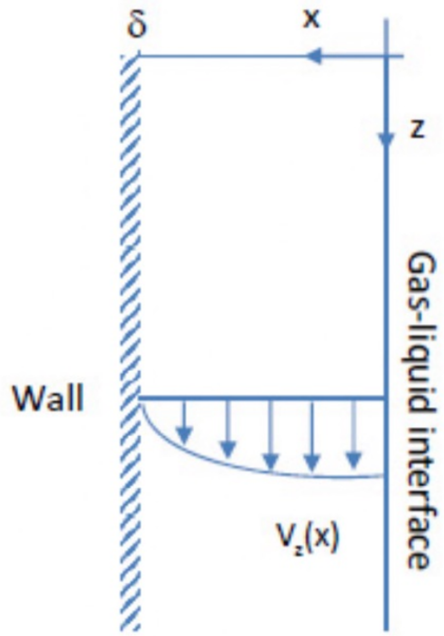
## Exercise 1

The steady-state velocity profile in a falling film (Figure 1) can be expressed as:

$$v_z(x) = \frac{\rho g \delta^2}{2\mu}\left[1 - \left(\frac{x}{\delta}\right)^2\right]$$

where $\delta$ is the is the film thickness, $x$ is the is the coordinate normal to the wall, $g$ is the gravitational acceleration, $\rho$ denotes the fluid density and $\mu$ represents the fluid dynamic viscosity.

Starting out from the general equation of motion and the continuity equation in Cartesian coordinates, which can be simplified for incompressible fluids having constant $\rho$ and $\mu$, show how to derive the given relation for the velocity profile. Assume constant pressure and an infinite system in the $y$ dimension.




Assumptions:

1. $\rho$ and $\mu$ is constant: Any $\partial$ og $d$ operator applied to $\rho$ or $\mu$ becomes zero
2. Constant pressure: $\partial P$ and $dP$ is zero
3. Infinite system in y-direction: $\frac{\partial}{\partial y} = 0$
4. We want the steady state equations: $\frac{\partial}{\partial t} = 0$
5. Assuming infinite y-direction, laminar flow, and no forces in y-direction: $V_y = 0$
6. Constant film thickness: Can't have movement in the x-direction $\Rightarrow V_x = 0$
7. Assuming equilibrium between liquid and gas: Forces are equal in x-direction $\sigma_x(l) = \sigma_x(g)$

$$\sigma_x = (\underbrace{\cancel{\sigma_{xx}}}_{V_x = 0\ (\nabla \cdot V = 0,\ \text{shown later})}, \overbrace{\cancel{\sigma_{xy}}}^{\text{Infinity y-direction}}, \sigma_{xz})$$

$$\Rightarrow \sigma_{xz}(l) = \sigma_{xz}(g) \quad \text{at } x = 0$$

8. Assuming only gravity in the z-direction: $g_x = 0,\ g_y = 0$ (gravity vector parallel to z-direction)

### Continuity equation in cartesian coordinates

$$\overbrace{\cancel{\frac{\partial \rho}{\partial t}}}^{\text{Assumption 4}} + \frac{\partial}{\partial x}(\rho v_x) + \frac{\partial}{\partial y}(\rho v_y) + \frac{\partial}{\partial z}(\rho v_z) = 0$$

Using $\rho$ = constant

$$\rho\left(\frac{\partial V_x}{\partial x} + \frac{\partial V_y}{\partial y} + \frac{\partial V_z}{\partial z}\right) = 0 \qquad \rho \neq 0$$

$$\frac{\partial V_x}{\partial x} + \frac{\partial V_y}{\partial y} + \frac{\partial V_z}{\partial z} = 0$$

$\Rightarrow$ $\boxed{\nabla \cdot V = 0}$, and using assumption 5 and 6, $V_x = V_y = 0 \Rightarrow \boxed{\frac{\partial V_z}{\partial z} = 0}$

### Equation of motion in cartesian coordinates

x-component:

$$\overbrace{\cancel{\frac{\partial}{\partial t}(\rho v_x)}}^{4} + \overbrace{\cancel{\frac{\partial}{\partial x}(\rho v_x v_x)}}^{6} + \overbrace{\cancel{\frac{\partial}{\partial y}(\rho v_y v_x)}}^{5} + \overbrace{\cancel{\frac{\partial}{\partial z}(\rho v_z v_x)}}^{6}$$

$$= -\overbrace{\cancel{\frac{\partial p}{\partial x}}}^{2} - \frac{\partial \sigma_{xx}}{\partial x} - \frac{\partial \sigma_{yx}}{\partial y} - \frac{\partial \sigma_{zx}}{\partial z} + \overbrace{\cancel{\rho g_x}}^{8}$$

