

WHEN YOU NEED TO BE SURE

SGS

CyFlex® Knowledge Article

Determining Gas Mixture Composition

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Objective

Compute the mass flow rates for each of three supply gases that can be blended to produce a single gas mixture which meets two desired gas characteristics. The two characteristics of the blended gas are Methane Number and Lower Heating Value. The mixture will be supplied to an engine as a gaseous fuel. The desired values of Methane Number and Heating Value will be varied during a test to investigate engine performance.

Inputs

1. Composition of each of the three supply gases. These are available as CyFlex composition variables.
2. The desired Heating Value. This can be expressed as either heating value per unit of mass or volume. The specification file will allow this to be entered either way as CyFlex real variables.
3. The desired Methane Number for either. This is available as a CyFlex real variable. The target Methane Number could be for rich burn or lean burn. Specify both and a selector to say which one to use.
4. The identification of the input and output variables is through a specification file that the application reads when it is launched and initialized. The filename will be a command line input.
5. A CyFlex periodic timer event to trigger a periodic evaluation to compute the desired outputs.
6. Desired priority of the application.
7. Optional command line argument to indicate whether or not the application should be considered to be "critical" by the `scheduler` app.

Outputs

1. Desired mass fractions of each of the three supply gases.
2. The composition of the desired mixture. This will be output as a CyFlex composition variable.
3. The computed methane number of the mixture. This will be output as a CyFlex real variable. Both the rich and lean burn Methane Numbers should be output. If the target Methane Number is not achievable, the closest value at the target heating value will be output.
4. The heating value for each of the component gases should be output both per unit mass and per unit standard volume. Might want to only output the min and max. Both the rich and lean burn Methane numbers at the ends of the line of constant heating value should be output. The target Methane number would have to be bounded by these values.

Process Requirements

The application will register with the scheduler task and can be run as "critical" if specified on the command line.

Inputs and outputs will be converted to or from SI units so that internal computations are done in base-SI units.

Computational Method

The mixing equation for non-reacting gas streams may be written as:

$$a(y_{A,a}A + y_{B,a}B + y_{C,a}C + \dots) + b(y_{A,b}A + y_{B,b}B + y_{C,b}C + \dots) + \dots \quad \text{ter.1}$$

$$\Rightarrow \alpha(y_A A + y_B B + y_C C + \dots)$$

where:

a , b , ... are the number of moles per unit time in the gas streams being mixed and α is the number of moles in the resulting mixture.

$y_{X,i}$ is the mole fraction of component X in the i th stream.

The mole flow rates may be determined from the measured stream mass flow rates and the calculated stream molecular weights using:

$$a = \frac{\dot{m}_a}{M_a} \quad b = \frac{\dot{m}_b}{M_b} \quad \dots \quad \text{ter.2}$$

The molecular weight of a given stream may be calculated using

$$M_a = y_{A,a}M_A + y_{B,a}M_B + \dots \quad \text{ter.3}$$

$$M_b = y_{A,b}M_A + y_{B,b}M_B + \dots$$

$$\vdots$$

where

M_A, M_B, \dots = molecular weight of the various stream components.

Mass is conserved in the mixing process, so we can write

$$\dot{m}_\alpha = \dot{m}_a + \dot{m}_b + \dots \quad \text{ter.4}$$

Since no reactions take place, the total number of moles is conserved and we can write

$$\alpha = a + b + \dots \quad \text{ter.5}$$

Since no reactions take place, the number of moles of each component is also conserved and we can write

$$\begin{aligned} \alpha y_A &= \alpha y_{A,a} + b y_{A,b} + \dots && \text{ter.6} \\ \alpha y_B &= \alpha y_{B,a} + b y_{B,b} + \dots \\ &\vdots \end{aligned}$$

Because of the generalized treatment we have presented, it is not possible at this point to make a meaningful statement about the number of equations we have derived and the number of unknowns we might have to solve for. In real-world applications, we will be faced with a variety of scenarios. We may know one or more of the mass flow rates, the ratio of various mass flow rates, the concentration on a wet or a dry basis of a given component in one or more streams or perhaps the composition of all but one stream. For an example of a useful application of this generalized approach, see [Exhaust Gas Recirculation \(EGR\) Calculations](#).

