



051176 - Computational Techniques for Thermochemical Propulsion
Master of Science in Aeronautical Engineering

Basic Concepts of Fluid Flows

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Fluids are substances whose molecular structure offers no resistance to external shear forces: even the smallest force causes deformation of a fluid particle.

Although a significant distinction exists between liquids and gases, both types of fluids obey the same laws of motion. In most cases of interest, a fluid can be regarded as *continuum*.

- Fluid flow is caused by the action of externally applied forces. Common **driving forces** include: pressure differences, gravity, shear, rotation, surface tension.
- They can be classified as:
 - **surface forces** (e.g. the shear force due to wind blowing above the ocean or pressure and shear forces created by a movement of a rigid wall relative to the fluid)
 - **body forces** (e.g. gravity and forces induced by rotation).

While all fluids behave similarly under action of forces, their macroscopic properties differ considerably. The most important properties of simple fluids are the *density* and *viscosity*. Others, such as Prandtl number, specific heat, and surface tension affect fluid flows only under certain conditions, e.g. when there are large temperature differences.

Fluid properties are functions of other thermodynamic variables, (e.g. temperature and pressure) and of the chemical composition.

The speed of a flow affects its properties in a number of ways:

- *at low enough speeds, the inertia of the fluid may be ignored and we have creeping flow.* This regime is of importance in flows containing small particles (suspensions), in flows through porous media or in narrow passages (coating techniques, micro-devices);
- *as the speed is increased, inertia becomes important but each fluid particle follows a smooth trajectory; the flow is then said to be laminar. Further increases in speed may lead to instability that eventually produces a more random type of flow that is called turbulent. The process of laminar-turbulent transition is an important area in its own right.*

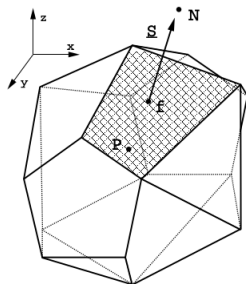
Finally, the *ratio of the flow speed to the speed of sound in the fluid (the Mach number)* determines whether exchange between kinetic energy of the motion and internal degrees of freedom needs to be considered:

- for $Ma < 0.3$, the flow may be considered incompressible; otherwise, it is compressible;
- if $Ma < 1$, the flow is called subsonic; when $Ma > 1$, the flow is supersonic and shock waves are possible; finally, for $Ma > 5$, the compression may create high enough temperatures to change the chemical nature of the fluid; such flows are called *hypersonic*.

These distinctions affect the mathematical nature of the problem and therefore the solution method. Note that we call the flow compressible or incompressible depending on the Mach number, even though compressibility is a property of the fluid. This is common terminology since the flow of a compressible fluid at low Mach number is essentially incompressible.

CONSERVATION LAWS

- Conservation laws can be derived by considering a given quantity of matter or control mass (CM) and its extensive properties, such as mass, momentum and energy.
- This approach is used to study the dynamics of solid bodies, where the CM (sometimes called the system) is easily identified.



In fluid flows, however, it is difficult to follow a parcel of matter: it is more convenient to deal with the **flow within a certain spatial region we call a control volume (CV): this method of analysis is called the control (or finite) volume approach.**

The conservation law for an extensive property relates the rate of change of the amount of that property in a given control mass to externally determined effects.

- For mass, which is neither created nor destroyed in the flows of engineering interest, the conservation equation can be written:

$$\frac{Dm}{Dt} = 0$$

- On the other hand, momentum can be changed by the action of forces and its conservation equation is Newton's second law of motion:

$$\frac{D(mu)}{Dt} = \sum f$$

In the Finite Volume (FV) framework, these laws must be written into a control volume form.

The fundamental variables will be *intensive* rather than extensive properties; the former are properties which are independent of the amount of matter considered: examples are density ρ (mass per unit volume) and velocity v (momentum per unit mass).

If ϕ is any conserved intensive property, then the corresponding extensive property Φ can be expressed as:

$$\Phi = \int_{\Omega_{CV}} \rho \phi d\Omega \quad (1)$$

where Ω_{CV} stands for the volume of the Control Volume (CV); sometimes the symbol CM (Control Mass) is used also.

Note:

- for mass conservation, $\phi = 1$;
- for momentum conservation, $\phi = \mathbf{u}$;
- for conservation of a scalar, ϕ represents the conserved property per unit mass).

