- In this module, we will deal with advanced modeling capabilities.
- Advanced modeling capabilities rely a lot in physical models, such as, turbulence, multiphase flows, porous media, combustion, radiation, heat transfer, phase change, acoustics, cavitation, and so on.
- Therefore, it is extremely important to get familiar with the theory behind the models.

> "Essentially, all models are wrong,
> but some are useful"
>
> G. E. P. Box

George Edward Pelham Box
18 October 1919 – 28 March 2013. Statistician, who worked in the areas of quality control, time-series analysis, design of experiments, and Bayesian inference. He has been called *"one of the great statistical minds of the 20th century"*.

What are compressible flows?

- In few words, compressible flows are flows where the density change.
- The changes in density can be due to velocity, pressure, or temperature variations.
- Compressible flows can happen at low speed (subsonic) or high speed (transonic, supersonic, hypersonic and so on).
- Buoyancy-driven flows are also considered compressible flows. After all, the buoyancy is due to temperature gradients.
- In compressible flows, the viscosity also change with temperature.
- In compressible flows, the thermodynamical variables are related via an equation of state (e.g., ideal gas law).
- In principle, all flows are compressible.
- Usually compressibility effects start to become significant when the Mach number is higher than 0.3.

A few compressible flows applications

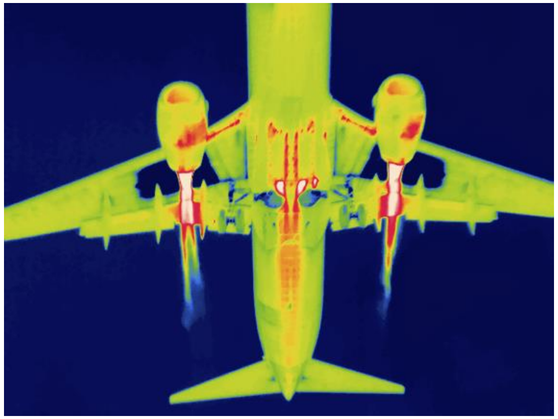
- The following applications fall within the compressible flows classification:
    - External and internal aerodynamics (high speed).
    - Heat transfer and conjugate heat transfer
    - Fire dynamics.
    - Buoyancy driven flows
    - Heating, ventilation, and air conditioning (HVAC).
    - Thermal comfort.
    - Turbomachinery.
    - Combustion.
    - Chemical reactions.
    - Condensation, evaporation, and melting.
    - And many more.
- As you can see, the range of applicability is very wide.

A crash introduction to compressible flows modeling OpenFOAM®

Large Natural Convection Plume, as effect of combustion of excess non-useable gases behind oilfield.
https://en.wikipedia.org/wiki/Plume_(fluid_dynamics)#/media/File:Naturalconvectionplume.JPG