$\underline{LHS = 0}$

$$RHS = -\frac{\partial \sigma_{xx}}{\partial x} - \frac{\partial \sigma_{yx}}{\partial y} - \frac{\partial \sigma_{zx}}{\partial z}$$

$$\sigma_{xx} = -\mu\left[2\cancelto{6}{\frac{\partial v_x}{\partial x}} - \frac{2}{3}\underbrace{(\nabla \cdot \mathbf{v})}_{=0 \text{ from continuity eq}}\right] \Rightarrow \frac{\partial \sigma_{xx}}{\partial x} = \frac{\partial}{\partial x}(-\mu \cdot 0) = 0$$

$$\sigma_{yx} = -\mu\left[\cancelto{6}{\frac{\partial v_x}{\partial y}} + \cancelto{5}{\frac{\partial v_y}{\partial x}}\right] = 0 \Rightarrow \frac{\partial \sigma_{yx}}{\partial y} = 0$$

Result from continuity equation

$$\sigma_{zx} = \sigma_{xz} = -\mu\left[\frac{\partial v_z}{\partial x} + \cancelto{6}{\frac{\partial v_x}{\partial z}}\right] = -\mu\frac{\partial v_z}{\partial x} \Rightarrow \frac{\partial \sigma_{zx}}{\partial z} = \frac{\partial}{\partial z}\left(-\mu\frac{\partial v_z}{\partial x}\right) \overset{1.}{=} -\mu\frac{\partial}{\partial z}\left(\frac{\partial v_z}{\partial x}\right) = -\mu\frac{\partial}{\partial x}\left(\cancel{\frac{\partial v_z}{\partial z}}\right) = 0 \Rightarrow \frac{\partial \sigma_{zx}}{\partial z} = 0$$

$V_z$ is continous
$\partial$ is distributive

$\Rightarrow$ LHS = RHS = 0 ok!

y-component:

$$\cancelto{4}{\frac{\partial}{\partial t}(\rho v_y)} + \cancelto{5}{\frac{\partial}{\partial x}(\rho v_x v_y)} + \cancelto{5}{\frac{\partial}{\partial y}(\rho v_y v_y)} + \cancelto{5}{\frac{\partial}{\partial z}(\rho v_z v_y)}$$
$$= -\cancelto{2}{\frac{\partial p}{\partial y}} - \frac{\partial \sigma_{xy}}{\partial x} - \frac{\partial \sigma_{yy}}{\partial y} - \frac{\partial \sigma_{zy}}{\partial z} + \cancelto{8}{\rho g_y}$$

$\Rightarrow \underline{LHS = 0}$

$$RHS = -\frac{\partial \sigma_{xy}}{\partial x} - \frac{\partial \sigma_{yy}}{\partial y} - \frac{\partial \sigma_{zy}}{\partial z}$$

$$\sigma_{xy} = \sigma_{yx} = -\mu\left[\cancelto{3}{\frac{\partial v_x}{\partial y}} + \cancelto{5}{\frac{\partial v_y}{\partial x}}\right] = 0 \Rightarrow \frac{\partial \sigma_{xy}}{\partial x} = 0$$

$$\sigma_{yy} = -\mu\left[2\cancelto{3 \text{ or } 5}{\frac{\partial v_y}{\partial y}} - \frac{2}{3}\underbrace{(\nabla \cdot \mathbf{v})}_{=0 \text{ from continuity equation}}\right] = 0 \Rightarrow \frac{\partial \sigma_{yy}}{\partial y} = 0$$

$$\sigma_{yz} = \sigma_{zy} = -\mu\left[\cancelto{5}{\frac{\partial v_y}{\partial z}} + \cancelto{3}{\frac{\partial v_z}{\partial y}}\right] = 0 \Rightarrow \frac{\partial \sigma_{zy}}{\partial y} = 0$$

$\Rightarrow \underline{RHS = 0}$

$\Rightarrow$ LHS = RHS = 0 ok!

z-component:

$$\cancel{\frac{\partial}{\partial t}(\rho v_z)}^{4} + \cancel{\frac{\partial}{\partial x}(\rho v_x v_z)}^{6} + \cancel{\frac{\partial}{\partial y}(\rho v_y v_z)}^{5} + \frac{\partial}{\partial z}(\rho v_z v_z)$$
$$= -\cancel{\frac{\partial p}{\partial z}}^{2} - \frac{\partial \sigma_{xz}}{\partial x} - \frac{\partial \sigma_{yz}}{\partial y} - \frac{\partial \sigma_{zz}}{\partial z} + \rho g_z$$

$$LHS = \frac{\partial}{\partial z}(\rho V_z V_z) \underset{\text{Assumption 1}}{=} \rho \frac{\partial}{\partial z}(V_z V_z) = 2\rho V_z \frac{\partial V_z}{\partial z} = 0$$