From Eq. (1), the total time derivative can be expanded by the *Reynolds Transport Theorem*:

$$\frac{D}{Dt} \int_{\Omega_{CV}} \rho \phi d\Omega = \frac{\partial}{\partial t} \int_{\Omega_{CV}} \rho \phi d\Omega + \int_{S_{CV}} \rho \phi (\mathbf{u} - \mathbf{u}_b) \cdot \mathbf{n} dS \quad (2)$$

where Ω_{CV} is the CV volume, S_{cv} is the surface enclosing CV, \mathbf{n} is the unit vector orthogonal to S_{cv} and directed outwards, \mathbf{u} is the fluid velocity and \mathbf{v}_b is the velocity with which the CV surface is moving (\rightarrow *moving mesh*!).

The last term is usually called the convective (or sometimes, advective) flux of ϕ through the CV boundary. If the CV moves so that its boundary coincides with the boundary of a control mass, then $\mathbf{u} = \mathbf{v}_b$ and this term will be zero as required.

The integral form of the mass conservation (continuity) equation follows directly from the control volume equation, by setting $\phi = 1$:

$$\frac{\partial}{\partial t} \int_{\Omega} \rho d\Omega + \int_S \rho(\mathbf{u} - \mathbf{u}_b) \cdot \mathbf{n} dS = 0$$

By applying the Gauss' divergence theorem to the convection term, we can transform the surface integral into a volume integral. Allowing the control volume to become infinitesimally small leads to a differential coordinate-free form of the continuity equation:

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

For the differential form of the conservation of mass:

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

The Cartesian form using the Einstein convention that whenever the same index appears twice in any term, summation over the range of that index is implied:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = \frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_x)}{\partial x} + \frac{\partial (\rho u_y)}{\partial y} + \frac{\partial (\rho u_z)}{\partial z} = 0$$

$$\frac{\partial}{\partial t} \int_{\Omega} \rho \mathbf{u} \, d\Omega + \int_S \rho \mathbf{u} (\mathbf{u} - \mathbf{u}_b) \cdot \mathbf{n} \, dS = \sum f \quad (3)$$

To express the right hand side in terms of intensive properties, one has to consider the forces which may act on the fluid in a CV:

- surface forces (pressure, normal and shear stresses, surface tension etc.);
- body forces (gravity, centrifugal and Coriolis forces, electromagnetic forces, etc.).

The surface forces due to pressure and stresses are, from the molecular point of view, the microscopic momentum fluxes across a surface. If these fluxes cannot be written in terms of the properties whose conservation the equations govern (density and velocity), the system of equations is not closed; that is there are fewer equations than dependent variables and solution is not possible.

With the body forces (per unit mass) being represented by \mathbf{b} , the integral form of the momentum conservation equation becomes:

$$\int_{\Omega} \rho \mathbf{u} \, d\Omega + \int_S \rho \mathbf{u} (\mathbf{u} - \mathbf{u}_b) \cdot \mathbf{n} dS = \int_S \mathbf{T} \cdot \mathbf{n} dS + \int_{\Omega} \rho \mathbf{b} \, d\Omega$$

A coordinate-free vector form of the momentum conservation equation is readily obtained by applying Gauss' divergence theorem to the convective and diffusive flux terms:

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \rho \mathbf{u} (\mathbf{u} - \mathbf{u}_b) = \nabla \cdot \mathbf{T} + \rho \mathbf{b}$$

For **newtonian fluids**, the stress tensor T , which is the molecular rate of transport of momentum, can be written:

$$T = - \left(p + \frac{2}{3} \mu \nabla \cdot \mathbf{u} \right) \mathbf{I} + 2\mu D$$

where μ is the dynamic viscosity, \mathbf{I} is the unit tensor, p is the static pressure and D is the rate of strain (deformation) tensor:

$$D = \frac{1}{2} \left[\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right]$$

In index (Einstein) notation, we can write:

$$T_{ij} = - \left(p + \frac{2}{3} \mu \frac{\partial u_j}{\partial x_j} \right) \delta_{ij} + 2\mu D_{ij}$$

$$D = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

where δ_{ij} is Kronecker symbol ($\delta_{ij}=1$ if $i=j$ and $\delta_{ij}=0$ otherwise). The following notation is often used in literature to describe the **viscous part of the stress tensor**:

$$\tau_{ij} = 2\mu D_{ij} - \frac{2}{3} \mu \delta_{ij} \operatorname{div} \mathbf{u}$$