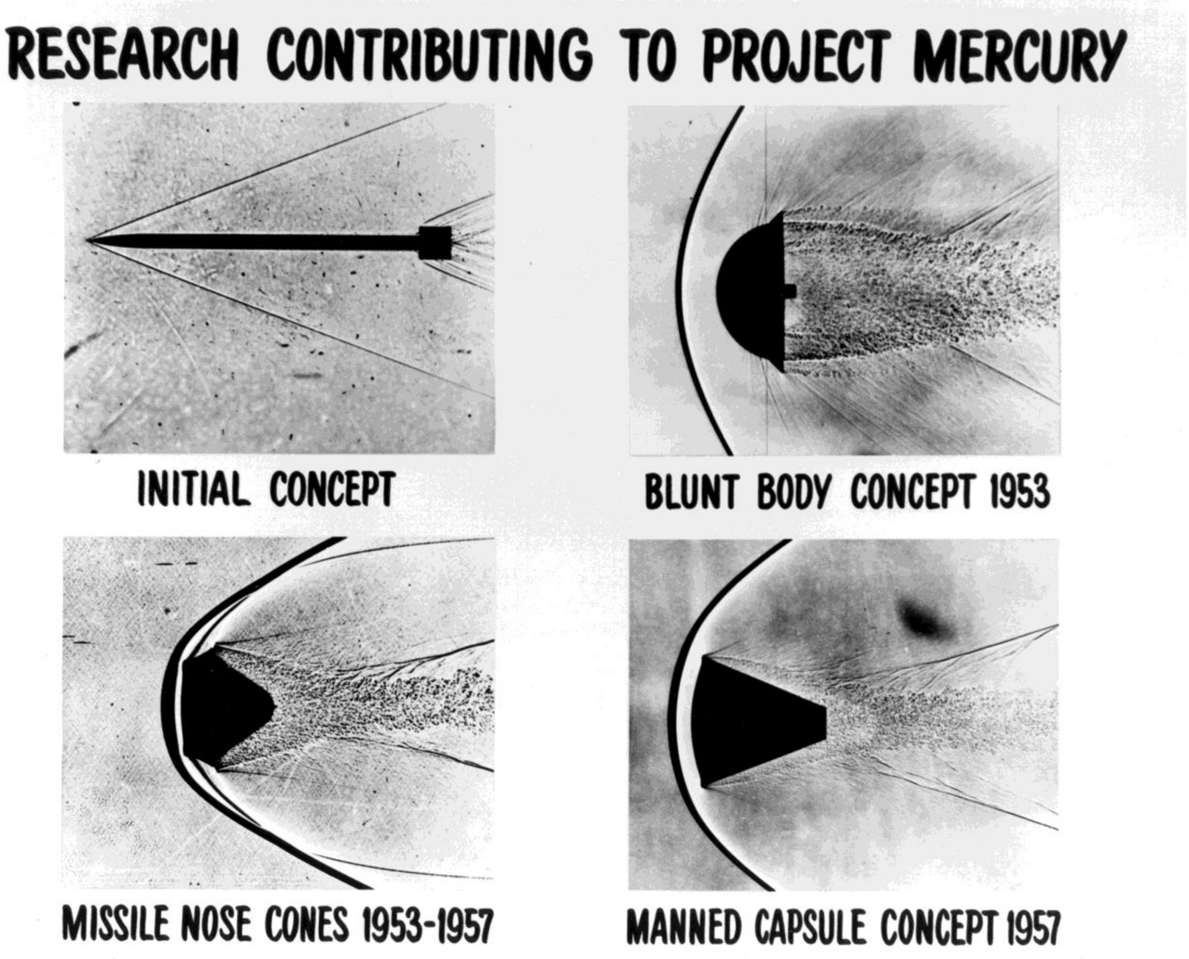
Rayleigh–Bénard convection cells
https://en.wikipedia.org/wiki/File:B%C3%A9nard_cells_convection.ogv

Iron melting
https://commons.wikimedia.org/wiki/File:Iron_-melting.JPG



Airplane thermal image
http://www.blackroc.com/wp-content/uploads/2016/03/thermal-image.jpg

A crash introduction to compressible flows modeling OpenFOAM®



Shadowgraph Images of Re-entry Vehicles
Photo credit: NASA on the Commons.
https://www.flickr.com/photos/nasacommons/

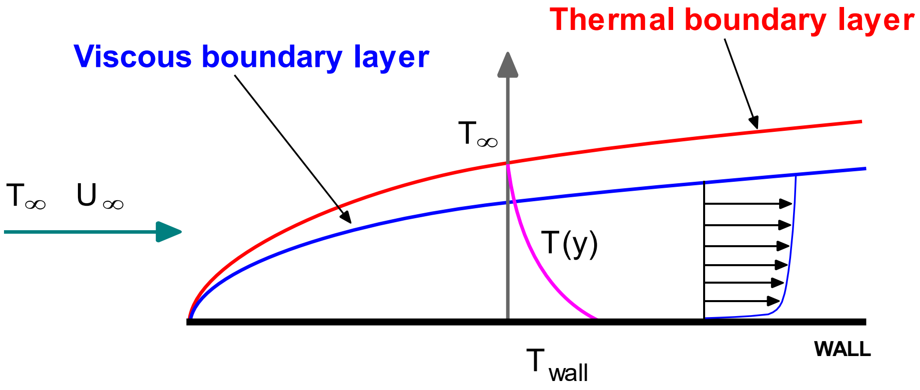
Compressible flows – Starting equations

$$
\textbf{NSE} \quad \left\{
\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0, \\
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla p + \nabla \cdot \tau, \\
\frac{\partial (\rho e_t)}{\partial t} + \nabla \cdot (\rho e_t \mathbf{u}) &= \nabla \cdot q - \nabla \cdot (p \mathbf{u}) + \tau \mathbf{:} \nabla \mathbf{u},
\end{aligned}
\right.
$$

