Flow
Problem Formulation

Aspects of Formulation

The formulation of the internal flow problem has several aspects:

1. What are the Objectives?
2. What is Known?
    - Geometry
    - Flow Conditions
3. What Analysis Approach to Use? → CFD
    - Fluid Models
    - Flow Equation
    - Frame of Reference
    - Flow Domain
    - Boundary Conditions
    - Initial Conditions

Aerodynamic Features of Flows

The features of flows of interest may include:

- Mach number range (static, Mach 0 → hypersonic, Mach 10+)
- Shock waves
- High Reynolds numbers (laminar transitioning to turbulent)
- Turbulent boundary and shear layers
- Shock / boundary layer interactions
- Boundary layer separation
- High-temperature effects at hypersonic Mach numbers
- Compressor face / engine effects
- Unsteady flows (hammershocks, unstart)

Levels of the Use of CFD Results

1. Provide Qualitative Information.

   Provide features of flow field (conceptual, rough estimates of quantities). Accuracy requirements are low.

2. Provide Incremental Quantities, ΔP.

   - $P = P_{baseline} + \Delta P$
   - Errors partially cancel for ΔP
   - $\Delta P = (P_2 - P_1)_{actual} + (E_2 - E_1) = P_{actual} + \Delta E$
   - Moderate accuracy requirement.

3. Provide Absolute Quantities, P.

   Requires high level of accuracy.

Objectives

CFD analysis is conducted to provide data for the design of an inlet operating as part of a propulsion system. Two aspects:

Performance / Engine Compatibility

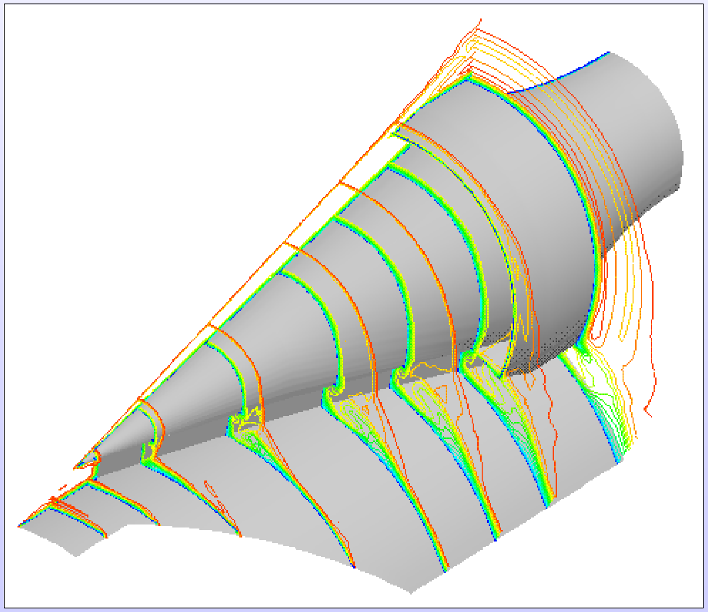
- Engine / inlet mass flow
- Total pressure recovery (recovery)
- Distortion (total pressure, total temperature)
- Bleed requirements (slots, bleed holes)
- Spillage (side walls, cowl)
- Features of the shock system (positions, cowl stand-off)
- Features of the boundary layers (thickness, separation)
- Drag (vehicle integration)
- Aerodynamic and thermal loads

