Thermally-Perfect Gas Calculations

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1 Governing equations

Starting equations, with some assumed known $c_{p(T)}$:

$$\mathrm{d}h \; - \; v\,\mathrm{d}p \; = \; T\,\mathrm{d}s \tag{1}$$

$$pv \; = \; RT \tag{2}$$

$$\mathrm{d}h \; = \; c_{p(T)}\,\mathrm{d}T \tag{3}$$

2 Complete enthalpy calculation

The complete enthalpy function is obtained by integration of the known $c_{p(T)}$ function,

$$h_{(T)} \; \equiv \; \Delta h_f \; + \; \int_{T_s}^{T} c_{p(T)}\,\mathrm{d}T \tag{4}$$

where Δh_f is the heat of formation, and T_s is the standard condition at which Δh_f is defined, typically $T_s = 298\,\mathrm{K}$.

3 Pressure calculation

For an adiabatic compressor or turbine, the entropy change is specified via a polytropic efficiency

$$T\,\mathrm{d}s \; = \; \left(1 - \eta_{\mathrm{pol}}^{\pm 1}\right) c_p\,\mathrm{d}T \tag{5}$$

with η_{pol}^{+1} used when $\mathrm{d}T > 0$ as in a compressor, and η_{pol}^{-1} used when $\mathrm{d}T < 0$ as in a turbine, so that $\mathrm{d}s$ is always positive. All the above relations above are combined into the definition of an entropy-complement variable $\sigma_{(T)}$, which then defines $p_{(T)}$.

$$\frac{\mathrm{d}p}{p} \; = \; \eta_{\mathrm{pol}}^{\pm 1}\,\frac{c_p}{R}\,\frac{\mathrm{d}T}{T} \; = \; \eta_{\mathrm{pol}}^{\pm 1}\,\frac{\mathrm{d}\sigma}{R} \tag{6}$$

$$\sigma_{(T)} \; \equiv \; \int_{T_s}^{T} c_{p(T)}\,\frac{\mathrm{d}T}{T} \; = \; \int_{\ln T_s}^{\ln T} c_{p(\ln T)}\,\mathrm{d}(\ln T) \tag{7}$$

$$p_{(T)} \; = \; p_0\,\exp\!\left(\eta_{\mathrm{pol}}^{\pm 1}\,\frac{\sigma_{(T)} - \sigma_{(T_0)}}{R}\right) \tag{8}$$

The compression or expansion process is assumed to occur over $p_0 \ldots p$ and $T_0 \ldots T$.

4   Properties of a gas mixture

A gas mixture is specified with the mass fraction vector $\vec{\alpha}$, whose components are the mass fractions of the mixture constituents. Similarly, the components of $\vec{R}$, $\vec{c}_p$, $\vec{h}$, $\vec{\sigma}$ are gas properties of the constituents. The overall properties are then

$$R \;=\; \vec{\alpha} \cdot \vec{R} \tag{9}$$

$$c_{p(T)} \;=\; \vec{\alpha} \cdot \vec{c}_{p(T)} \tag{10}$$

$$h_{(T)} \;=\; \vec{\alpha} \cdot \vec{h}_{(T)} \tag{11}$$

$$\sigma_{(T)} \;=\; \vec{\alpha} \cdot \vec{\sigma}_{(T)} \tag{12}$$

5   Calculations for turbomachine components

The $()_t$ total-quantity subscript will be omitted here for convenience.

5.1   Compressor

In a compressor, the total-pressure ratio between the exit station 3 and inlet station 2

$$\pi_{\mathrm{c}} \;\equiv\; \frac{p_3}{p_2} \tag{13}$$

is typically specified. The inlet conditions p_2 and T_2 are also assumed known. The objective here is to determine the corresponding exit total temperature T_3.