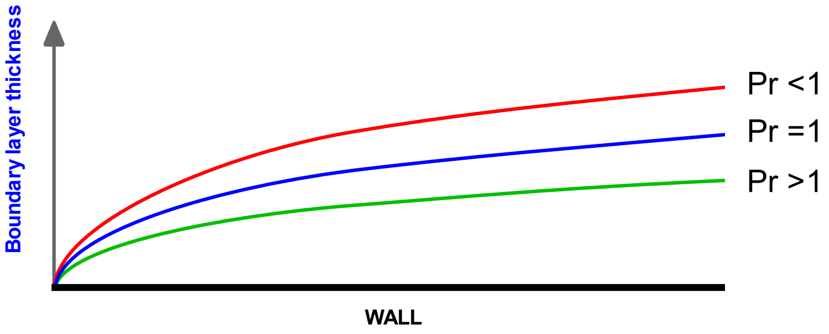
$$+$$

Additional closure equations for:
turbulence models, multiphase models, combustion, particles, source terms, equation of state, and so on

Compressible flows – Boundary layer



Thermal boundary layer vs. Viscous boundary layer
Forced convection

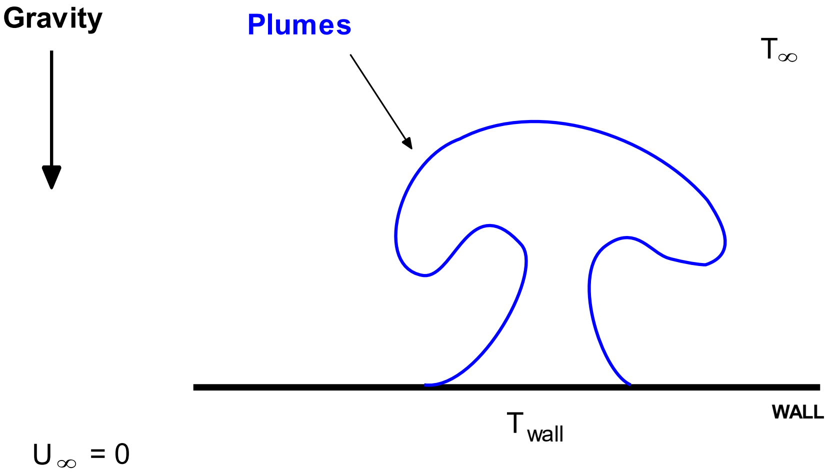


Thermal boundary layer in function of Prandtl number (Pr)

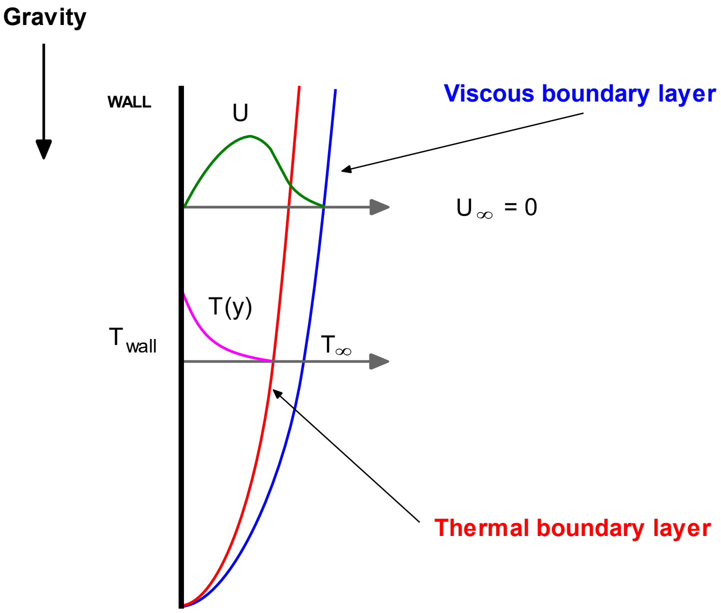
Momentum and thermal boundary layer

- Just as there is a viscous boundary layer in the velocity distribution (or momentum), there is also a thermal boundary layer.
- Thermal boundary layer thickness is different from the thickness of the viscous sublayer (momentum), and is fluid dependent.
- The thickness of the thermal sublayer for a high Prandtl number fluid (e.g. water) is much less than the momentum sublayer thickness.
- For fluids of low Prandtl numbers (*e.g.*, air), it is much larger than the momentum sublayer thickness.
- For Prandtl number equal 1, the thermal boundary layer is equal to the momentum boundary layer.

Compressible flows – Boundary layer



Horizontal heated plate immersed in a quiescent fluid.
Natural convection



Vertical heated plate immersed in a quiescent fluid.
Natural convection.