The corresponding equation for the i th Cartesian component is:

$$\frac{\partial (\rho u_i)}{\partial t} + \nabla \cdot \rho u_i (u_i - u_b) = \nabla \cdot \mathbf{t}_i + \rho b_i$$

where:

$$\mathbf{t}_i = \mu \nabla u_i + \mu (\nabla \mathbf{u})^T \cdot \mathbf{i}_j - \left(p + \frac{2}{3} \mu \frac{\partial u_j}{\partial x_j} \right) \cdot \mathbf{i}_i = \tau_{ij} \mathbf{i}_j - p \mathbf{i}_i$$

Here b_i stands for the i th component of the body force, T superscript means transpose and \mathbf{i}_i is the Cartesian unit vector in the direction of the coordinate x_i . In Cartesian coordinates one can write the above expression as:

$$t_i = \mu \nabla u_i + \mu (\nabla \mathbf{u})^T \cdot \mathbf{i}_j - \left(p + \frac{2}{3} \mu \frac{\partial u_j}{\partial x_j} \right) \cdot \mathbf{i}_i$$

- The momentum equations are said to be in **strong conservation form** if all terms have the form of the divergence of a vector or tensor. This is possible for the component form of the equations only when *components in fixed directions* are used.
- The strong conservation form of the equations, when used together with a finite volume method, automatically insures global momentum conservation in the calculation.
- A coordinate-oriented vector component turns with the coordinate direction and an "apparent force" is required to produce the turning; these forces are non-conservative in the sense defined above.

If the expression for the viscous part of the stress tensor,

$$\tau_{ij} = 2\mu D_{ij} - \frac{2}{3}\mu\delta_{ij} \operatorname{div} \mathbf{u}$$

is substituted into

$$\frac{\partial (\rho u_i)}{\partial t} + \nabla \cdot \rho u_i (u_i - u_b) = \nabla \cdot \mathbf{t}_i + \rho b_i$$

and if gravity is the only body force, the momentum equation for Cartesian coordinates is:

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i$$

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i$$

SOME NOTES:

- For the case of constant density and gravity, the term $\rho \mathbf{g} \Delta h$ can be written as $\nabla(\rho \mathbf{g} \cdot \mathbf{r})$, where \mathbf{r} is the position vector, $\mathbf{r} = x_i \mathbf{i}_i$; usually, gravity is assumed to act in the negative z -direction, i.e. $\mathbf{g} = g_z \mathbf{k}$, g_z being negative; in this case, $\mathbf{g} \cdot \mathbf{r} = g_z z$.
- $-\rho g_z z$ is the hydrostatic pressure, and it is convenient (and for numerical solution more efficient) to define $\tilde{p} = p - \rho g_z z$ as the *head* and use it in place of the pressure. The term $\rho \mathbf{g}_i$ then disappears from the above equation. If the actual pressure is needed, one has only to add $\rho g_z z$ to \tilde{p} .

The integral form of the equation describing conservation of a scalar quantity ϕ is:

$$\frac{\partial}{\partial t} \int_{\Omega} \rho \phi \mathbf{u} \, d\Omega + \int_S \rho \phi \cdot \mathbf{n} dS = \sum f_{\phi}$$

where f_{ϕ} represents transport of ϕ by mechanisms other than convection and any sources or sinks of the scalar.

Diffusive transport is always present (even in stagnant fluids), and it is usually described by a gradient approximation, e.g. Fourier's law for heat diffusion and Fick's law for mass diffusion:

$$f_{\phi}^d = \int_S \Gamma \, grad \, \phi \cdot \mathbf{n} dS$$

where Γ is the diffusivity for the quantity ϕ .

NOTE: equations for the conservation of scalar quantities are very common in CFD. Typical examples are the track of the chemical species in reactive flows!

- The conservation equations for mass and momentum are non-linear, coupled, and difficult to solve:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0$$
$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot \rho \mathbf{u} (\mathbf{u} - \mathbf{u}_b) = \nabla \cdot \mathbf{T} + \rho \mathbf{b}$$

- Only in a small number of cases - mostly fully developed flows in simple geometries, e.g. in pipes, between parallel plates etc. - is it possible to obtain an analytical solution of the Navier-Stokes equations. These flows are important for studying the fundamentals of fluid dynamics, but their practical relevance is limited. In all cases in which such a solution is possible, many terms in the equations are zero.
- For other flows some terms are unimportant and we may neglect them; this simplification introduces an error. **In most cases, even the simplified equations cannot be solved analytically; one has to use numerical methods;** the computing effort may be much smaller than for the full equations, which is a justification for simplifications.