$\frac{\partial V_z}{\partial z} = 0$ from continuity equation

$$\underline{LHS = 0}$$

$$RHS = -\frac{\partial \sigma_{xz}}{\partial x} - \frac{\partial \sigma_{yz}}{\partial y} - \frac{\partial \sigma_{zz}}{\partial z} + \rho g_z$$

$$\sigma_{zx} = \sigma_{xz} = -\mu \left[\frac{\partial v_z}{\partial x} + \cancel{\frac{\partial v_x}{\partial z}}^{6}\right] = -\mu \frac{\partial V_z}{\partial x} \Rightarrow -\frac{\partial \sigma_{xz}}{\partial x} = -\frac{\partial}{\partial x}\left(-\mu \frac{\partial V_z}{\partial x}\right) \underset{\text{Assumption 1}}{=} \mu \frac{\partial^2 V_z}{\partial x^2} \Rightarrow \boxed{-\frac{\partial \sigma_{xz}}{\partial x} = \mu \frac{\partial^2 V_z}{\partial x^2}}$$

$$\sigma_{yz} = \sigma_{zy} = -\mu \left[\cancel{\frac{\partial v_y}{\partial z}}^{5} + \cancel{\frac{\partial v_z}{\partial y}}^{3}\right] = 0 \Rightarrow \boxed{\frac{\partial \sigma_{yz}}{\partial y} = 0}$$

$\frac{\partial V_z}{\partial z} = 0$ from continuity eq

$$\sigma_{zz} = -\mu \left[2\cancel{\frac{\partial v_z}{\partial z}} - \underbrace{\frac{2}{3}(\nabla \cdot \mathbf{v})}_{=0 \text{ from the continuity eq}}\right] = 0 \Rightarrow \boxed{\frac{\partial \sigma_{zz}}{\partial z} = 0}$$

$$\Rightarrow RHS = \mu \frac{\partial^2 V_z}{\partial x^2} + \rho g_z$$

$$RHS = LHS \Rightarrow \mu \frac{\partial^2 V_z}{\partial x^2} + \rho g_z = 0$$

$$\frac{\partial^2 V_z}{\partial x^2} = -\frac{\rho g_z}{\mu} \qquad / \text{"Integrating"}$$

$$\int \frac{\cancel{\partial}}{\partial x}\left(\frac{\partial V_z}{\partial x}\right) \cancel{dx} = -\int \frac{\rho g_z}{\mu} dx$$

$$\frac{\partial V_z}{\partial x} = -\frac{\rho g_z}{\mu} x + C_1 \qquad / \text{"Integrating"}$$

$$\int \frac{\cancel{\partial}}{\cancel{\partial x}} V_z \cancel{dx} = \int \left(-\frac{\rho g_z}{\mu} x + C_1\right) dx$$

$$\underline{V_z(x) = -\frac{\rho g_z}{2\mu} x^2 + C_1 x + C_2}$$

Must determine $C_1$ and $C_2$ => Need suitable boundary conditions

- No slip condition at the wall => $V_z(x=\delta)=0$
- Assumption 7: Assuming equilibrium between liquid and gas => $\sigma_{xz}(l)=\sigma_{xz}(g)$ at $x=0$ (shown on first page)

$$\sigma_{xz}(l)=\sigma_{xz}(g) \Rightarrow -\mu_{liq}\left(\frac{\partial V_z}{\partial x}+\frac{\partial V_x}{\partial z}\right)_{liq} = -\mu_{gas}\left(\frac{\partial V_z}{\partial x}+\frac{\partial V_x}{\partial z}\right)_{gas} \quad / \cdot \frac{1}{\mu_{liq}}$$

$$\left(\frac{\partial V_z}{\partial x}+\frac{\partial V_x}{\partial z}\right)_{liq} = \frac{\mu_{gas}}{\mu_{liq}}\left(\frac{\partial V_z}{\partial x}+\frac{\partial V_x}{\partial z}\right)_{gas}$$