The ASME document “Standard Practice for Calculating Heat Value, Compressibility Factor, and Relative Density of Gaseous Fuels, Designation: D3588-98 (Reapproved 2011)”, lists the molar masses and heating values for many of the components of natural gas, which allows us to calculate the heating value per unit mass of a natural gas mixture using

$$HVM = \frac{\sum_{j=1}^n y_j M_j H_{m,j}}{\sum_{j=1}^n y_j M_j} \quad \text{ter.7}$$

The heating value per unit standard volume is given by

$$HVV = \sum_{j=1}^n y_j H_{v,j} \quad \text{ter.8}$$

The ASME document lists both the higher and lower heating values and in the above formulas, we make no distinction between the two. The customer is only interested in the lower heating values for this application, so only those values will be calculated.

By definition, the sum of the mole fractions of the three component gases must equal one, so we can solve for the mole fraction of one of the gases in terms of the other two.

$$1 = a + b + c \Rightarrow a = 1 - b - c \quad \text{ter.9}$$

The mole fraction of any component gas in the final mixture is given by

$$y_j = a y_{j,a} + b y_{j,b} + c y_{j,c} \quad \text{ter.10}$$

Combining the above two equations gives

$$\begin{aligned} y_j &= (1 - b - c) y_{j,a} + b y_{j,b} + c y_{j,c} && \text{ter.11} \\ &= y_{j,a} + b (y_{j,b} - y_{j,a}) + c (y_{j,c} - y_{j,a}) \end{aligned}$$

Substituting this result into the equation for heating value per unit mass gives us

$$HVM = \frac{\sum_{j=1}^n [y_{ja} + b(y_{jb} - y_{ja}) + c(y_{jc} - y_{ja})] M_j H_{mj}}{\sum_{j=1}^n [y_{ja} + b(y_{jb} - y_{ja}) + c(y_{jc} - y_{ja})] M_j} \quad \text{ter.12}$$

or

$$\begin{aligned} HVM \sum_{j=1}^n y_{ja} M_j + b HVM \sum_{j=1}^n (y_{jb} - y_{ja}) M_j + c HVM \sum_{j=1}^n (y_{jc} - y_{ja}) M_j & \quad \text{ter.13} \\ = \sum_{j=1}^n y_{ja} M_j H_{mj} + b \sum_{j=1}^n (y_{jb} - y_{ja}) M_j H_{mj} + c \sum_{j=1}^n (y_{jc} - y_{ja}) M_j H_{mj} \end{aligned}$$

Solving this equation for the mole fraction of component gas b in terms of the target HVM and the mole fraction of component gas c gives.

$$b = \frac{\sum_{j=1}^n y_{ja} M_j H_{mj} - HVM \sum_{j=1}^n y_{ja} M_j + c \left[\sum_{j=1}^n (y_{jc} - y_{ja}) M_j H_{mj} - HVM \sum_{j=1}^n (y_{jc} - y_{ja}) M_j \right]}{HVM \sum_{j=1}^n (y_{jb} - y_{ja}) M_j - \sum_{j=1}^n (y_{jb} - y_{ja}) M_j H_{mj}} \quad \text{ter.14}$$

Essentially the same result can be found by solving for c

$$c = \frac{\sum_{j=1}^n y_{ja} M_j H_{mj} - HVM \sum_{j=1}^n y_{ja} M_j + b \left[\sum_{j=1}^n (y_{jb} - y_{ja}) M_j H_{mj} - HVM \sum_{j=1}^n (y_{jb} - y_{ja}) M_j \right]}{HVM \sum_{j=1}^n (y_{jc} - y_{ja}) M_j - \sum_{j=1}^n (y_{jc} - y_{ja}) M_j H_{mj}} \quad \text{ter.15}$$

