Combustion Chamber Flow Modeling

Last Updated: 9/10/2022

## Rocket Nozzle Principles

An important principle of the converging-diverging rocket nozzle is the concept of flow choking and compressibility at high speeds. One of the biggest limiting factors on the flow of mass through the system is the choked flow through the nozzle.

The flow induced through any duct or orifice (e.g. a rocket nozzle) is governed primarily by the difference in pressure between the upstream and downstream points above and below the orifice, leaving aside the effects of the cross sectional area of the flow for a moment. Specifically, subsonic, incompressible flows are governed by the scalar difference in pressure between the entrance and the exit of the orifice. Therefore, in order to achieve higher mass flow rates, higher pressure differences are necessitated. However, after decreasing the downstream pressure past a certain point (outlined in equation 3) the flow accelerates to sonic conditions, after which the downstream conditions no longer affect the upstream flow. This condition is known as choked flow.

For a choked flow through a duct or orifice, the flow reaches a mach number of 1, or travels at the speed of sound through the fluid, at the narrowest point in the flow volume, referred to as the “throat” in a rocket nozzle. Past the throat, as the nozzle diverges, the gas is allowed to expand, decreasing drastically in pressure and density, and accelerating as it does so. This is the basic principle of a converging-diverging nozzle. This allows for the expulsion of exhaust gasses to very high, supersonic velocities necessary for rocket propulsion.

## Choked Flow Modeling

While the section above was focused primarily on the qualitative aspects of the nozzle flow, this section will focus more on the quantitative aspects and equations involved in predicting flow characteristics within the nozzle. The equations for doing so are relatively straightforward, if arithmetically tedious. For the purpose of brevity, the derivation of such equations will be spared in this document.

A convenient relation used below can relate the combustion temperature (which can be obtained as per existing flame temperature documentation [A]), the gas properties specific gas constant , and ratio of specific heats (see their respective sections below) to the chamber pressure and the mass flow rate through the nozzle. The following equation (3-24) was retrieved from page 59 of Sutton.

(1)

Where:

* is the mass flow rate in kg/s
* is the stagnation temperature at the injector, or chamber pressure, in Pa
* is the minimum area of the nozzle, or the throat area, in m^2
* is the unitless ratio of specific heats of the gas at the given temperature
* is the specific gas constant of the exhaust in J/kg-K
* is the temperature after combustion

Similarly, in the event that the mass flow rate through the injector is known, by the conservation of mass this must equal the mass flow rate through the nozzle. Thus, if the mass flow rate is known (and fixed) then the equation can be rewritten to obtain the resulting pressure:

(2)

Note that these equations assume that flow is choked. As mentioned above, the choked condition is governed by the pressure difference between the upstream and downstream conditions, provided that the mass flow rate can be increased into perpetuity to maintain a sufficiently high chamber pressure for some arbitrary throat area. The pressure difference required for the choked flow condition is defined by a critical pressure ratio, as a function of the specific heat ratio, as shown in equation 3.

(3)

…where is the critical downstream pressure (which becomes the throat pressure after upstream pressure rises above critical pressure ratio) and is the stagnation/upstream pressure. So, for example, considering a rocket nozzle at sea level where ambient pressure is about 1 bar, assuming an exhaust gas specific heat ratio of ~1.2, choked flow occurs at chamber pressures above 1.77 bar.

Since the pressure differences/ratios seen in rocketry tend to be far greater than those necessitated by this relation, assuring that flow chokes in the nozzle is not usually a concern, provided that any chamber pressure achieved is even remotely above ambient pressure.

## Fixed-Temperature Mass Flow Balancing

As mentioned above, the mass flow rate through the injector is conserved through the nozzle. Assuming for a moment that the propellant mixture ratio, and by extension combustion temperature, is not variable with pressure (not a wholly unreasonable assumption for non-cavitating propellants), the following relation can be created by pulling equation 3 from existing injector documentation[B] and assuming that, due to conservation of mass, the mass flow rate through the injector and rocket nozzle must be equal in a steady-state flow.

(4)

(5)

(6)

Equation 5 can then be rearranged to resemble a quadratic equation of the form:

(7)

…which can then be solved closed-form via the quadratic formula, or numerically using zero-finding methods. In the case of the quadratic formula, the formula can be expressed analytically as Equation 7 below.

(8)

Noting that the solution should theoretically be positive, the minus component of the plus-or-minus can be neglected in favor of simple addition.

Again, this method neglects the effect of variable pressure on combustion. While it presents a neat closed-form solution which would produce an accurate result for non-cavitating injectors with flow rates governed as such, in reality the temperature and product gas properties of the combustion reaction are affected by pressure, and as such this equation is not wholly accurate, *especially* if the chamber pressure is above the vapor pressure of one propellant but not the other (see internal reference [B] for more detail).

## Variable Temperature and Iterative Methods

Due to the cavitating flows of high vapor pressure propellants through the injector plate, the effect of pressure on combustion and exhaust gas produced, and the numerical nature of most tools/methods which yield these properties, the closed-form solution above cannot be expected to reliably predict chamber conditions. As a result, a method which can account for the variation of propellant mixture ratios, and subsequently temperature, must be selected. To this end, an iterative method was devised to converge chamber temperature, mass flow rate, and chamber pressure. The iterative method for modeling the chamber conditions is described qualitatively in Figure 1 below.



**Figure 1: Iterative Chamber Pressure Modeling Flowchart**

In this case, the approximate error can be obtained simply as the absolute value difference between the previous and current iteration of pressure divided by the current iteration of pressure, or as described in the equation below:

(9)

Where:

* is the pressure in the current iteration
* is the pressure in the previous iteration

The maximum tolerable approximate error is not something which can be necessarily calculated, but depends generally on how precise of a convergence is attainable for the computational power available and how precise of a result is required. This particular method converges relatively quickly with little computational strain, so a relative error on the order of magnitude of 0.01% or 0.001% can yield quite precise results without requiring significant computational power.

