What the PROPEP 3 results mean

Understanding the PROPEP results

The results text-file is an awful mixture of metric and American units.

Included in this zip file is the very useful program 'convert.exe' This will convert metric to American and back again. It has only one error I've spotted: it thinks that 1 Bar is 14.50377 psi, whereas I think it's 14.5 psi.

Here's what the numbers mean:

The first few lines (after the date and time) say:

CODE	WEIGHT	D-H	DENS	COMPOSITION
780 NITROUS OXIDE (LIQUID) -RMN-	86.500	408	0.02680	2N 1O
866 POLYETHYLENE	13.500	-453	0.03250	2C 4H

'CODE' is the code number of the propellants in the file pepcoded.daf

'WEIGHT' is the system weight (total propellant weight), which is expressed in grams.
In the following explanations, we'll assume this is 100 grams.

'D-H' is the heat (enthalpy) of formation of the propellant in calories per gram from the file pepcoded.daf.
This can be negative, as 'zero' has been standardized at quite a high value.

'DENS' is the density of the propellant in pounds per cubic inch (this can be zero without affecting the program).

'COMPOSITION' is the molecular composition, for example Polyethylene is a repeating chain of 2 carbon atoms and 3 hydrogen atoms.

'NUMBER OF GRAM ATOMS OF EACH ELEMENT PRESENT IN INGREDIENTS'
Shows the number of gram atoms of each element present per system weight (e.g. per 100 grams)

Next come the results for the combustion chamber:

***************************CHAMBER RESULTS FOLLOW   *****************************

T(K)	T(F)	P(ATM)	P(PSI)	ENTHALPY	ENTROPY	CP/CV	GAS	RT/V
3327.	5529.	68.02	1000.00	29.18	229.93	1.2467	3.788	17.956

From left to right are: the chamber (stagnation) gas temperature in Kelvin then degrees Fahrenheit.
Next are the chamber pressure in atmospheres and pounds per cubic inch (PSI).

Next are the chamber gas's enthalpy and entropy: the enthalpy is in kilocalories per system weight and the entropy is in calories per degree Kelvin per system weight.
So if the system weight is 100 grams, multiply by 10 to get enthalpy and entropy per kilo.

CP/CV is the ratio of specific heats (γ) for the chamber gasses.

GAS identifies the number of moles of gas produced per system weight (e.g. per 100 grams).

Suppose the molecular weight (also known as the molecular mass, nowadays known as the relative molecular mass) of the combustion chamber gas was 26. Then the number of moles in 100 grams of chamber gas = 100 / 26 = 3.85 which is the value given by GAS.
Therefore the effective molecular weight is obtained by dividing the system weight (e.g. 100 grams) by GAS: 100 / 3.85 = 26
Note that although non-gases are not included in this computation this is the proper molecular weight to use in gas dynamic (rocketry) equations.

RT/V is the Universal (for any gas) gas constant R_0 (in astonishingly horrible units: 0.08205 litre-atmospheres/mole/K) times the chamber temperature in Kelvin, divided by the volume of the combustion chamber in litres. It's used later.

From the ideal gas law: $R_0 = \frac{PV}{nT}$ where P is pressure, V is volume, n is number of moles, and T is temperature in Kelvin.
So R_0 has the units of (PV)/mole/K
PROPEP uses the horrible units of atmosphere-litres for PV whereas in the metric system we'd use Pascal-cubic metres. As a Pascal has units of N/m^2 and a cubic metre has units of m^3 then multiplying the two together gives units of Nm, which are the units of Work energy, and so are equivalent to Joules.
So in metric units, the universal gas constant, is 8.314 Joules/mole/K

So multiply PROPEP's RT/V by $\frac{8.314 \times 1000}{0.08205} = 101329$ to convert to metric: J/(mole-cubic metre).

Note that from the ideal gas law, $\frac{RT}{V} = \frac{P}{n}$ i.e. $\frac{RT}{V}$ equals chamber pressure divided by the number of moles of gas in the combustion chamber.

Note that the metric value of R_0 = 8.314 Joules/mole/K is expressed per gram because moles are in grams.
So it's usual to multiply this by 1000 to get R_0 = 8314 Joules/kg mole/K
Using this larger value, we can now calculate the density ρ of the combustion chamber gasses as:

$\rho = \frac{PM}{R_0 T}$ in kg per cubic metre where ***M*** is the molecular weight calculated above.