Natural convection in a heated plate

- As the fluid is warmed by the plate, its density decreases and a buoyant force arises which induces flow motion in the vertical or horizontal direction.
- The force is proportional to $(\rho - \rho_\infty) \times g$, therefore gravity must be considered.

Compressible solvers in OpenFOAM®

- Dealing with compressible flows in OpenFOAM® is not so different from what we have done so far.
- The new steps are:
    - Define the thermophysical variables.
    - Define the boundary conditions and initial conditions for temperature.
    - If you are dealing with turbulence, you will need to define the boundary conditions and initial conditions for the turbulent thermal diffusivity.
    - Define discretization schemes and linear solvers for the new variables and equations.

- Remember to choose the near-wall treatment.
- FYI, we have found that it is tricky to achieve convergence using a low-RE approach with compressible flows (high speed) and steady solvers.

Compressible solvers in OpenFOAM®

- Additionally, the numerics of compressible solvers is a little bit more delicate.
  - Temperature is a bounded quantity, so we need to use accurate and stable methods (preferably TVD).
  - If you are in the presence of shock waves, you need to use TVD methods and gradient limiters.
  - The solvers are very sensitive to overshoots and undershoots in the gradients, so you need to use very aggressive limiters.
  - If you are dealing with chemicals reactions or combustion, you need to use accurate and stable methods (preferably TVD).
  - TVD methods requires good meshes and CFL number below 1 for good accuracy and stability.
  - Using steady solvers requires tuning of the under-relaxation factors. Usually, the default values do not work well.
  - The use local time stepping to reach steady state can improve the convergence rate.

Compressible solvers in OpenFOAM®

- OpenFOAM® comes with many solvers and models that can address a wide physics.
- Compressibility can be introduced in all the modeling capabilities we have seen so far (turbulence modeling and multiphase flows).
- It is also possible to add source terms, deal with moving bodies or use adaptive mesh refinement.

- You will find the source code of all the compressible solvers in the directories:
    - **`OpenFOAM-6/applications/solvers/compressible`**
    - **`OpenFOAM-6/applications/solvers/combustion`**
    - **`OpenFOAM-6/applications/solvers/heatTransfer`**
    - **`OpenFOAM-6/applications/solvers/lagrangian`**
    - **`OpenFOAM-6/applications/solvers/multiphases`**
- You will find the source code of the thermophysical models in the directory:
    - **`OpenFOAM-6/src/thermophysicalModels`**

Compressible solvers in OpenFOAM®

- These are the compressible solvers that you will use most of the time in OpenFOAM®.

- HVAC and low speed aerodynamics:
  - rhoSimpleFoam, rhoPimpleFoam

- High speed aerodynamics:
  - sonicFoam, rhoSimpleFoam, rhoPimpleFoam

- Buoyancy driven flows (including Boussinesq approximation):
  - buoyantBoussinesqPimpleFoam buoyantBoussinesqSimpleFoam, buoyantSimpleFoam, buoyantPimpleFoam

- Conjugate heat transfer
  - chtMultiRegionFoam

Selecting thermophysical properties

```
1      thermoType
2      {
3          type            hePsiThermo;
4          mixture         pureMixture;
5          transport       const;
6          thermo          hConst;
7          equationOfState perfectGas;
8          specie          specie;
9          energy          sensibleEnthalpy;
10     }
11
12     mixture
13     {
14         specie
15         {
16             nMoles      1;
17             molWeight   28.9;
18         }
19         thermodynamics
20         {
21             Cp          1005;
22             Hf          0;
23         }
24         transport
25         {
26             mu          1.84e-05;
27             Pr          0.713;
28         }
29     }
```

- The thermophysical properties are set in the dictionary *thermophysicalProperties*.
- This dictionary file is located in the directory **`constant`**.
- Thermophysical models are concerned with energy, heat and physical properties.
- In the sub-dictionary **thermoType** (lines 1-10), we define the thermophysical models.
- The entries in lines 3-4, are determined by the choice of the solver (they are hardwired to the solver).
- The **transport** keyword (line 5). concerns evaluating dynamic viscosity. In this case the viscosity is constant.
- The thermodynamic models (**thermo** keyword) are concerned with evaluating the specific heat Cp (line 6). In this case Cp is constant.
- The **equationOfState** keyword (line 7) concerns to the equation of state of the working fluid. In this case,

$$\rho = \frac{p}{RT}$$

- Line 8 is a fixed option (hardwired to the solver).