We first recast the specified pressure ratio definition in residual form.

$$\ln \pi_{\mathrm{c}} \;=\; \ln \frac{p_3}{p_2} \;=\; \frac{\eta_{\mathrm{pol}}}{R}\left(\sigma_3 - \sigma_2\right) \tag{14}$$

$$\mathcal{R}_{(T_3)} \;\equiv\; \frac{\sigma_{(T_3)}}{R} - \frac{\sigma_2}{R} - \frac{\ln \pi_{\mathrm{c}}}{\eta_{\mathrm{pol}}} \;=\; 0 \tag{15}$$

$$\mathcal{R}'_{(T_3)} \;\equiv\; \frac{\mathrm{d}\mathcal{R}}{\mathrm{d}T}_{(T_3)} \;=\; \frac{c_{p(T_3)}}{R T_3} \tag{16}$$

This is then solved for the unknown T_3 by the standard Newton method, with the sequence of progressively better iterates $T_3^1, T_3^2 \ldots T_3^n$. A good initial guess T_3^0 is obtained by assuming a fixed isentropic exponent $(\gamma-1)/\gamma = R/c_p$ taken from the known $()_2$ condition.

$$c_{p_2} \;=\; c_{p(T_2)} \tag{17}$$

$$T_3^0 \;=\; T_2\,\pi_{\mathrm{c}}^{R/(c_{p_2}\eta_{\mathrm{pol}})} \tag{18}$$

$$T_3^{n+1} \;=\; T_3^n - \frac{\mathcal{R}_{(T_3^n)}}{\mathcal{R}'_{(T_3^n)}} \tag{19}$$
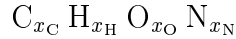
After convergence, the exit h_3 is evaluated directly.

$$h_3 \;=\; h_{(T_3)} \tag{20}$$

5.2 Combustor

In a combustor, both the inlet total temperature T_3 and exit total temperature T_4 are typically specified. The objective is to determine the fuel mass fraction which gives this temperature change.

It will be assumed that the fuel has the chemical form

$$C_{x_C}\, H_{x_H}\, O_{x_O}\, N_{x_N}$$

and the combustion reaction is limited to the fuel and atmospheric oxygen, and is complete (i.e. nitrogen oxide and carbon monoxide production is neglected).

$$C_{x_C}\, H_{x_H}\, O_{x_O}\, N_{x_N}\ +\ n_{O_2}\, O_2\ \rightarrow\ n_{CO_2}\, CO_2\ +\ n_{H_2O}\, H_2O\ +\ n_{N_2}\, N_2 \tag{21}$$

Equating the atom numbers gives the reaction mole numbers.

$$n_{O_2}\ =\ x_C\ +\ x_H/4\ -\ x_O/2 \tag{22}$$
$$n_{CO_2}\ =\ x_C \tag{23}$$
$$n_{H_2O}\ =\ x_H/2 \tag{24}$$
$$n_{N_2}\ =\ x_N/2 \tag{25}$$

Using mole numbers together with the atomic masses

$$m_C\ =\ 12.01$$
$$m_H\ =\ \ 1.01$$
$$m_O\ =\ 16.00$$
$$m_N\ =\ 14.01$$

gives the reactant masses.

$$M_{O_2}\ =\ n_{O_2}\,(2m_O) \tag{26}$$
$$M_{CO_2}\ =\ n_{CO_2}\,(m_C + 2m_O) \tag{27}$$
$$M_{H_2O}\ =\ n_{H_2O}\,(2m_H + m_O) \tag{28}$$
$$M_{N_2}\ =\ n_{N_2}\,(2m_N) \tag{29}$$
$$M_{fuel}\ =\ x_C\, m_C\ +\ x_H\, m_H\ +\ x_O\, m_O\ +\ x_N\, m_N \tag{30}$$

The reaction change fraction vector components γ_i in the following table are then calculated,

	i	α_i	β_i	γ_i
N_2	1	0.7532	0	$\eta_b\, M_{N_2}/M_{fuel}$
O_2	2	0.2315	0	$-\eta_b\, M_{O_2}/M_{fuel}$
CO_2	3	0.0006	0	$\eta_b\, M_{CO_2}/M_{fuel}$
H_2O	4	0.0020	0	$\eta_b\, M_{H_2O}/M_{fuel}$
Ar	5	0.0127	0	0
fuel	6	0	1	$1-\eta_b$

where the burner efficiency η_b is the fraction of fuel that undergoes reaction. Note that the fraction vector component sums must all be exactly unity: $\sum \alpha_i = 1$, $\sum \beta_i = 1$, $\sum \gamma_i = 1$.

