabla Y_k + \frac{Y_k}{W} \nabla W \right) = -\frac{D_k}{Y_k} \nabla Y_k - \frac{D_k}{W} \nabla W \\ V_k &= -\frac{D_k}{X_k} \nabla X_k + V_c = \left(-\frac{D_k}{Y_k} \nabla Y_k - \frac{D_k}{W} \nabla W \right) + \frac{1}{W} \sum_{j=1}^{KK} D_k W_k \nabla X_k \\ &= \left(-\frac{D_k}{Y_k} \nabla Y_k - \frac{D_k}{W} \nabla W \right) + \frac{1}{W} \sum_{j=1}^{KK} D_k W_k \left(\nabla Y_k + \frac{Y_k}{W} \nabla W \right) \frac{W}{W_k} \\ &= \left(-\frac{D_k}{Y_k} \nabla Y_k - \frac{D_k}{W} \nabla W \right) + \left(\sum_{j=1}^{KK} D_k \nabla Y_k + \frac{\nabla W}{W} \sum_{j=1}^{KK} D_k Y_k \right) \\ &= \left(-\frac{D_k}{Y_k} \nabla Y_k \right) + \left(-\frac{D_k}{W} \nabla W + \sum_{j=1}^{KK} D_k \nabla Y_k + \frac{\nabla W}{W} \sum_{j=1}^{KK} D_k Y_k \right) = \left(-\frac{D_k}{Y_k} \nabla Y_k \right) + V_c' \end{aligned}$$

Then $Y_k V_k = -D_k \nabla Y_k + Y_k V_c'$ in the mass fraction form.

Some details in stress tensor τ :

For Newtonian fluid,

$$\boldsymbol{\tau} = 2\mu\boldsymbol{\sigma} + \lambda(\nabla \cdot \mathbf{V})\mathbf{I} = \mu \left\{ [\nabla\mathbf{V} + (\nabla\mathbf{V})^T] - \frac{2}{3}(\nabla \cdot \mathbf{V})\mathbf{I} \right\} + \lambda(\nabla \cdot \mathbf{V})\mathbf{I}$$

$$\boldsymbol{\sigma} = \frac{1}{2} [\nabla\mathbf{V} + (\nabla\mathbf{V})^T] - \frac{1}{3}(\nabla \cdot \mathbf{V})\mathbf{I}$$

μ is dynamic viscosity.

λ is secondary viscosity/bulk viscosity/dilatational viscosity.

The first term $2\mu\boldsymbol{\sigma}$ is **deviatoric** stress, related to flow deformation, and $\boldsymbol{\sigma}$ is strain rate.

The second term $\lambda(\nabla \cdot \mathbf{V})\mathbf{I}$ is **isotropic** stress, related to flow expansion/dilatational.

Note that rotation does not induce viscous force.

The stress can also be written as

$$\boldsymbol{\tau} = \mu[\nabla\mathbf{V} + (\nabla\mathbf{V})^T] + \left(\lambda - \frac{2}{3}\mu \right) (\nabla \cdot \mathbf{V})\mathbf{I}$$

The bulk viscosity, $\lambda(\nabla \cdot \mathbf{V})\mathbf{I}$, is often neglected, i.e. λ is set to be 0.

In incompressible ($\nabla \cdot \mathbf{V} = \mathbf{0}$), neglecting the bulk viscosity

$$\boldsymbol{\tau} = 2\mu\boldsymbol{\sigma} = 2\mu \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{1}{2} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & \frac{1}{2} \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \\ \frac{1}{2} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & \frac{\partial v}{\partial y} & \frac{1}{2} \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \\ \frac{1}{2} \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) & \frac{1}{2} \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) & \frac{\partial w}{\partial z} \end{bmatrix}$$

In incompressible ($\nabla \cdot \mathbf{V} = \mathbf{0}$) AND irrotational flow ($\boldsymbol{\omega} = \frac{1}{2}\boldsymbol{\Omega} = \mathbf{0}$, $\boldsymbol{\Omega}$ is vorticity), the bulk viscosity can be neglected, resulting in

$$\boldsymbol{\tau} = 2\mu\nabla\mathbf{V} = 2\mu \begin{bmatrix} \frac{\partial u}{\partial x} & 0 & 0 \\ 0 & \frac{\partial v}{\partial y} & 0 \\ 0 & 0 & \frac{\partial w}{\partial z} \end{bmatrix}$$