Selecting thermophysical properties

```
1     thermoType
2     {
3         type            hePsiThermo;
4         mixture         pureMixture;
5         transport       const;
6         thermo          hConst;
7         equationOfState perfectGas;
8         specie          specie;
9         energy          sensibleEnthalpy;
10    }
11
12    mixture
13    {
14        specie
15        {
16            nMoles      1;
17            molWeight   28.9;
18        }
19        thermodynamics
20        {
21            Cp          1005;
22            Hf          0;
23        }
24        transport
25        {
26            mu          1.84e-05;
27            Pr          0.713;
28        }
29    }
```

- The form of the energy equation to be used is specified in line 9 (**energy**).
- In this case we are using enthalpy formulation (**sensibleEnthalpy**).
- In this formulation, the following equation is solved,

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho \mathbf{u} h) + \frac{\partial \rho K}{\partial t} + \nabla \cdot (\rho \mathbf{u} K) - \frac{\partial p}{\partial t} = \nabla \cdot (\alpha_{eff} \nabla e) + \rho \mathbf{g} \cdot \mathbf{u} + S$$

- Alternatively, we can use the **sensibleInternalEnergy** formulation, where the following equation is solved for the internal energy,

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho \mathbf{u} e) + \frac{\partial \rho K}{\partial t} + \nabla \cdot (\rho \mathbf{u} K) + \nabla \cdot (\mathbf{u} p) = \nabla \cdot (\alpha_{eff} \nabla e) + \rho \mathbf{g} \cdot \mathbf{u} + S$$

- In the previous equations, the effective thermal diffusivity is equal to,

$$\alpha_{eff} = \alpha_{turbulent} + \alpha_{laminar} = \frac{\rho \nu_t}{Pr_t} + \frac{\mu}{Pr} = \frac{\rho \nu_t}{Pr_t} + \frac{k}{c_p}$$

- And $K \equiv |\mathbf{u}|^2/2$ is the kinetic energy per unit mass.

Selecting thermophysical properties

```
1      thermoType
2      {
3          type            hePsiThermo;
4          mixture         pureMixture;
5          transport       const;
6          thermo          hConst;
7          equationOfState perfectGas;
8          specie          specie;
9          energy          sensibleEnthalpy;
10     }
11
12     mixture
13     {
14         specie
15         {
16             nMoles      1;
17             molWeight   28.9;
18         }
19         thermodynamics
20         {
21             Cp          1005;
22             Hf          0;
23         }
24         transport
25         {
26             mu          1.84e-05;
27             Pr          0.713;
28         }
29     }
```

- When we use the sensible formulation (**sensibleEnthalpy** or **sensibleInternalEnergy**), the heat of formation is not included in the energy equation.
- In the sub-dictionary **mixture** (lines 12-29), we define the thermophysical properties of the working fluid.
- In line 17, we define the molecular weight.
- In line 21, we define the specific heat.
- The heat of formation is defined is line 22 (not used in the sensible formulation).
- In this case, we are defining the properties for air at 20° Celsius and at a sea level.
- As we are using the transport model **const** (line 5), we need to define the dynamic viscosity and Prandtl number (lines 26 and 27).
- If you set the viscosity to zero, you solve the Euler equations.
- Remember, transport modeling (line 5), concerns evaluating dynamic viscosity, thermal conductivity and thermal diffusivity.

Selecting thermophysical properties

```
1      thermoType
2      {
3          type             hePsiThermo;
4          mixture          pureMixture;
5          transport        sutherland;
6          thermo           hConst;
7          equationOfState  perfectGas;
8          specie           specie;
9          energy           sensibleEnthalpy;
10     }
11
12     mixture
13     {
14         specie
15         {
16             nMoles       1;
17             molWeight    28.9;
18         }
19         thermodynamics
20         {
21             Cp           1005;
22             Hf           0;
23         }
24         transport
25         {
26             As           1.4792e-06;
27             Ts           116;
28         }
29     }
```

- When we use the sensible formulation (**sensibleEnthalpy** or **sensibleInternalEnergy**), the heat of formation is not included in the energy equation.
- If you want to include the heat of formation, you must use the **absoluteEnthalpy** formulation (line 6).
- If you use the transport model **sutherland** (line 5), you will need to define the coefficients of the Sutherland model.
- The Sutherland model is defined as follows (OpenFOAM® uses the 2 coefficients formulation):

$$\mu = \frac{A_s\sqrt{T}}{1 + T_s/T}$$

- The Sutherland coefficients are defined in lines 26-27.
- **Remember, you can use the banana method to know all the options available.**