We list now some flow types for which the equations of motion can be simplified.

- **In many applications the fluid density may be assumed constant.** This is true for:
 - liquids, whose compressibility may indeed be neglected;
 - for gases if the Mach number is below 0.3

Such flows are said to be incompressible.

The governing equations for mass and momentum become:

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

$$\nabla (u_i, \mathbf{u}) = \nabla (\nu \nabla u_i) - \frac{1}{\rho} \nabla (p \mathbf{i}_i) + b_i$$

where $\nu = \mu/\rho$ is the kinematic viscosity. This simplification is generally not of a great value, as the equations are hardly any simpler to solve. However, it does help in numerical solution.

If the flow is also isothermal, the viscosity is also constant.

In flows far from solid surfaces, the effects of viscosity are usually very small. If viscous effects are neglected altogether, i.e. if we assume that the stress tensor reduces to $\mathbf{T} = -p\mathbf{I}$, the Navier-Stokes equations reduce to the Euler equations. The continuity equation does not change its form, while the momentum equations are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot \rho \mathbf{u} (\mathbf{u} - \mathbf{u}_b) = \text{div} (\mathbf{p} \mathbf{i}_i) + \rho \mathbf{b}$$

- Since the fluid is assumed to be inviscid, it cannot stick to walls and slip is possible at solid boundaries. The Euler equations are often used to study compressible flows at high Mach numbers. At high velocities, the Reynolds number is very high and viscous and turbulence effects are important only in a small region near the walls. These flows are often well predicted using the Euler equations.
- Although the Euler equations are not easy to solve, the fact that no boundary layer near the walls need be resolved allows the use of coarser grids. Thus flows over the whole aircraft have been simulated using Euler equations; accurate resolution of the viscous region would require much more computer resource; such simulations are being done on a research basis at present.

One of the simplest flow models is potential flow. *The fluid is assumed to be inviscid (as in the Euler equations);* however, an additional condition is imposed:

$$\text{rot } \mathbf{u} = 0$$

From this condition it follows that there exists a *velocity potential* Φ , such that the velocity vector can be defined as:

$$\mathbf{v} = -\nabla \Phi$$

The continuity equation for an incompressible flow, $\nabla \cdot \mathbf{v} = 0$, then becomes a Laplace equation for the potential Φ :

$$\nabla \cdot (\nabla \Phi) = 0$$

The momentum equation can then be integrated to give the Bernoulli equation, an algebraic equation that can be solved once the potential is known. Potential flows are therefore described by the scalar Laplace equation.

- For each velocity potential Φ one can also define the corresponding streamfunction Ψ . The velocity vectors are tangential to streamlines (lines of constant streamfunction); the streamlines are orthogonal to lines of constant potential, so these families of lines form an orthogonal flow net.
- Potential flows are important but not very realistic. For example, the potential theory leads to D'Alembert's paradox, i.e. a body experiences neither drag nor lift in a potential flow.

When the flow velocity is very small, the fluid is very viscous, or the geometric dimensions are very small (i.e. when the Reynolds number is small):

- **the convective (inertial) terms** in the Navier-Stokes equations play a minor role and **can be neglected**. Due to the **low velocities, the unsteady term can also be neglected**;
- *the flow is then dominated by the viscous, pressure, and body forces and is called creeping flow*. If the fluid properties can be considered constant, the momentum equations become linear; they are usually called Stokes equations.

While the continuity equation does not change, the momentum equations become:

$$\nabla (\mu \nabla u_i) - \frac{1}{\rho} \nabla (p \mathbf{i}_i) + b_i = 0$$

Examples of creeping flows are porous media, coating technology, micro-devices, etc.

In flows accompanied by heat transfer, the fluid properties are normally functions of temperature. The variations may be small and yet be the cause of the fluid motion.