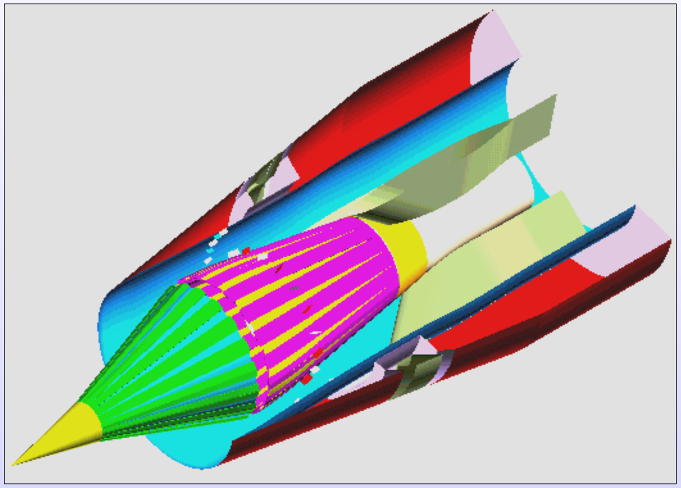
Stability

- Stability of the shock system (unstart)
- Off-design

Geometry

Define the aerodynamic surfaces about which the flow is to be determined.





More on this later…

Flow Conditions

Define what fluids are involved

- Air
- Combustion reactants

Define the operational environment / requirements

- Mach number, M
- Altitude, h
- Angle-of-attack, α
- Angle-of-sideslip, β
- Mass flows
- Pressures
- Temperatures

Fluid Models: Perfect Gas

A perfect gas is defined as "*A gas where intermolecular forces are negligible*". A gas that is not perfect is called a real gas. Some use the term "*real gas effects*" for describing high-temperature effects of vibration, dissociation, and chemical reactions associated with high Mach number flows. The suggested term is "*high-temperature effects*".

WIND only simulates perfect gases.

Perfect Gas Equation of State:

$$p = \rho R T$$

$$R = \frac{\Re}{M}$$

$\Re$, Universal gas constant

M, Molecular weight

For air, R = 1716 ft lbf / (slug °R) = 287 J / (kg K)

Mixtures of Perfect Gases

A gas may be a *mixture* of other gases. A mixture of several *species* of perfect gases is still a perfect gas. The *composition* of a gas mixture is defined by the *mass fraction*, c_i

$$c_i = \frac{m_i}{m} = \frac{\rho_i}{\rho}$$

where m_i is the mass of species i and m is the total mass of all species. One condition for a mixture with ns species is that

$$\sum_{i=1}^{ns} c_i = 1$$

The *molecular weight*, M, of the mixture is determined as

$$M = \frac{1}{\sum_{i=1}^{ns} \frac{c_i}{M_i}} \qquad R = \frac{\Re}{M}$$

Partial Pressures

Perfect gas equation of state applies to each species to determine the *partial pressure* of species i, p_i

$$p_i = \rho_i R_i T$$

Dalton's Law of Partial Pressures states that

$$p = \sum_{i=1}^{ns} p_i$$

Note also that

$$\rho = \sum_{i=1}^{ns} \rho_i \qquad R = \sum_{i=1}^{ns} c_i R_i$$

Specific Enthalpy & c_p

The *specific enthalpy* for a gas mixture is determined as

$$h = \sum_{i=1}^{ns} c_i \, h_i$$

where for each species

$$h_i = h_{f_i} + \int_{T_{ref}}^{T} c_{p_i} \, dT$$

The h_{fi} is the *specific enthalpy of formation* of species i at the reference temperature T_{ref}. The c_{pi} is the specific heat, which is defined using a polynomial

$$\frac{c_{p_i}}{R_i} = \sum_{k=0}^{K} a_{k_i} \, T^k$$

Transport Properties

The transport properties of a fluid are coefficients in physical models that govern the "transport" of

1) molecular kinetic energy: $\Rightarrow \mu$, molecular viscosity
2) thermal energy: $\Rightarrow k$, thermal conductivity
3) mass: $\Rightarrow D_{ij}$, binary diffusion

Sutherland’s Formula

Sutherland’s formula computes the *coefficient of molecular viscosity* μ for an perfect gas with fixed composition as a function of temperature

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

Where C_1 and C_2 are constants.

WIND uses C_1 = 2.269578E-08 slug / (ft-s-°$R^{1/2}$) and C_2 = 216.0 °R.