Assuming $\mu_{gas} \ll \mu_{liq} \Rightarrow \frac{\mu_{gas}}{\mu_{liq}} \approx 0$
This holds true in most cases

$$\Rightarrow \left(\frac{\partial V_z}{\partial x}+\cancelto{6}{\frac{\partial V_x}{\partial z}}\right)_{liq} = 0$$

$$\Rightarrow \boxed{\frac{\partial V_z}{\partial x}=0 \text{ at } x=0}$$

Applying $\frac{\partial V_z}{\partial x}=0$ at $x=0$ to $\frac{\partial V_z}{\partial x}$:

$$\frac{\partial V_z}{\partial x}(x=0) = -\frac{\rho g_z}{\mu}\cdot 0 + C_1 = C_1 = 0$$

$$\Rightarrow \boxed{C_1=0}$$

We then have $V_z(x) = -\frac{\rho g_z}{2\mu}x^2 + C_2$, applying $V_z(x=\delta)=0$:

$$V_z(x=\delta) = -\frac{\rho g_z}{2\mu}\delta^2 + C_2 = 0$$

$$\Rightarrow \boxed{C_2 = \frac{\rho g_z}{2\mu}\delta^2}$$

$V_z(x)$ becomes:

$$V_z(x) = -\frac{\rho g_z}{2\mu}x^2 + \frac{\rho g_z}{2\mu}\delta^2 = \frac{\rho g_z}{2\mu}\left(\delta^2 - x^2\right)\cdot\frac{\delta^2}{\delta^2} = \frac{\rho g_z}{2\mu}\left(1-\left(\frac{x}{\delta}\right)^2\right)$$

Finally

$V_z(x) = \frac{\rho g_z}{2\mu}\left(1-\left(\frac{x}{\delta}\right)^2\right)$, which is what we wanted to show

**Exercise 2: Conservation of Total Energy**

a) Formulate the first law of thermodynamics in the Langrangian frame of reference.

The first law of thermodynamics: $\frac{DE_{total}}{Dt} = \dot{Q}_{heat} + \dot{W}_{work}$

Where $E_{total} = \int_{V(t)} \rho\left(e + \frac{1}{2}v^2 + \phi\right) dV$ ← V or v? What is the correct notation here?

And $e$ is the internal energy
$\frac{1}{2}v^2$ is the kinetic energy
$\phi$ is the potential energy
} Per unit mass

$\dot{Q}_{heat} = -\int_{A(t)} \mathbf{q} \cdot \mathbf{n} \, da$, where $\mathbf{q}$ is the heat flux across the surface of the control volume

$$\dot{W}_{work} = -\int_{A(t)} \Big[\underbrace{(T \cdot v) \cdot n}_{\text{Mechanical work}} + \underbrace{\sum_{c=1}^{N} (\rho_c v_c \phi_c) \cdot n}_{\text{Potential work}}\Big] da,$$

Inserted into the 1st law of thermodynamics, we get the lagrangian frame formulation

$$\frac{D}{Dt} \int_{V(t)} \rho\left(e + \frac{1}{2}v^2 + \phi\right) dV = -\int_{A(t)} \mathbf{q} \cdot \mathbf{n} \, da - \int_{A(t)} \left[(T \cdot v) \cdot n + \sum_{c=1}^{N} (\rho_c v_c \phi_c) \cdot n\right] da$$

b) The corresponding formulation of the first law of thermodynamics in the Eulerian frame of reference becomes:

This term must be a scalar in order to have equal tensor order in the sum

$$\frac{\partial}{\partial t}\left[\rho\left(e + \frac{1}{2}\mathrm{v}^2 + \mathbf{\Phi}\right)\right] = -\nabla \cdot \left[\rho\left(e + \frac{1}{2}\mathrm{v}^2 + \mathbf{\Phi}\right)\mathbf{v}\right] - \nabla \cdot \mathbf{q} - \nabla \cdot (p\mathbf{v})$$
$$- \nabla \cdot (\overline{\boldsymbol{\sigma}} \cdot \mathbf{v}) - \nabla \cdot \left(\sum_{c=1}^{N} \rho_c \mathbf{v}_{c,d} \mathbf{\Phi}_c\right) \quad (1)$$

Identify the different energy, heat and work terms in the equation above.