This method does not only have applications in injectors where the O/F ratio is coupled with the chamber pressure. Combustion temperature is also affected by pressure, namely due to enthalpies of vaporization of different propellants at different pressures, and especially when accounting for chemical equilibrium and minor combustion products. Thus, this method may also be employed when trying to obtain a significantly more accurate result.

## Specific Gas Constant

Unlike the universal gas constant, denoted by convention as or , nearly every equation utilized in this project uses the specific gas constant . The specific gas constant varies with the gas considered, where the universal gas constant is, of course, universal. The specific gas constant of a gas is defined as follows:

Where:

* is the specific gas constant in J/kg-K
* is the universal gas constant 8.31 J/mol-K
* is the average molar weight of the gas

This value is useful because given that molar weight is defined as the ratio below, the molar specific ideal gas law can be rearranged to the mass specific ideal gas law, which is far more useful for applications outside of chemistry.

Where:

* is the mass in kg
* is the number of moles

Thus:

This mass specific ideal gas law is what is used to derive essentially all equations relevant to this project. Therefore, it is important to be able to determine the specific gas constant of the exhaust gas. The exhaust, however will be a mixture of gasses, meaning that is not a single defined value in any chemical table. Fortunately, the molar weight of a mixture can simply be taken to be an average weighted by molar fraction. The general expression of this is:

…

Where:

* is the molar weight of component gas , usually obtainable from any chemical table or by summing the molar weights of constituent atoms as given by a periodic table
* is the molar fraction of gas within the mixture, or the amount of moles of gas divided by the total amount of moles within the mixture

Thus, the specific gas constant of the exhaust mixture becomes:

Where:

* is the *mass* fraction of gas within the mixture, or the amount of kilograms of gas divided by the total number of kilograms of the mixture.
* is the *molar* fraction of gas within the mixture, or the amount of moles of gas divided by the total amount of moles within the mixture
* is the specific gas constant of gas

## Specific Heats and Ratio of Specific Heats

For solids, the concept of specific heat is rather simple: the specific heat is the amount of thermal energy required to raise one unit mass of the substance by one unit temperature. With gasses, however, heat capacity becomes more complex. Whenever heat is added to a gas, depending on the circumstances, the thermal energy can cause the gas to expand or to raise in temperature at varying rates depending on the circumstances. Thus, enthalpy and energy are two separate ways of quantifying the energy within a gas. “Energy”, by convention, refers to the pure thermal energy within the gas. “Enthalpy”, however, refers to the thermal energy within the gas *and* the potential energy within the gas due to the pressure within the gas (i.e. the isothermal potential work the pressure within a gas of a given volume could produce). These two quantities are related as follows:

Where:

* is the mass specific enthalpy of the gas, in J/kg
* is the mass specific energy of the gas, in J/kg
* is the pressure of the gas, in Pa or J/m^3
* is the specific volume of the gas, in m^3/kg
* is the density of the gas, in kg/m^3

Note that the units Pa and N/m^2 and J/m^3 are algebraically equivalent.

There are two ways to measure the specific heat of a gas: the specific heat of a gas at constant pressure (gas is allowed to expand and some heat drives expansion), and the specific heat of a gas at constant volume (i.e. gas is not allowed to expand and all heat added goes into raising temperature). In the case of a gas, is the amount of *enthalpy* required to raise a unit mass of the gas by a unit temperature, while describes only the amount of *energy* required to raise a unit mass by a unit temperature, such that and . It is important to note that for isolated thermal systems *energy* is not conserved as defined here, but *enthalpy is*.

These specific heats are somewhat less commonly used in compressible flow modeling, particularly . Instead, the ratio of these specific heats is more commonly used. The ratio of specific heats is defined as , and is generally a unitless number a little above 1, e.g. 1.2, 1.4 for air, etc.

While CoolProp does not explicitly contain the ratio of specific heats, it does contain both and at any given temperature and pressure. and , then, can be obtained using the following commands as per CoolProp documentation [C], demonstrated below. Note that despite needing pressure as a second input variable, the ratio of specific heats generally varies primarily with temperature.

*py.CoolProp.CoolProp.PropsSI(“Cpmolar”, “P”, p, “T”, T, “fluidName”)*

*py.CoolProp.CoolProp.PropsSI(“Cvmolar”, “P”, p, “T”, T, “fluidName”)*

Since this method involves using molar-specific heat capacity, the ratio of specific heats of a mixture can be obtained by first obtaining the ratio of specific heats of each component gas and then finding the molar-weighted average specific heat ratio of the mixture as expressed in general form below in Equation 8.

…

Where:

* is the molar fraction of gas within the mixture
* is the specific heat ratio of component gas

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## References and Sources

[1] [Sutton, Rocket Propulsion Elements](https://drive.google.com/file/d/1muyScRo6bWxT6AzNZnpIaxudrqsAPFAy/view?usp=sharing)

## Related Documentation

[A] [Flame Temperature Documentation](https://docs.google.com/document/d/1d_NiXlDQG8T_QP-7L1u7jTly_aJhEoFRetvkPETi3QE/edit?usp=sharing)

[B] [Injector Flow Documentation](https://docs.google.com/document/d/1EwtdHJscOhw51d0kd1JRHDjzPgklcJx-H6rjGxaLMqE/edit?usp=sharing)

[C] [CoolProp Quick Reference](https://docs.google.com/document/d/1SwY_JbAcMK3dY37hVzANKK0KHyNtMjkAvfUAsUOoy1Y/edit?usp=sharing)