Thermal Conductivity

The definition of the *Prandtl number*

$$\Pr \equiv \frac{\mu c_p}{k}$$

is used to compute the *coefficient of thermal conductivity*, k

$$k = \frac{\mu c_p}{\Pr}$$

where the Prandtl number is considered a constant. Thus k is only a

WIND uses $Pr = 0.72$.

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Wilke’s Law

Wilke’s Law computes the transport properties μ and k for a mixture

$$\mu = \sum_{i=1}^{ns} \frac{x_i \, \mu_i}{\sum_{j=1}^{ns} x_j \, \phi_{ij}}$$

$$k = \sum_{i=1}^{ns} \frac{x_i \, k_i}{\sum_{j=1}^{ns} x_j \, \phi_{ij}}$$

where ϕ_{ij} is the *inter-collisional parameter*

$$\phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j} \right)^{-1/2} \left[1 + \left(\frac{\mu_i}{\mu_j} \right)^{1/2} \left(\frac{M_j}{M_i} \right)^{1/4} \right]^2$$

Diffusion

The coefficient of diffusion for a binary mixture of two species *i* and *j* of dilute gases is provided by the Chapman-Enskog formula

$$D_{ij} = 0.0018583 \sqrt{\frac{1}{M_i} + \frac{1}{M_j}} \left(\frac{1}{d_{ij}^2} \right) \frac{T^{3/2}}{p \Omega_{ij}}$$

where the effective diffusion collision integral factor is

$$\Omega_{ij} = \frac{1}{T_D^{0.145}} + \frac{1}{(T_D + 0.5)^2} \qquad T_D = \frac{T}{T_{\varepsilon_{ij}}} \qquad d_{ij} = \frac{1}{2}(d_i + d_j)$$

For the mixture of gases,

$$D_{im} = {1 - X_i} \Big/ {\sum_{j \neq i}^{ns} \frac{X_j}{D_{ij}}}$$

Air

Air is the most common gas (default gas) used in CFD simulations with WIND. Air is a mixture of mostly nitrogen (N_2) and oxygen (O_2) with other trace gases (Argon, water vapor).

Usually assume air to have a fixed composition with constant R, γ, c_p, and c_v, which is assuming air behaving as an *calorically (ideal) perfect gas*.

Simulations with hypersonic Mach numbers and higher temperatures (>1440 ^{o}R) involve changes in the energy states and composition of air. The relations for a mixture of perfect gases need to be used and models for the chemical reactions need to be used to determine the thermodynamic and transport properties.

Air (continued)

The behavior of air with temperature can be summarized as

T < 1440 °R. Air behaves as a *calorically perfect gas*.

T > 1440 °R. Vibrational energy states of molecules become significant and the specific heats become a function of temperature. Air behaves as a *thermally perfect gas*.

T > 4500 °R. Air chemically reacts to dissociate O_2 to form atomic oxygen O.

T > 7200 °R. Air chemically reacts to dissociate N_2 to form atomic oxygen N.

T > 16200 °R. Both N and O begin to ionize to form a plasma.

The above temperatures assume the air pressure is 1 atm. If the the air pressure is lower, the on-set temperatures (except the 1440 °R) will be lower, and vice versa. Once air chemically reacts, the chemical composition (species) of the air mixture will need to be tracked and the chemical reactions modeled.

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Gas Models

The following gas models provide specific relations for the thermodynamic properties (p, T, ρ, h, e, …) and the transport properties (μ, k, D):

Constant Property Fluid

Calorically Perfect (Ideal) Gas

Thermally Perfect Gas

Equilibrium Chemistry

Finite-Rate Chemistry

Constant Property Fluid Model

- Composition remains constant.
- Specific heats c_p and c_v are constant, maybe the same, c.
- Molecular viscosity μ and thermal conductivity k are constant.
- Density ρ may be constant (incompressible).
- Used for simulating liquid flow.