The total enthalpies of all the constituents are known from the specified T_3 and T_4, and also at the known fuel temperature T_f.

$$\vec{h}_3 = h_{i(T_3)} \tag{31}$$

$$\vec{h}_4 = h_{i(T_4)} \tag{32}$$

$$\vec{h}_\mathrm{f} = h_{i(T_\mathrm{f})} \tag{33}$$

The enthalpy balance across the combustor is

$$\dot{m}_\mathrm{air}\, \vec{\alpha} \cdot \vec{h}_3 \; + \; \dot{m}_\mathrm{fuel}\, \vec{\beta} \cdot \vec{h}_\mathrm{f} \;\; = \;\; \dot{m}_\mathrm{air}\, \vec{\alpha} \cdot \vec{h}_4 \; + \; \dot{m}_\mathrm{fuel}\, \vec{\gamma} \cdot \vec{h}_4 \tag{34}$$

from which the fuel mass fraction is obtained directly.

$$f \; \equiv \; \frac{\dot{m}_\mathrm{fuel}}{\dot{m}_\mathrm{air}} \;\; = \;\; \frac{\vec{\alpha} \cdot \vec{h}_4 \; - \; \vec{\alpha} \cdot \vec{h}_3}{\vec{\beta} \cdot \vec{h}_\mathrm{f} \; - \; \vec{\gamma} \cdot \vec{h}_4} \tag{35}$$

The mass fraction vector $\vec{\lambda}$ of the combustion products is obtained from the mass balance across the combustor,

$$(\dot{m}_\mathrm{air} + \dot{m}_\mathrm{fuel})\, \vec{\lambda} \;\; = \;\; \dot{m}_\mathrm{air}\, \vec{\alpha} \; + \; \dot{m}_\mathrm{fuel}\, \vec{\gamma} \tag{36}$$

$$\vec{\lambda} \;\; = \;\; \frac{\vec{\alpha} + f\vec{\gamma}}{1 + f} \tag{37}$$

which can then be used to obtain the net properties of the combustion products.

$$R_4 \;\; = \;\; \vec{\lambda} \cdot \vec{R}_4 \tag{38}$$

$$c_{p_4} \;\; = \;\; \vec{\lambda} \cdot \vec{c}_{p_4} \tag{39}$$

5.3   Mixer

Mixing will typically occur between the combustor discharge flow and the turbine cooling flow. In general, the two streams will have two different chemical compositions specified by their mass fraction vectors $\vec{\lambda}_a$ and $\vec{\lambda}_b$, two different temperatures T_a and T_b, and two different constituent enthalpy vectors $\vec{h}_a = h_{i(T_a)}$ and $\vec{h}_b = h_{i(T_b)}$. The species mass flow balance gives the composition mass fraction vector $\vec{\lambda}$ of the mixed gas.

$$(\dot{m}_a + \dot{m}_b)\, \vec{\lambda} \;\; = \;\; \dot{m}_a\, \vec{\lambda}_a \; + \; \dot{m}_b\, \vec{\lambda}_b \tag{40}$$

$$\vec{\lambda} \;\; = \;\; \frac{\dot{m}_a\, \vec{\lambda}_a \; + \; \dot{m}_b\, \vec{\lambda}_b}{\dot{m}_a + \dot{m}_b} \tag{41}$$

Assuming no chemical reaction takes place, the enthalpy balance equation is

$$(\dot{m}_a + \dot{m}_b)\, \vec{\lambda} \cdot \vec{h}_{(T)} \;\; = \;\; \dot{m}_a\, \vec{\lambda}_a \cdot \vec{h}_a \; + \; \dot{m}_b\, \vec{\lambda}_b \cdot \vec{h}_b \tag{42}$$

which can be numerically inverted for the mixed temperature T.

5.4 Turbine

In a turbine, the total-enthalpy difference between the exit station 5 and inlet station 4 is typically known from the compressor–turbine work balance.

$$(\dot{m}_{\text{air}} + \dot{m}_{\text{fuel}})(h_5 - h_4) = \dot{m}_{\text{air}}(h_2 - h_3) \tag{43}$$

$$\Delta h \equiv h_5 - h_4 = \frac{h_2 - h_3}{1 + f} \tag{44}$$

The objective here is to determine the corresponding total-pressure ratio.

$$\pi_{\text{t}} \equiv \frac{p_5}{p_4} \tag{45}$$

The procedure is similar to that for the compressor, except that $h_{(T)}$ is used in the Newton residual.