$\frac{\partial}{\partial t}\left[\rho\left(e + \frac{1}{2}v^2 + \phi\right)\right]$ is the change in total energy with respect to time

$-\nabla \cdot \left[\rho\left(e + \frac{1}{2}v^2 + \phi\right)v\right]$ is the convection term, the energy input due to convection

$-\nabla \cdot \mathbf{q}$ is heat change due to conduction

$-\nabla \cdot (pv)$ is the mechanical work done by pressure/volume changes

$-\nabla \cdot (\overline{\sigma} \cdot v)$ is the mechanical work done by viscous forces (stress)

$-\nabla \cdot \left(\sum_{c=1}^{N} \rho_c v_{c,d} \phi_c\right)$ is the potential work done by external energy fields (and diffusion inside said fields)

c) Balances for the various energy forms can be derived. The *potential energy equation* is:

$$\frac{\partial(\rho\Phi)}{\partial t} + \nabla\cdot(\rho\mathbf{v}\Phi) + \nabla\cdot\left(\sum_{c=1}^{N}\rho_c\mathbf{v}_{c,d}\Phi_c\right) = -\sum_{c=1}^{N}\rho_c(\mathbf{v_c}\cdot\mathbf{g_c}) \qquad (2)$$

Use the *potential energy equation* to show that the *total energy equation* can be transformed to the *equation of internal- and kinetic energy*:

$$\begin{aligned}\frac{\partial}{\partial t}\left[\rho\left(e+\frac{1}{2}v^2\right)\right] &= -\nabla\cdot\left[\rho\left(e+\frac{1}{2}v^2\right)\mathbf{v}\right]-\nabla\cdot\mathbf{q}\\ &- \nabla\cdot(p\mathbf{v})-\nabla\cdot(\overline{\sigma}\cdot\mathbf{v})+\sum_{c=1}^{N}\rho_c(\mathbf{v_c}\cdot\mathbf{g_c}) \qquad (3)\end{aligned}$$

As the total energy consists of internal, kinetic and potential energy, the internal and kinetic energy can be expressed as $E_i + E_k = E_{tot} - E_p$

Goal: • Factor out the terms of the potential energy balance from the total energy balance

• Subtract the potential energy balance from the total energy balance to get the answer.

Starting from the total energy balance in the eulerian frame:

$$\frac{\partial}{\partial t}\left[\rho\left(e+\tfrac{1}{2}v^2+\phi\right)\right] = -\nabla\cdot\left[\rho\left(e+\tfrac{1}{2}v^2+\phi\right)V\right]-\nabla\cdot q-\nabla\cdot(pV)-\nabla\cdot(\overline{\sigma}\cdot V)-\nabla\cdot\left(\sum_{c=1}^{N}\rho_c V_{c,d}\phi_c\right)$$

Using that $\nabla\cdot$, the partial derivative $\frac{\partial}{\partial t}$, and the dyadic vector product are distributive, we can write:

One of the terms in the potential energy balance

$$\frac{\partial}{\partial t}\left[\rho\left(e+\tfrac{1}{2}v^2+\phi\right)\right] = \frac{\partial}{\partial t}\left[\rho\left(e+\tfrac{1}{2}v^2\right)\right] + \frac{\partial(\rho\phi)}{\partial t}$$

$\phi$ is a scalar => The order doesn't matter

$$-\nabla\cdot\left[\rho\left(e+\tfrac{1}{2}v^2+\phi\right)V\right] = -\nabla\cdot\left[\rho\left(e+\tfrac{1}{2}v^2\right)V\right]-\nabla\cdot(\rho\phi V) = -\nabla\cdot\left[\rho\left(e+\tfrac{1}{2}v^2\right)V\right]-\nabla\cdot(\rho V\phi)$$

We now have the entire LHS of the potential energy balance

moving all terms of the potential energy balance to the left hand side, we get that the total energy balance becomes:

$$\frac{\partial}{\partial t}\left[\rho\left(e+\frac{1}{2}v^2\right)\right] + \frac{\partial(\rho\phi)}{\partial t} + \nabla\cdot(\rho v\phi) + \nabla\cdot\left(\sum_{c=1}^{N}\rho_c V_{c,d}\phi_c\right) =$$

$$-\nabla\cdot\left[\rho\left(e+\frac{1}{2}v^2\right)v\right] - \nabla\cdot q - \nabla\cdot(pv) - \nabla\cdot(\bar{\sigma}\cdot v)$$

Recognizing the terms in grey to be the LHS of the potential energy balance, we subtract the potential energy balance from the total energy balance.

Finally, we get:

$$\frac{\partial}{\partial t}\left[\rho\left(e+\frac{1}{2}v^2\right)\right] = -\nabla\cdot\left[\rho\left(e+\frac{1}{2}v^2\right)v\right] - \nabla\cdot q - \nabla\cdot(pv) - \nabla\cdot(\bar{\sigma}\cdot v) + \overbrace{\sum_{c=1}^{N}\rho_c(V_c\cdot g_c)}^{=-\text{RHS of potential energy balance}}$$

d) The *kinetic energy equation* is derived by taking the scalar product of the velocity with the momentum equation. The equation becomes:

$$\begin{aligned} \frac{\partial}{\partial t}\left(\rho\frac{1}{2}\mathbf{v}^2\right) &= -\nabla\cdot\left(\rho\frac{1}{2}\mathbf{v}^2\mathbf{v}\right) - \nabla\cdot(p\mathbf{v}) + p(\nabla\cdot\mathbf{v}) \\ &- \nabla\cdot(\bar{\boldsymbol{\sigma}}\cdot\mathbf{v}) + (\bar{\boldsymbol{\sigma}}:\nabla\mathbf{v}) + \mathbf{v}\cdot\sum_{c=1}^{N}(\rho_c\mathbf{g_c}) \end{aligned} \tag{4}$$