Calorically Perfect Gas Model

- Ideally Perfect (Ideal) Gas
- Composition remains constant, thus R is constant.
- Assumes the specific heats c_p and c_v are constant

$$\beta = \frac{h}{e} = \frac{c_p}{c_v} = \gamma \qquad c_p = \frac{\gamma R}{\gamma - 1} \qquad c_v = \frac{R}{\gamma - 1}$$

- Given ρ and e,

$$p = \rho e (\gamma - 1) \qquad T = \frac{p}{\rho R}$$

- Molecular viscosity μ is computed using Sutherland's formula
- Thermal conductivity k computed assuming a constant Prandtl number, Pr.

This model is the default model and is probably used 95-99% of time for WIND applications.

Thermally Perfect Gas Model

- Vibrational energy modes of gas molecules are significant.
- Composition is *frozen*, and so, gas constant, *R*, remain constant.
- Specific heats c_p and c_v are functions of static temperature, *T*.

$$\frac{c_p}{R} = \sum_{k=0}^{K} a_k T^k \qquad c_v = c_p - R \qquad h = h_{ref} + \int_{T_{ref}}^{T} c_p(T)\,dT$$

- Given ρ and *e*,

$$\beta = \frac{h}{e} \qquad p = \rho e(\beta - 1) \qquad T = \frac{p}{\rho R}$$

- Molecular viscosity μ is computed using Sutherland's formula
- Thermal conductivity *k* computed assuming a constant Prandtl number, Pr.

Equilibrium Chemistry Model

The equilibrium chemistry model considers changes in the chemical composition; however, the chemical reactions are assumed to happen instantaneously such that the flow remains in local thermodynamic and chemical equilibrium.

- Chemical composition varies, but is a function of two properties (p, T)
- Curve fits (Liu & Vinokur) are available for thermodynamic and transport properties.
- Applicable when fluid motion time scale is much greater than chemical reaction time scale.
- For air, chemical reactions occur above 4500 ^{o}R (2500 K).

Finite-Rate Chemistry Model

The finite-rate chemistry model considers changes in chemical composition when the time scales of chemical reactions are comparable or greater with the fluid motion time scale. Requires the specification of the chemical reactions in the model

$$\sum_{i=1}^{n} a_i [X_i] \underset{K_b}{\overset{K_f}{\leftrightarrow}} \sum_{i=1}^{n} b_i [X_i]$$

a_i and b_i are the stoichiometric mole numbers of the reactants and products of species i, respectively.

$$X_i = \frac{\rho c_i}{M_i} \qquad K_f = C T^n \exp\left[-E / K T\right] \qquad K_b = \frac{K_f}{K_e}$$

Each species has a continuity equation that must be solved as part of the system of conservation equation.

Flow Equations

The dynamics of fluid flow is described by several conservation principles:

- Mass (mass of system and species)
- Momentum
- Energy (internal, turbulent, chemical)

Fluid motion requires determining the fluid velocity components $\vec{v}$ and additional static properties (p, T, ρ, c_i). The flow may be time-invariant (steady) or time-variant (unsteady).

In addition to the equations, a complete description of the dynamic equations requires:

Frame of Reference
Control Volume and Control Surface (Flow Domain)
Boundary Conditions
Initial Conditions

Conservation Statement

An integral formulation of the conservation statement helps visualize the nature of the conservation:

$$\frac{d}{dt}\int_{V(\vec{r},t)} Q\,dV = -\oint_{S(\vec{r},t)} \left[\left(\vec{v}-\vec{g}\right)Q-\mathbf{D}\right]\cdot\hat{n}\,dS + \int_{V(\vec{r},t)} P\,dV$$

Time-rate of change of Q in the control volume.

Flux of Q leaving the control volume through the control surface.

Production of Q within the control volume.