Adjusting the numerical method

- If you choose the **sensibleEnthalpy** formulation, you need to define the convective discretization schemes and linear solvers of the energy equation (enthalpy formulation).

fvSchemes

```
divSchemes
{
        div(phi,K) Gauss linear;
        div(phi,h) Gauss linear;
        …
        …
        …
}
```

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho \mathbf{u} h) + \frac{\partial \rho K}{\partial t} + \nabla \cdot (\rho \mathbf{u} K) - \frac{\partial p}{\partial t} = \nabla \cdot (\alpha_{eff} \nabla e) + \rho \mathbf{g} \cdot \mathbf{u} + S$$

fvSolution

```
"(h|rho)"
{
        solver          PBiCGStab;
        preconditioner  DILU;
        tolerance       1e-8;
        relTol          0.01;
}
        …
        …
        …
```

- Remember, temperature is a bounded quantity so you need to use non-oscillatory methods.
- For low speed flows, the kinetic energy **K** and the enthalpy **h** can be discretized using the linear method. For high speed flows, is better to use bounded methods.
- Remember to use gradient limiters.
- If you are using a steady solver, remember to set the under-relaxation factors for **h** and **rho**.

Adjusting the numerical method

- If you choose the **sensibleInternalEnergy** formulation, you need to define the convective discretization schemes and linear solvers of the energy equation (internal energy formulation).

fvSchemes

```
divSchemes
{
        div(phi,K) Gauss linear;
        div(phi,e) Gauss linear;
        div(phiv,p) Gauss linear;
        …
        …
        …
}
```

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho \mathbf{u} e) + \frac{\partial \rho K}{\partial t} + \nabla \cdot (\rho \mathbf{u} K) + \nabla \cdot (\mathbf{u} p) = \nabla \cdot (\alpha_{eff} \nabla e) + \rho \mathbf{g} \cdot \mathbf{u} + S$$

fvSolution

```
"(e|rho)"
{
        solver          PBiCGStab;
        preconditioner  DILU;
        tolerance       1e-8;
        relTol          0.01;
}
        …
        …
        …
```

- Remember, temperature is a bounded quantity so you need to use non-oscillatory methods.
- For low speed flows, the kinetic energy **K** and the internal energy **e** can be discretized using the linear method. For high speed flows, is better to use bounded methods.
- Remember to use gradient limiters.
- If you are using a steady solver, remember to set the under-relaxation factors for **e** and **rho**.

Transport properties – Boussinesq solvers

```
transportModel Newtonian;

// Laminar viscosity
nu              nu [0 2 -1 0 0 0 0] 1e-05;

// Thermal expansion coefficient
beta            beta [0 0 0 -1 0 0 0] 3e-03;

// Laminar Prandtl number
Pr              Pr [0 0 0 0 0 0 0] 0.9;

// Turbulent Prandtl number
Prt             Prt [0 0 0 0 0 0 0] 0.7;

// Reference temperature
TRef            TRef [0 0 0 1 0 0 0] 300;
```

- If you use the family of solvers that uses the Boussinesq approximation, you do not need to define the thermodynamical properties.
- Instead, you need to define the transport properties (as for incompressible flows) and a reference temperature.
- You will need to define the following fluid properties: laminar viscosity, thermal expansion coefficient, laminar Prandtl number, and turbulent Prandtl number.
- The following solvers use the Boussinesq approximation:
    - buoyantBoussinesqPimpleFoam
    - buoyantBoussinesqSimpleFoam.
- Remember, the Boussinesq approximation is a way to solve natural convection problems, without having to solve the compressible NSE.
- It assumes that variations in density have no effect on the flow field, except when they give rise to buoyancy forces.
- This approximation is accurate when density variations are small.

Final remarks

- When solving the enthalpy formulation of the energy equation,

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho \mathbf{u} h) + \frac{\partial \rho K}{\partial t} + \nabla \cdot (\rho \mathbf{u} K) - \frac{\partial p}{\partial t} = \nabla \cdot (\alpha_{eff} \nabla e) + \rho \mathbf{g} \cdot \mathbf{u} + S$$

  the pressure work term $\partial p / \partial t$ can be excluded from the solution.

- This has a stabilizing effect on the solution, specially if you are using steady solvers.
- To turn off the pressure work term $\partial p / \partial t$, set the option dpdt to no (**dpdt no;**) in the *`thermophysicalProperties`* dictionary.

- Finally, when you work with compressible solvers you use absolute pressure and the working units are in Pascals.