Use this equation to show that the *internal energy equation* can be written as:

$$\frac{\partial}{\partial t}(\rho e) = -\nabla\cdot(\rho\mathbf{v}e) - \nabla\cdot\mathbf{q} - p(\nabla\cdot\mathbf{v}) - (\bar{\boldsymbol{\sigma}}:\nabla\mathbf{v}) + \sum_{c=1}^{N}(\mathbf{J_c}\cdot\mathbf{g_c}) \tag{5}$$

where

$$\sum_{c=1}^{N}(\mathbf{J_c}\cdot\mathbf{g_c}) = \sum_{c=1}^{N}\rho_c(\mathbf{v_c}\cdot\mathbf{g_c}) - \mathbf{v}\cdot\sum_{c=1}^{N}\rho_c\mathbf{g_c} \tag{6}$$

Starting out with the internal and kinetic energy equation, and factoring the LHS and convection terms using the distributive properties as done in c):

Grey = Terms in eq (4); kinetic energy equation

$$\frac{\partial(\rho e)}{\partial t} + \frac{\partial}{\partial t}\left(\rho\frac{1}{2}v^2\right) = -\nabla\cdot(\rho v e) - \nabla\cdot\left(\rho\frac{1}{2}v^2 v\right) - \nabla\cdot q - \nabla\cdot(pv) - \nabla\cdot(\bar{\sigma}\cdot v) + \sum_{c=1}^{N}\rho_c(V_c\cdot g_c)$$

Subtracting the kinetic energy equation from the expression above gives:

$$\frac{\partial(\rho e)}{\partial t} = -\nabla\cdot(\rho v e) - \nabla\cdot q + \underline{\sum_{c=1}^{N}\rho_c(V_c\cdot g_c)} - p(\nabla\cdot v) - (\bar{\sigma}:\nabla v) \underline{- v\cdot\sum_{c=1}^{N}(\rho_c g_c)}$$

Where the grey part came from the kinetic energy equation.

Finally, recognizing that the underlined terms are the same as in eq. (6)

$$\Rightarrow \sum_{c=1}^{N}\rho_c(V_c\cdot g_c) - v\cdot\sum_{c=1}^{N}(\rho_c g_c) = \sum_{c=1}^{N}(J_c\cdot g_c)$$

We end up with:

$$\frac{\partial(\rho e)}{\partial t} = -\nabla\cdot(\rho V e) - \nabla\cdot q - p(\nabla\cdot V) - (\bar{\sigma} : \nabla V) + \sum_{c=1}^{N}(J_c \cdot g_c)$$ , which is the equation we wanted.

e) Derive the *enthalpy equation* by introducing the enthalpy quantity into the *internal energy equation*:

$$h = e + \frac{p}{\rho} \tag{7}$$

Rewriting (7): $e = h - \frac{p}{\rho}$

Inserting into the answer from d):

$$\frac{\partial}{\partial t}\left(\rho\left(h-\frac{p}{\rho}\right)\right) = -\nabla\cdot\left(\rho V\left(h-\frac{p}{\rho}\right)\right) - \nabla\cdot q - p(\nabla\cdot V) - (\bar{\sigma} : \nabla V) + \sum_{c=1}^{N}(J_c \cdot g_c)$$

Separating terms

$$\frac{\partial(\rho h)}{\partial t} - \frac{\partial p}{\partial t} = -\nabla\cdot(\rho V h) + \nabla\cdot(Vp) - \nabla\cdot q - p(\nabla\cdot V) - (\bar{\sigma} : \nabla V) + \sum_{c=1}^{N}(J_c \cdot g_c)$$

We now want to combine the pressure terms into $\frac{Dp}{Dt} = \frac{\partial p}{\partial t} + V\cdot\nabla p$