Q is conserved quantity, scalar or vector (i.e. mass, momentum)

V is the control volume (time-varying)

S is the control surface (time-varying)

$\hat{n}$ is surface normal vector with positive direction out of volume

D is non-convective terms of the flux (vector or tensor)

The control volume can translate and rotate, as well as, change shape and deform. Gauss' theorem relates control surface and control volume.

Equations Sets

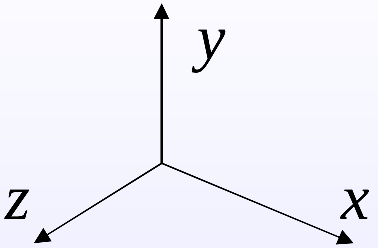
The dynamics can be expressed in the following equation sets:

$$Q = \begin{pmatrix} Q_{NS} \\ Q_{turb} \\ Q_{chem} \\ Q_{MFD} \end{pmatrix} \qquad \mathbf{D} = \begin{pmatrix} \mathbf{D}_{NS} \\ \mathbf{D}_{turb} \\ \mathbf{D}_{chem} \\ \mathbf{D}_{MFD} \end{pmatrix} \qquad P = \begin{pmatrix} P_{NS} \\ P_{turb} \\ P_{chem} \\ P_{MFD} \end{pmatrix}$$

Q, **D**, and *P* can be scalars or an algebraic vectors with elements as vectors. **D** can be a vector or dyadic, depending on whether Q is a scalar or vector.

Frames of Reference

Some frames of reference:



Inertial Cartesian Frame $(\hat{\imath}, \hat{\jmath}, \hat{k})$

$$\vec{r} = x\hat{\imath} + y\hat{\jmath} + z\hat{k} \qquad \vec{v} = u\hat{\imath} + v\hat{\jmath} + w\hat{k} \qquad \vec{g} = x_t\hat{\imath} + y_t\hat{\jmath} + z_t\hat{k}$$

Cylindrical Frame $(\hat{e}_x, \hat{e}_r, \hat{e}_\theta)$

Rotating Frame $\vec{g} = \vec{\omega} \times \vec{r}$

6 DOF Frame (generalized translation and rotation)

Navier-Stokes Equations

The Navier-Stokes equation govern fluid dynamics. They consist of the statements of conservation of mass, momentum, and internal energy:

$$Q_{NS} = \begin{pmatrix} \rho \\ \rho \vec{v} \\ \rho e_t \end{pmatrix} \qquad \mathbf{D}_{\mathrm{NS}} = \begin{pmatrix} 0 \\ \boldsymbol{\sigma} \\ \vec{v} \cdot \boldsymbol{\sigma} - \vec{q} \end{pmatrix} \qquad P_{NS} = \begin{pmatrix} 0 \\ -\rho \vec{G} \\ 0 \end{pmatrix}$$

The total internal energy is defined as

$$e_t = e + \frac{1}{2}\left(\vec{v} \cdot \vec{v}\right)$$

The gravitational acceleration is defined by $\vec{G}$.

Navier-Stokes Equations (continued)

The total internal stress tensor is

$$\boldsymbol{\sigma} = -p\,\mathrm{I} + \boldsymbol{\tau}$$

and includes the isotropic pressure component plus the viscous shear stress tensor. The **I** is the identity matrix. Assuming a Newtonian fluid in local thermodynamic equilibrium, the constitutive equation is

$$\boldsymbol{\tau} = \tau_{ij} = \mu\left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right]$$

This expression incorporates Stoke’s hypothesis that the bulk coefficient of viscosity is negligible for gases, and so, the second coefficient of viscosity is directly related to the coefficient of viscosity μ.

