Principles of Nitrous Oxide-Ethane Combustion

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## Perfect Combustion Reaction of Nitrous Oxide and Ethane

Not accounting for chemical equilibrium in imperfect combustion, the perfect combustion formula for nitrous oxide and ethane is expressed as the following formula:

Using this formula and the second chapter of *An Introduction to Combustion*[1] (pages 9-27) a value of temperature increase can be retrieved using the thermochemical properties available from either the *CoolProp* MATLAB wrapper[A] or the thermochemical tables available at the end of *Intro to Combustion*.

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## Enthalpy of Reaction

To summarize the Enthalpy of Combustion section of Chapter 2[1], the heat of reaction (or ) can be expressed in the general form:

(1)

Where:

- is the total change in enthalpy for the given amount of products and reactants in moles

- is the molar standard enthalpy of formation of the reactants

- is the molar standard enthalpy of formation of the products

From this, the *exhaust* molar specific change in enthalpy can be expressed generally as

(2)

Where:

- is the stoichiometric coefficient of an *exhaust* product *i*

- is the molar weight in kg/mol of an *exhaust* product *i*

For our perfect combustion formula of ethane and nitrous oxide, these two equations become:

(3)

*Note that*  *is 0 since it is a diatomic gas*

## Adiabatic Flame Temperature

The generalized form for for a given is as follows:

(4)

Where:

- is the change in gas enthalpy due to the reaction

- is the total heat capacity of the exhaust products

- is the change in temperature from the initial to final temperature

Note that the value of must be obtained as , or the sum of the stoichiometric coefficient of each species times its respective molar specific heat capacity at the approximate midpoint of between the initial temperature *T0* and final temperature *Tf*. For our purposes, this *Tmid* can be assumed to be around 1500K ([1], pg 33).

So, expressing in terms of and and the perfect N2O-Ethane combustion reaction:

(5)

For perfect combustion like this, the enthalpy of combustion is assumed to be roughly equal to the enthalpy of reaction . Plugging in Equation 4 for and expressing as a molar weighted fraction of the of each product yields:

(6)

Pulling the enthalpies of formation from the *Intro to Combustion* appendix and getting the of each species from CoolProp in MATLAB allows for the calculation of a perfect adiabatic flame temperature of a stoichiometric mixture (a theoretical maximum temperature).

## Flame Temperature with an Excess Propellant

The stoichiometric adiabatic flame temperature tends to be quite high - high enough to melt the engine or subject it to undue thermal stress (bar extreme cooling measures). So, our engine will be running fuel rich - more fuel will be injected into the combustion chamber than can be combusted by the amount of oxidizer available in the combustion chamber. This means that, again neglecting minor reaction products, the fuel will remain uncombusted and absorb some excess heat.

Typically, the mix ratio of fuel is given in terms of mass, usually the variable *r*, where . For these purposes, however, a molar mix ratio is ideal. This can be found using the ratio .

Assuming that we will be running fuel rich under pretty much any circumstance (because running ox rich would cause the excess oxidizer to react with the steel in the engine), the combustion reaction can then be expressed as:

…where

In this case, the nitrous oxide can be assumed to be a constant since we’re assuming there will be excess fuel varying with a mixture ratio less than the stoichiometric mix ratio.

Plugging this new reaction back into Equation 6 yields:

(7)

Again, assuming perfect combustion, this will allow for the calculation of adiabatic flame temperature as a continuous function of the molar mix ratio up to a stoichiometric mix ratio of .

## Enthalpy of Vaporization

For any liquid at a given pressure, there is a certain amount of enthalpy (energy “input”) required to boil the liquid into a vapor. This enthalpy is referred to as the “enthalpy of vaporization”. This value is most often expressed in molar specific terms () or mass specific terms (). In other words, is the amount of enthalpy required to vaporize a mole of water already at saturation pressure and temperature.

Most gasses in our exhaust products do not need to account for enthalpy absorbed by vaporization - water, however, may initially form as a liquid and absorb enthalpy until it becomes steam.

Assuming different levels of water vaporization immediately after combustion produces two possible values of heat produced: the “upper heating value”, in which it is assumed that no enthalpy is absorbed by water vaporization (i.e. ), and the “lower heating value”, in which it is assumed that all the water absorbs all the theoretically possible enthalpy produced by vaporization. The lower heating value can be acquired by simply subtracting the number of moles of water times the molar specific enthalpy of vaporization of water at the given pressure (which can be retrieved from CoolProp), as in Equation 8.

(8)

In this case, for caution’s sake, we will be using the upper heating value to provide a worst-case estimate of the combustion temperature. Building an engine around an estimate of the temperature that is higher than the actual experimental temperature is safer than building one around a lower temperature

## Other Vaporization Considerations

Water is not the only fluid in this reaction which is expected to change phases. Both liquid propellants are stored relatively near their vapor pressure for our purposes, and once injected and subjected to the heat of the gas in the combustion chamber, will evaporate and absorb some amount of enthalpy. This means that regardless of our heating value, our propellants will evaporate and effectively lower our total enthalpy of reaction. Note that just as the molar enthalpy of vaporization of water can be found using CoolProp for water, so too can the enthalpy of vaporization be found for nitrous oxide and ethane.

Since in this case we are modeling combustion using a chemical formula, the enthalpy of combustion using the upper heating value including vaporization effects can be written as Equation 9.

(9)

…and the enthalpy of combustion using the *lower* heating value can be expressed as in Equation 10.

(10)

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## References and Sources

[1] [Introduction to Combustion](https://drive.google.com/file/d/1V93_c_ekuT-lM256LfNEVRspmNPMu8Vh/view?usp=sharing)

## Related Documentation

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