Vector identity: $\nabla\cdot(ab) = a\nabla\cdot b + b\cdot\nabla a$

$\Rightarrow \nabla\cdot(Vp) = V\cdot\nabla p + p(\nabla\cdot V)$

Rearranging a bit then gives

$$\frac{\partial(\rho h)}{\partial t} + \nabla\cdot(\rho V h) = -\nabla\cdot q + \underbrace{\frac{\partial p}{\partial t} + V\cdot\nabla p}_{=\frac{Dp}{Dt}} \underbrace{\left(+p(\nabla\cdot V) - p(\nabla\cdot V)\right)}_{=0} - (\bar{\sigma} : \nabla V) + \sum_{c=1}^{N}(J_c \cdot g_c)$$

$$\frac{\partial(\rho h)}{\partial t} + \nabla\cdot(\rho V h) = -\nabla\cdot q + \frac{Dp}{Dt} - (\bar{\sigma} : \nabla V) + \sum_{c=1}^{N}(J_c \cdot g_c)$$

Which is equivalent to the enthalpy equation (67) from governing equations.

f) The enthalpy, H, is a function of pressure, p, temperature, T, and mass fraction, $w_c$. Applying the chain rule of partial differantiation on the enthalpy variable, we get:

$$dH = \left(\frac{\partial H}{\partial T}\right)_{p,w} dT + \left(\frac{\partial H}{\partial p}\right)_{T,w} dp + \sum_{c=1}^{N} \left(\frac{\partial H}{\partial w_c}\right)_{p,T} dw_c \tag{8}$$

By applying appropriate Maxwell relations and the heat capacity definition, the equation above becomes:

$$dH = C_p dT + \left[\frac{1}{\rho} - T\left(\frac{\partial \rho^{-1}}{\partial T}\right)_{p,w}\right] dp + \sum_{c=1}^{N} \left(\frac{\partial H}{\partial w_c}\right)_{p,T} dw_c \tag{9}$$

Introducing the local instantaneous equilibrium hypothesis, assuming that h(t,**r**)=h(p(t,**r**),T(t,**r**),$w_c(t,\mathbf{r})$) and by use of the chain rule of calculus, the relation becomes:

$$\begin{aligned}\frac{Dh}{Dt} &= C_p\frac{DT}{Dt} + \left[\frac{1}{\rho} - T\left(\frac{\partial \rho^{-1}}{\partial T}\right)_{p,w}\right]\frac{Dp}{Dt} \\ &- \frac{1}{\rho}\left[\sum_{c=1}^{N} \bar{h}_c \nabla\cdot\frac{\boldsymbol{J_c}}{M_{w_c}} + \sum_{r=1}^{q} r_{r,c_{ref}}(-\Delta\bar{H}_{r,c_{ref}})\right]\end{aligned} \tag{10}$$

Show that this equation together with the equation derived in part e) gives:

$$\begin{aligned}\rho C_p\frac{DT}{Dt} &= -\nabla\cdot\boldsymbol{q} - \frac{T}{\rho}\left(\frac{\partial\rho}{\partial T}\right)_{p,w}\frac{Dp}{Dt} - (\boldsymbol{\sigma}:\nabla\mathbf{v}) + \sum_{c=1}^{N}(\mathbf{J_c}\cdot\mathbf{g_c}) \\ &+ \sum_{c=1}^{N}\bar{h}_c\nabla\cdot\frac{\boldsymbol{J_c}}{M_{w_c}} + \sum_{r=1}^{q} r_{r,c_{ref}}(-\Delta\bar{H}_{r,c_{ref}})\end{aligned} \tag{11}$$

Identify the different terms in the equation above.

Starting from the answer from e)

$$\frac{\partial(\rho h)}{\partial t} + \nabla\cdot(\rho V h) = -\nabla\cdot q + \frac{Dp}{Dt} - (\bar{\sigma}:\nabla V) + \sum_{c=1}^{N}(J_c\cdot g_c)$$

Factoring terms

$$\frac{\partial(\rho h)}{\partial t} = \rho\frac{\partial h}{\partial t} + h\frac{\partial \rho}{\partial t}$$

$$\nabla\cdot(\rho V h) = \rho V\cdot(\nabla h) + h\nabla\cdot(\rho V)$$

$$\Rightarrow LHS = \rho\frac{\partial h}{\partial t} + \rho V\cdot(\nabla h) + h\frac{\partial\rho}{\partial t} + h\nabla\cdot(\rho V) = \rho\frac{Dh}{Dt} + h\underbrace{\left(\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho V)\right)}_{=0 \text{ by the continuity equation}} = \rho\frac{Dh}{Dt}$$

We then have that:

$$\rho\frac{Dh}{Dt} = -\nabla\cdot q + \frac{Dp}{Dt} - (\bar{\sigma}:\nabla V) + \sum_{c=1}^{N}(J_c\cdot g_c)$$