Navier-Stokes Equations (continued)

The non-convective term of the flux can be separated into inviscid and viscous components in the form

$$\mathbf{D}_{NS} = \mathbf{D}^{I}_{NS} + \mathbf{D}^{V}_{NS} \qquad \mathbf{D}^{I}_{NS} = \begin{pmatrix} 0 \\ -p\,\mathbf{I} \\ -\vec{v}\cdot p\,\mathbf{I} \end{pmatrix} \qquad \mathbf{D}^{V}_{NS} = \begin{pmatrix} 0 \\ \tau \\ \vec{v}\cdot\tau - \vec{q} \end{pmatrix}$$

The heat flux vector can be expressed as

$$\vec{q} = q_j = -k\frac{\partial T}{\partial x_j} + \sum_{i=1}^{ns} \rho_i \vec{U}_i h_i + \vec{q}_R$$

and includes components of heat transfer due to molecular dissipation, diffusion of species, and radiation.

Turbulence

When fluid dynamics exhibits instabilities, it is known as *turbulence*. Most aerospace flows of interest involve the transition of flow from a laminar condition to turbulent. Turbulence is defined as,

> *"…an irregular condition of flow in which the various quantities show a random variation with time and space coordinates, so that statistically distinct average values can be discerned" (Hinze, 1975).*

Turbulence can be visualized as eddies (local swirling motion):

- Size of eddy is turbulent length scale, but smallest still larger than molecular length scale.
- Length scales vary considerably.
- Eddies overlap in space with large eddies carrying small eddies.
- Cascading process transfers the turbulent kinetic energy from large eddies to smaller eddies where energy is dissipated as heat energy through molecular viscosity.
- Eddies convect with flow, and so, turbulence is not local – depend on history of the eddy.

Reynolds-Averaging

The fact that "*statistically distinct average values can be discerned*" allows us to apply a time-average over a time interval considered large with respect to the time scale of turbulence, but yet, small compared to the time scale of the flow. We use Reynolds-averaging, which replaces time-varying quantities with such relations as

$$u = \overline{u} + u'' \qquad p = \overline{p} + p'' \qquad \rho = \overline{\rho} + \rho''$$

With similar expressions for (v,w,h,T). This introduces Reynolds Stress

$$\overline{-\rho u_i'' u_j''}$$

into the time-averaged momentum and energy equations and the Reynolds Heat-Flux

$$\overline{-\rho u_j'' h''}$$

into the time-averaged energy equations.

Task of turbulence modeling is to model these terms.

Simplifications of the RANS Equations

Simplification of the full Reynolds-Averaged Navier-Stokes (RANS) equations can be employed to allow less computational effort when certain flow physics is not to be simulated:

Thin-Layer Navier-Stokes Equations

In the case of thin boundary layers along a solid surface, one can neglect viscous terms for coordinate directions along the surface, which are generally small.

Parabolized Navier-Stokes (PNS) Equations

In addition to the thin-layer assumption, if the unsteady term is removed from the equation and flow is supersonic in the streamwise direction, then the equations become parabolic in the cross-stream coordinates and a space-marching method can be used, which reduces computational effort significantly.

Euler (Inviscid) Equations

If all viscous and heat conduction terms are removed from the RANS equations, the equations become hyperbolic in time. This assumes viscosity effects are very small (high Reynolds numbers).

Turbulence Modeling

Turbulence Modeling is the process of closing the Navier-Stokes equations by providing required turbulence information. Turbulence Modeling has a few fundamental classifications:

1. Models that use the Boussinesq Approximation. These are the *eddy-viscosity models*, which will be the focus of this presentation.
2. Models that solve directly for the Reynolds Stresses. These become complicated fast by introducing further terms requiring modeling.
3. Models not based on time-averaging. These are the Large-Eddy Simulation (LES) and Direct Numerical Simulation (DNS) methods.