'SPECIFIC HEAT (MOLAR) OF GAS AND TOTAL = 10.038 10.041'
This is the molar specific heat capacity (I think) in unknown units (specific means per unit mass, though this might be per gram or per kilo).
TOTAL includes any gas species that have condensed into a liquid or a solid.

'NUMBER MOLS GAS AND CONDENSED = 3.7883 0.0000'
Is again the number of moles of chamber gas per system weight (e.g. per 100 grams).
GAS is chamber gasses only (identical to the 'GAS' result given earlier), and 'CONDENSED' includes any gas species that have condensed into a liquid or a solid.

Next come a list of all the gasses that occur in the chamber in units of moles per system weight (e.g. per 100 grams). If you prefer to obtain partial pressures in atmospheres, multiply each composition by RT/V from above. Species are solid if '&' follows the name and liquid if '*' follows the name.
To obtain mole fractions, divide each composition by the total of 'GAS' plus 'CONDENSED' given above.

Then the molecular weight (molecular mass, nowadays known as relative molecular mass) of the mixture is given, as calculated above from the 'GAS' variable.

Next come the results for the gas as it exhausts from the nozzle exit:

****************************EXHAUST RESULTS FOLLOW   ****************************

The first line is the same layout as mentioned above.

The exhaust gas's enthalpy is in kilocalories per system weight (e.g. per 100 grams, in which case multiply by 10 to get it per kilo).
Note that this enthalpy may be negative, as zero enthalpy has been internationally set at a high value. Subtract the combustion chamber enthalpy from this enthalpy to get the total enthalpy drop down the nozzle (per system weight). The shifting exhaust velocity (see below) is calculated from this.

Then come the figures you really want: how the rocket is performing. PROPEP assumes an ideal nozzle (no losses and the exit pressure exactly equals the outside atmospheric pressure).

**********PERFORMANCE: FROZEN ON FIRST LINE, SHIFTING ON SECOND LINE**********

The first line gives the results assuming that the flow through the nozzle is frozen (the mixture of gasses doesn't alter down the nozzle). The next line is the shifting results (the gasses do alter as the temperature drops down the nozzle).

IMPULSE	IS EX	T*	P*	C*	ISP*	OPT-EX	D-ISP	A*M	EX-T
305.4	1.2872	2909.	37.28	4966.5		1770.77	232.1	0.15440	255.
325.1	1.2349	2983.	37.94	5051.5	198.9	2925.20	247.0	0.15704	502.

IMPULSE is the specific impulse in seconds. Multiply by 9.81 (one gee in metric) to get the exhaust velocity in metres per second.

IS EX is the isentropic exponent (ratio of specific heats, γ) for the exhaust gas at the nozzle exit. It is also the gamma that can be used anywhere along the nozzle (such as at the throat) for the frozen flow, but not the shifting flow which changes its γ all down the nozzle.
The values of the nozzle IS EX and the chamber CP/CV do not agree, because the exhaust gas is not modeled as a perfect gas.

T* and P* are the temperature (in Kelvin) and the pressure (in atmospheres) at the nozzle throat.

C* is the characteristic velocity in feet per second. The nozzle thrust coefficient C_f can be calculated from:

$$C_f = \frac{32.17 \times IMPULSE}{C^*}$$ (32.17 is one gee in American units).

ISP* is the vacuum specific impulse(in seconds) to be obtained from a sonic nozzle (no exit cone). This is used in air-breathing propulsion work (otherwise, ignore it).

OPT-EX is the area ratio (nozzle exit area over throat area) that will give you an ideal nozzle (perfect expansion to outside air pressure, no pressure thrust).

D-ISP is the density specific impulse. This is the density (don't know in what units) of the propellants times the specific impulse; it tells you how big your propellant tanks are going to be.

A*M is particularly useful: it tells you how much nozzle throat area A* you need to pass each pound (mass) per second of nozzle mass flow rate. So if you wanted your nozzle mass flow rate to be 2 pounds (mass) per second, then multiply the given A* value by 2.

A* is given in square inches per mass flow rate in pounds (mass) per second. Multiply by 0.00142232 to convert to square metres per kilo per second.

EX T is the gas temperature in Kelvin at the nozzle exit.

Good luck!
Rick Newlands, July 2013