Inserting equation (10) for $\frac{Dh}{Dt}$:

$$\rho C_p\frac{DT}{Dt} + \rho\left[\frac{1}{\rho} - T\left(\frac{\partial\rho^{-1}}{\partial T}\right)_{p,w}\right]\frac{Dp}{Dt} - \sum_{c=1}^{N}\bar{h}_c\nabla\cdot\frac{J_c}{M_{w_c}} - \sum_{r=1}^{q} r_{r,c_{ref}}(-\Delta\bar{H}_{r,c_{ref}}) =$$

$$-\nabla\cdot q + \frac{Dp}{Dt} - (\bar{\sigma}:\nabla V) + \sum_{c=1}^{N}(J_c\cdot g_c)$$

Moving all terms except $\rho C_p \frac{DT}{Dt}$ to the right, and multiplying out the terms in the square brackets

$$\rho C_p \frac{DT}{Dt} = -\nabla \cdot q + \underbrace{\left(\frac{Dp}{Dt} - \frac{Dp}{Dt}\right)}_{=0} + T\rho \left(\frac{\partial \rho^{-1}}{\partial T}\right)_{p,w} \frac{Dp}{Dt} - (\bar{\sigma} : \nabla v) + \sum_{c=1}^{N} (J_c \cdot g_c) + \sum_{c=1}^{N} \bar{h}_c \nabla \cdot \frac{J_c}{Mw_c} + \sum_{r=1}^{q} r_{r,cref} (-\Delta \bar{H}_{r,cref})$$

Using the chain rule, using that $\rho$ is a function of $T$:

$$\frac{\partial(\rho^{-1})}{\partial T} = \frac{\partial}{\partial \rho}\left(\frac{1}{\rho}\right) \cdot \frac{\partial \rho}{\partial T} = -\frac{1}{\rho^2} \frac{\partial \rho}{\partial T}$$

$$\Rightarrow \quad T\rho \left(\frac{\partial \rho^{-1}}{\partial T}\right)_{p,w} \frac{Dp}{Dt} = -\frac{T}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_{p,w} \frac{Dp}{Dt}$$

Finally:

$$\rho C_p \frac{DT}{Dt} = -\nabla \cdot q - \frac{T}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_{p,w} \frac{Dp}{Dt} - (\bar{\sigma} : \nabla v) + \sum_{c=1}^{N} (J_c \cdot g_c) + \sum_{c=1}^{N} \bar{h}_c \nabla \cdot \frac{J_c}{Mw_c} + \sum_{r=1}^{q} r_{r,cref} (-\Delta \bar{H}_{r,cref})$$

Which is the equation we wanted to get.

In this equation:

- $\rho C_p \frac{DT}{Dt}$ is the rate of gain of heat content per unit volume
- $\nabla \cdot q$ is the heat flow due to convection/conduction
- $\frac{T}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_{p,w} \frac{Dp}{Dt}$ is the rate of pressure work from surroundings on CV
- $(\bar{\sigma} : \nabla v)$ is the viscous dissipation term; the rate of irreversible conversion from kinetic to internal energy
- $\sum_{c=1}^{N} (J_c \cdot g_c)$ is the rate of work done by body forces on the CV
- $\sum_{c=1}^{N} \bar{h}_c \nabla \cdot \frac{J_c}{Mw_c}$ is an energy flux caused by inter-diffusion
- $\sum_{r=1}^{q} r_{r,cref} (-\Delta \bar{H}_{r,cref})$ is thermal energy release by homogeneous chemical reactions.

g) Several of the terms in the equation derived in part f) can be neglected in common reactor modeling. Remove the terms that are negligible and write the z component of the resulting dispersion model.

For chemical, exothermal reactions, it is reasonable to assume time dependency of the temperature field, heat convection, heat conduction and transfer of energy due to the chemical reaction.

This means that $\rho C_p \frac{DT}{Dt}$, $\nabla \cdot q$ and $\sum_{r=1}^{q} r_{r,C_{ref}}(-\Delta \bar{H}_{r,C_{ref}})$ are not negligible

Generally, except for in very specific systems, the heat transfer of convection/conduction and the heat from the reaction is a lot bigger than the pressure work, viscous dissipation, work of body forces and the energy from interdiffusion. Therefore, unless the system has specific properties, they are negligible.

This means that the "surviving" terms are:

$$\underline{\underline{\rho C_p \frac{DT}{Dt} = -\nabla \cdot q + \sum_{r=1}^{q} r_{r,C_{ref}}(-\Delta \bar{H}_{r,C_{ref}})}}$$