Boussinesq Approximation

The Boussinesq Approximation essentially assumes the exchange of turbulent energy in the cascading process of eddies is analogous of that of molecular viscosity. Thus, the approximation is

$$\overline{-\rho u_i'' u_j''} \approx 2\mu_T \left(S_{ij} - \frac{1}{3}\frac{\partial \bar{u}_k}{\partial x_k} \right)$$

which is the same form as the laminar viscous tensor. This allows us to write an effective viscosity as

$$\mu \approx \mu_L + \mu_T$$

Similarly the Reynolds heat-flux vector is approximated by applying the Reynolds analogy between momentum and heat transfer

$$\overline{-\rho u_j'' h''} \approx -k_T \frac{\partial T}{\partial x_j} \quad \text{with} \quad k_T = \frac{\mu_T c_p}{\mathrm{Pr}_T} \quad \text{and} \quad k = k_L + k_T .$$

Thus, the objective of the turbulence model is to compute μ_T.

Turbulence Equations

There exist various turbulence models, which may be classified as

1. Algebraic Models
   - Cebeci-Smith
   - Baldwin-Lomax
   - PDT
2. One-Equation Models (1 PDE)
   - Baldwin-Barth
   - Spalart-Allmaras (S-A)
3. Two-Equation Models (2 PDEs)
   - SST
   - Chien k-epsilon

- Models mostly assume fully turbulent flow rather than accurately model transition from laminar to turbulence flow.
- One- and two-equation models attempt to model the time history of turbulence.
- Models integrate through boundary layers to the wall, but S-A and SST models allow use of a wall function.

Algebraic Models

Algebraic Models consist of algebraic relations to define the local eddy viscosity. The models are based on Prandtl's Mixing Length Model that was developed through an analogy with the molecular transport of momentum.

$$\mu_T = \rho\, l_{mix}^2 \left| \frac{\partial u}{\partial y} \right|$$

The Cebeci-Smith Model is a two-layer model for wall-bounded flows that computes the turbulent eddy viscosity based on the distance from a wall using Prandtl's model and empirical turbulence correlations.

The Baldwin-Lomax Model improves on the correlations of the Cebeci-Smith model and does not require evaluation of the boundary layer thickness. It is the most popular algebraic model.

The PDT Model improves on the Baldwin-Lomax model for shear layers.

Algebraic models work well for attached boundary layers under mild pressure gradients, but are not very useful when the boundary layer separates.

One-Equation Models

One-Equation Models consist of a single partial differential equation (pde) that attempts to capture some of the history of the eddy viscosity. The Baldwin-Barth and Spalart-Allmaras turbulence models are two popular models; however, the Baldwin-Barth model has some problems and its use is not recommended.

The Spalart-Allmaras Model can be used when the boundary layer separates and has been shown to be a good, general-purpose model (at least robust to be used for a variety of applications).

Two-Equation Models

Two-Equation Models consist of two partial differential equations (pde) that attempts to capture some of the history of the eddy viscosity. The Menter SST and Chien k-ε turbulence models are two popular models.

As the number of equations increases, the computational effort increases and one has to balance improvements in modeling with the capture of important turbulence information.

Use of Turbulence Models

- Models were mainly formulated for external flows assuming incompressible flows and low adverse pressure gradients.
- Inlet flows have an adverse pressure gradient and our applications have been compressible flow with shocks, and so, large separation regions. *Bad area for models.*
- Compressibility corrections useful in some cases.
- Our use has settled with default models (Spalart-Allmaras & SST). S-A seems a little more consistent than SST?
- Amount of error with turbulence model can be estimated by simulating with S-A and SST and then comparing differences.