We would like to find the values of a, b and c on the ‘boundaries’ where the mole fraction of one component gas is zero. The line of constant heating value will intersect only two of the boundaries. On the remaining boundary, one of the mole fractions will be negative, so that combination can be ignored. If we set a=0, we can solve for either b or c using

$$c = \frac{\sum_{j=1}^n y_{jb} M_j H_{mj} - HVM \sum_{j=1}^n y_{jb} M_j}{\sum_{j=1}^n y_{jb} M_j H_{mj} - HVM \sum_{j=1}^n y_{jb} M_j - \sum_{j=1}^n y_{jc} M_j H_{mj} + HVM \sum_{j=1}^n y_{jc} M_j} \Bigg|_{a=0, b=1-c} \quad \text{ter.16}$$

or

$$b = \frac{\sum_{j=1}^n y_{jc} M_j H_{mj} - HVM \sum_{j=1}^n y_{jc} M_j}{\sum_{j=1}^n y_{jc} M_j H_{mj} - HVM \sum_{j=1}^n y_{jc} M_j - \sum_{j=1}^n y_{jb} M_j H_{mj} + HVM \sum_{j=1}^n y_{jb} M_j} \quad \left. \vphantom{b} \right|_{a=0, c=1-b} \quad \text{ter.17}$$

On the boundary where $b=0$, we can find c using

$$c = \frac{\sum_{j=1}^n y_{ja} M_j H_{mj} - HVM \sum_{j=1}^n y_{ja} M_j}{HVM \sum_{j=1}^n (y_{jc} - y_{ja}) M_j - \sum_{j=1}^n (y_{jc} - y_{ja}) M_j H_{mj}} \quad \left. \vphantom{c} \right|_{b=0, a=1-c} \quad \text{ter.18}$$

On the boundary where $c=0$, we can solve for b using

$$b = \frac{\sum_{j=1}^n y_{ja} M_j H_{mj} - HVM \sum_{j=1}^n y_{ja} M_j}{HVM \sum_{j=1}^n (y_{jb} - y_{ja}) M_j - \sum_{j=1}^n (y_{jb} - y_{ja}) M_j H_{mj}} \quad \left. \vphantom{b} \right|_{c=0, a=1-b} \quad \text{ter.19}$$

$$HVV = \sum_{j=1}^n [y_{ja} + b(y_{jb} - y_{ja}) + c(y_{jc} - y_{ja})] H_{vj} \quad \text{ter.20}$$

$$b = \frac{HVV - \sum_{j=1}^n [y_{ja} + c(y_{jc} - y_{ja})] H_{vj}}{\sum_{j=1}^n (y_{jb} - y_{ja}) H_{vj}} \quad \text{ter.21}$$

$$c = \frac{HVV - \sum_{j=1}^n [y_{ja} + b(y_{jb} - y_{ja})] H_{vj}}{\sum_{j=1}^n (y_{jc} - y_{ja}) H_{vj}} \quad \text{ter.22}$$

$$b = \frac{HVV - \sum_{j=1}^n y_{jc} H_{vj}}{\sum_{j=1}^n y_{jb} H_{vj} - \sum_{j=1}^n y_{jc} H_{vj}} \quad \left. \vphantom{b} \right|_{a=0, c=1-b} \quad \text{ter.23}$$

$$c = \frac{HVV - \sum_{j=1}^n y_{jb} H_{vj}}{\sum_{j=1}^n y_{jc} H_{vj} - \sum_{j=1}^n y_{jb} H_{vj}} \quad \left| \begin{array}{l} \text{ter.24} \\ a=0, b=1-c \end{array} \right.$$