- **If the density variation is not large, one may treat the density as constant in the unsteady and convection terms, and treat it as variable only in the gravitational term. This is called the Boussinesq approximation.**
- One usually assumes that the density varies linearly with temperature. If one includes the effect of the body force on the mean density in the pressure term, the remaining term can be expressed as:

$$(\rho - \rho_0) g_i = -\rho_0 g_i \beta (T - T_0)$$

where β is the coefficient of volumetric expansion. This approximation introduces errors of the order of 1% if the temperature differences are below e.g. 2° for water and 15° for air. The error may be more substantial when temperature differences are larger; the solution may even be qualitatively wrong.

NOTE: please check the source code of `buoyantBoussinesqSimpleFoam` in the folder `$FOAM_SOLVERS/heatTransfer!`

When the flow has a predominant direction (i.e. there is no reversed flow or recirculation) and the variation of the geometry is gradual, the flow is mainly influenced by what happened upstream. Examples are flows in channels and pipes and flows over plane or mildly curved solid walls. *Such flows are called thin shear layer or boundary layer flows.* The Navier-Stokes equations can be simplified for such flows as follows:

- diffusive transport of momentum in the principal flow direction is much smaller than convection and can be neglected;
- the velocity component in the main flow direction is much larger than the components in other directions;
- the pressure gradient across the flow is much smaller than in the principal flow direction.

The two-dimensional boundary layer equations reduce to:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_1 u_1)}{\partial x_1} + \frac{\partial(\rho u_2 u_1)}{\partial x_2} = \mu \frac{\partial^2 u_1}{\partial x_2^2} - \frac{\partial p}{\partial x_1}$$

which must be solved together with the continuity equation; the equation for the momentum normal to the principal flow direction reduces to $\partial p / \partial x_2 = 0$.

These techniques see considerable use in aerodynamics. **The methods are very efficient but can be applied only to problems without separation.**



The Navier-Stokes equations are a system of non-linear second order equations in four independent variables. Consequently the classification scheme does not apply directly to them.

Nonetheless, the Navier-Stokes equations do possess many of the properties outlined above and the many of the ideas used in solving second order equations in two independent variables are applicable to them but care must be exercised.

Hyperbolic Flows

To begin, consider the case of unsteady inviscid compressible flow. A compressible fluid can support sound and shock waves and it is not surprising that these equations have essentially hyperbolic character.

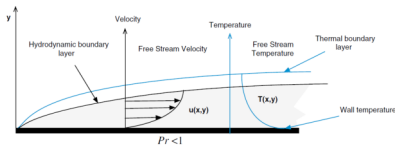
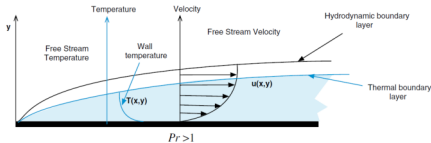
- Most of the methods used to solve these equations are based on the idea that the equations are hyperbolic and, given sufficient care, they work quite well.
- For **steady compressible flows**, the character depends on the speed of the flow:
 - if the flow is *supersonic*, the equations are hyperbolic while the equations for subsonic flow are essentially elliptic.
 - Equations for a viscous compressible flow are still more complicated. Their character is a mixture of elements of all of the types mentioned above; they do not fit well into the classification scheme and numerical methods for them are difficult to construct.

Mathematical Classification of Flows



Parabolic Flows

The boundary layer approximation described briefly above leads to a set of equations that have essentially parabolic character.



- Information travels only downstream in these equations and they may be solved using methods that are appropriate for parabolic equations.
- Note, however, that the boundary layer equations require specification of a pressure that is usually obtained by solving a potential flow problem.
- Subsonic potential flows are governed by elliptic equations (in the incompressible limit the Laplace equation suffices) so the overall problem actually has a mixed parabolic-elliptic character.

Elliptic Flows

When a flow has a region of recirculation i.e. flow in a sense opposite to the principal direction of flow, information may travel upstream as well as downstream. As a result, one cannot apply conditions only at the upstream end of the flow. The problem then acquires elliptic character.

- This situation occurs in subsonic (including incompressible) flows and makes solution of the equations a very difficult task.
- Unsteady incompressible flows actually have a combination of elliptic and parabolic character.
- the elliptic character comes from the fact that information travels in both directions in space;
- the parabolic character results from the fact that information can only flow forward in time. Problems of this kind are called incompletely parabolic.

What is missing?



The aim of this class is to look at **compressible reacting flows**. Today's lecture is only a (VERY IMPORTANT) part of the story: in reacting flows we have to solve carefully the energy equation, considering the changing properties of the compressible gas, which influence density.

Thank you for your attention!

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