$$\mathcal{R}_{(T_5)} \equiv h_{(T_5)} - h_4 - \Delta h = 0 \tag{46}$$

$$\mathcal{R}'_{(T_5)} \equiv \frac{d\mathcal{R}}{dT}_{(T_5)} = c_{p(T_5)} \tag{47}$$

The Newton method is started by assuming a fixed c_p taken from the known $()_4$ condition.

$$c_{p_4} = c_{p(T_4)} \tag{48}$$

$$T_5^0 = T_4 + \Delta h/c_{p_4} \tag{49}$$

$$T_5^{n+1} = T_5^n - \frac{\mathcal{R}_{(T_5^n)}}{\mathcal{R}'_{(T_5^n)}} \tag{50}$$

After convergence, the total-pressure ratio and p_5 are evaluated directly.

$$\pi_{\text{t}} = \exp\left(\frac{1}{\eta_{\text{pol}}} \frac{\sigma_{(T_5)} - \sigma_{(T_4)}}{R}\right) \tag{51}$$

$$p_5 = p_4 \, \pi_{\text{t}} \tag{52}$$

5.5 Inlet or Nozzle

An inlet or nozzle with losses can be considered as a turbine with zero efficiency, and is typically specified via a total-pressure drop ratio.

$$\pi_i \equiv \frac{p_2}{p_0} \tag{53}$$

In the limit $\eta_{\text{pol}} \to 0$, the turbine case above then reduces to the trivial relations

$$p_2 = p_0 \, \pi_i \tag{54}$$

$$T_2 = T_0 \tag{55}$$

$$h_2 = h_{(T_2)} = h_0 \tag{56}$$

with no need for Newton iteration.

Appendix: Spline representations

General

A cubic spline representation of a function $y_{(x)}$ requires the following discrete values at $i = 1, 2 \ldots N$ nodes:

$\quad x_i \qquad$ spline parameter values
$\quad y_i \qquad$ function values
$\quad y_i' \qquad$ function derivative values, $(\mathrm{d}y/\mathrm{d}x)_i$

On each interval $i-1 \ldots i$, the four end values y_{i-1}, y_i, y_{i-1}', y_i' uniquely define a cubic-polynomial $y_{(x)}$ over that interval. The union of all intervals then defines the overall $y_{(x)}$ function.

The derivative values y_i' are obtained from x_i, y_i by solving a linear system of equations expressing 2nd-derivative continuity across all the interior nodes $i = 2, 3 \ldots N-1$, together with two zero 3rd-derivative end conditions at $i = 1, N$. This system of equations produces a tridiagonal matrix which is very rapidly solved in $\mathcal{O}(N)$ arithmetic operations.

Current application

Two splines are first generated using the tabulated values T_i, c_{p_i}:

1) $c_{p(T)}$ spline:

$$
\begin{aligned}
x_i &= T_i & \text{(table values)} \\
y_i &= c_{p_i} & \text{(table values)} \\
y_i' &= (\mathrm{d}c_p/\mathrm{d}T)_i & \text{(via spline system solution)}
\end{aligned}
$$

2) $c_{p(\ln T)}$ spline:

$$
\begin{aligned}
x_i &= \ln(T_i) & \text{(table values)} \\
y_i &= c_{p_i} & \text{(table values)} \\
y_i' &= (\mathrm{d}c_p/\mathrm{d}\ln T)_i & \text{(via spline system solution)}
\end{aligned}
$$

Then two related splines $h_{(T)}$, $\sigma_{(\ln T)}$ are constructed as follows, with Δh_f being the heat of formation.

3) $h_{(T)}$ spline:

$$
\begin{aligned}
x_i &= T_i \\
y_i' &= c_{p_i} \\
y_i &= \Delta h_f + \int_{T_s}^{T_i} c_{p(T)} \; \mathrm{d}T
\end{aligned}
$$

4) $\sigma_{(\ln T)}$ spline:

$$
\begin{aligned}
x_i &= \ln(T_i) \\
y_i' &= c_{p_i} \\
y_i &= \int_{\ln T_s}^{\ln T_i} c_{p(\ln T)} \; \mathrm{d}(\ln T)
\end{aligned}
$$

Since the splined $c_{p(T)}$ and $c_{p(\ln T)}$ are piecewise-cubic, exact integrations can be used here to give perfect consistency between the related splines.