$$b = \frac{HVV - \sum_{j=1}^n y_{ja} H_{vj}}{\sum_{j=1}^n y_{jb} H_{vj} - \sum_{j=1}^n y_{ja} H_{vj}} \quad \left| \begin{array}{l} \text{ter.25} \\ c=0, a=1-b \end{array} \right.$$

$$c = \frac{HVV - \sum_{j=1}^n y_{ja} H_{vj}}{\sum_{j=1}^n y_{jc} H_{vj} - \sum_{j=1}^n y_{ja} H_{vj}} \quad \left| \begin{array}{l} \text{ter.26} \\ b=0, a=1-c \end{array} \right.$$

$$x_z = \frac{\dot{m}_z}{\dot{m}_{total}} = z \frac{\sum_{j=1}^n y_{jz} M_j}{\sum_{j=1}^n y_j M_j} \quad \text{ter.27}$$

$$\text{if } (MN(b_{1,boundary}) \geq MN(b_{2,boundary})) \text{ then } (b_1 = b_{hi}, b_2 = b_{lo}) \text{ else } (b_2 = b_{hi}, b_1 = b_{lo}) \quad \text{ter.28}$$

$$b_{new} = \frac{b_{hi} + b_{lo}}{2} \quad \text{ter.29}$$

$$\text{if } (MN(b_{new}) - MN_{target} > 0) \text{ then } (b_{hi} = b_{new}, b_{lo} = b_{lo}) \text{ else } (b_{hi} = b_{hi}, b_{lo} = b_{new}) \quad \text{ter.30}$$

Calculate and save $\sum_{j=1}^n y_j M_j H_{mj}$ and $\sum_{j=1}^n y_j M_j$ for each of the component gases. Calculate

the HVM for each component gas using ter.7 and the stored values from the previous step. Update the minimum and maximum allowable target heating value variables based on the minimum and maximum HVM values for the component gases.

Calculate and save $\sum_{j=1}^n (y_{jb} - y_{ja})M_j$, $\sum_{j=1}^n (y_{jb} - y_{ja})M_j H_{mj}$, $\sum_{j=1}^n (y_{jc} - y_{ja})M_j$ and

$\sum_{j=1}^n (y_{jc} - y_{ja})M_j H_{mj}$ for use in subsequent calculations.

Calculate the values of a, b and c for the target HVM when one of the component gas mole fractions is zero using equations ter.17, ter.18 and ter.19 to define the end points of a line of constant HVM that touch the mixture 'boundaries'. One of the three equations should produce a negative mole fraction. The line of constant HVM does not touch that boundary. Theoretically, there is a possibility that component gases could be specified that would have two identical values of HVM on one boundary. This is very unlikely to happen if this task is used for its intended use and we will not try to handle this condition until we find it causes a problem.

Calculate the mole fraction of each species in the gas mixture formed by the combinations of a, b and c that have endpoints on the boundaries using ter.10. Use these values to calculate the customer Methane Index Number, MN , for the combinations of a, b and c that have endpoints on the boundaries using the equations specified in the [Methane Index Calculation - Version 8 8_Rev07](#) document.

We can be confident that the target MN can be achieved if it is bracketed by the values at the endpoints. Update the minimum and maximum MN boundary output variables using the endpoint values.

The value of MN is not linear between the endpoints and it is theoretically possible to have a combination of component gases along the line of constant HVM that would have a MN value outside the endpoints. In that case, is possible that the interval halving method we are about to use will not find the value closest to the target along the line of constant HVM. Again, this is unlikely to happen with reasonable component gas selections, so we will not deal with the possibility at this time.

Arrange the values of b according to the logic in ter.28, then calculate a new value for b at the midpoint using ter.29. Use ter.15 to calculate a new value of c at the midpoint and ter.9 to calculate the corresponding value of a. Use the new values to calculate MN at the midpoint.

Use the logic in ter.30 to shift the endpoints to bracket the half of the segment that contains the MN value closest to the target. Calculate a new value for b at the midpoint using ter.29. Continue iterating until the value of MN from one iteration to the next changes less than a specified amount.