Chemistry Equations

The chemistry equations govern multi-species diffusion and chemical reactions for a finite-rate fluids model. The equations consist of species continuity equations:

$$Q_{chem} = \begin{pmatrix} \rho c_1 \\ \vdots \\ \rho c_i \\ \vdots \\ \rho c_{ns-1} \end{pmatrix} \qquad \mathbf{D}_{chem} = \begin{pmatrix} \mathbf{j}_1 \\ \vdots \\ \mathbf{j}_i \\ \vdots \\ \mathbf{j}_{ns-1} \end{pmatrix} \qquad P_{chem} = \begin{pmatrix} r_1 \\ \vdots \\ r_i \\ \vdots \\ r_{ns-1} \end{pmatrix}$$

Where $\mathbf{j}_i$ is the mass flux of species *i* defined by Fick's first law of diffusion

$$\mathbf{j}_i = -\rho D_{im} \nabla c_i$$

The rate of formation of species *i* is

$$r_i = M_i \frac{dX_i}{dt}$$

Chemistry Equations

The net rate of formation of species *i* is

$$r_i = M_i \frac{dX_i}{dt}$$

which is not zero for non-equilibrium flows. For the set of chemical reactions specified for the fluid, the net rate of formation can be determined from

$$\frac{d[X_i]}{dt} = \left.\frac{d[X_i]}{dt}\right|_f + \left.\frac{d[X_i]}{dt}\right|_b = (b_s - a_s)\left\{K_f \Pi_s [X_s]^{a_s} - K_b \Pi_s [X_s]^{b_s}\right\}$$

where Π denotes the product. Again, note that $X_i = \frac{\rho c_i}{M_i}$.

Normalization of the Equations

The equations can be normalized (non-dimensionalized) so that non-dimensional parameters (Reynolds and Prandtl number) are explicit in the equations and values are approximately unity. Usual reference quantities are

$$T_{ref} = T_\infty \quad \text{and} \quad \rho_{ref} = \rho_\infty$$

with velocities non-dimensionalized by $a_{ref}^2 = \gamma R T_\infty$.

To allow $\tilde{a}$ when $\tilde{T}$ requires $\tilde{R} = 1/\gamma$.

The non-dimensionalized equation of state becomes $\tilde{p} = \tilde{\rho}\,\tilde{R}\,\tilde{T}$.

Where at reference (freestream) conditions $\tilde{p}_\infty = \tilde{R} = 1/\gamma$.

This results in the relations $p_{ref} = e_{ref} = \rho_{ref}\, a_{ref}^2$.

Decoding the Conserved Variables

The solutions of the equations yields

$$Q_{NS} = \left(\rho, \rho\vec{v}, \rho e_t\right) \qquad Q_{chem} = \left(\rho c_i\right) \qquad \text{for } (i = 1, ns\text{-}1)$$

Those variables are then “decoded” to determine other flow properties:

$$\vec{v} = \frac{\rho\vec{v}}{\rho} \qquad e = e_t - \frac{1}{2}\vec{v}\cdot\vec{v} \qquad c_{ns} = 1 - \sum_{i=1}^{ns-1} c_i \qquad R = \sum_{i=1}^{ns} c_i R_i$$

A system of equations are iterated on temperature *T* to determine *p*, *h*, and *T*

$$h_i = h_{f_i} + \int_{T_{ref}}^{T} c_{p_i}\, dT \qquad h = \sum_{i=1}^{ns} c_i h_i \qquad \beta \equiv \frac{h}{e} \qquad p = \rho e\left(\beta - 1\right)$$

$$T = \frac{p}{\rho R} \qquad \textit{(repeat)}$$

Flow Domain

The flow problem formulation requires specification of a control volume bounded by a control surface that defines the flow domain on which the equations are solved. While in general this is a three-dimensional (3D) control volume, approximations may allow the use of planar (2D, axisymmetric) volumes.

More on this later…

Boundary Conditions

The flow conditions and constraints on the boundary of the control surface of the flow domain are the Boundary Conditions for the equations.   Aspects include:

Wall boundary conditions
Inflow / outflow boundary conditions
Compressor / engine face modeling
Bleed / blowing modeling
Vortex generator modeling

More on this later…

Initial Conditions

The type of Initial Conditions for the equations depend on the solution method. Time-marching or iterative methods require an initial flow field solution throughout the domain. Space-marching methods require the flow field solution at the starting marching surface.

More on this later…