Introduction to Numerical Optimization – Project

Data reconciliation of an industrial boiler

We consider an industrial boiler system whose purpose is to turn water into steam to spin steam turbines. The boiler consists of a burner and a heat exchanger. In Section A., the project focuses on the burner, where the combustion of natural gas and air takes place. In Section B., the project adds a heat exchanger which uses the hot exhausts from the burner to heat water. Data reconciliation is used to provide accurate measurements which fulfill material and energy conservation laws.

A. Burner

Cf. Figure 1, natural gas and air enter a combustion chamber inside the burner where they are ignited. The natural gas is a mixture of methane (CH_4), ethane (C_2H_6) and propane (C_3H_8).
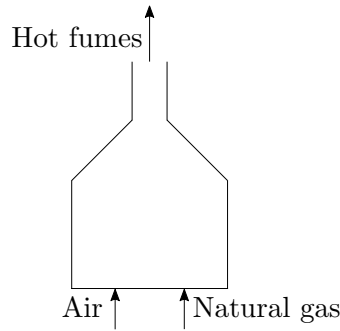
Figure 1: Burner

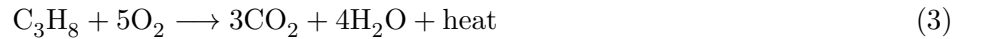Each hydrocarbon combustion reaction is summarized as follows:

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O + \text{heat} \tag{1}$$

$$2C_2H_6 + 7O_2 \longrightarrow 4CO_2 + 6H_2O + \text{heat} \tag{2}$$

$$C_3H_8 + 5O_2 \longrightarrow 3CO_2 + 4H_2O + \text{heat} \tag{3}$$

(1) reads: one mole of methane reacts with 2 moles of dioxygen (or *oxygen* for short) to form one mole of carbon dioxide and 2 moles of water vapor. However the burner does not have pure oxygen at its disposal, but can instead use air which is composed of 21% oxygen (O_2) and 79% nitrogen (N_2). The actual combustion reactions become

$$CH_4 + 2\left(O_2 + \frac{79}{21}N_2\right) \longrightarrow CO_2 + 2H_2O + 2\frac{79}{21}N_2 + \text{heat} \tag{4}$$

$$2C_2H_6 + 7\left(O_2 + \frac{79}{21}N_2\right) \longrightarrow 4CO_2 + 6H_2O + 7\frac{79}{21}N_2 + \text{heat} \tag{5}$$

$$C_3H_8 + 5\left(O_2 + \frac{79}{21}N_2\right) \longrightarrow 3CO_2 + 4H_2O + 5\frac{79}{21}N_2 + \text{heat} \tag{6}$$
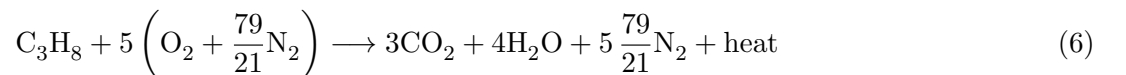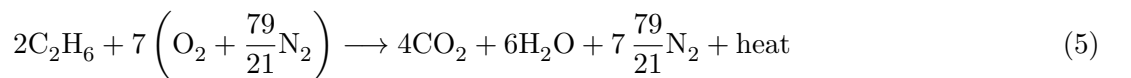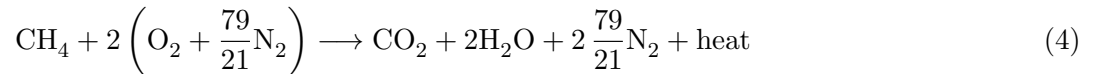
These equations ignore many effects, among which:

- at temperatures above 1400°C, oxygen and nitrogen may undergo an endothermic reaction inside the burner, producing various nitrogen oxides (NO_x), a major air pollutant;

- if there is not enough oxygen in the reactants, the combustion may be *incomplete* and release some toxic carbon monoxide (CO) instead of CO_2;

- in practice process engineers design the burners to use a slight excess of air to guarantee a complete combustion, and may preheat or superoxygenate air to improve efficiency.

Process engineers need reliable measurements to be able to meticulously adjust the burner to improve efficiency with as little harmful impact as possible on individuals and on the environment. This is the aim of the data reconciliation of this project.

All gases are assumed to obey the ideal gas law

$$PV = nRT$$

where P is the pressure in [atm], V is the volume in [m^3], n is the amount of substance in [mol], R is the gas constant ($8.2057 \times 10^{-5}\,m^3 \cdot atm \cdot K^{-1} \cdot mol^{-1}$) and T is the absolute temperature in [K].

The pressures and temperatures take the constant values depicted on Table 1.

Substance	Pressure	Temperature
Natural gas	1 atm	25 °C
Air	1 atm	25 °C
Hot fumes	1 atm	1600 °C

Table 1: Fixed temperatures and pressures

The amount of moles n in [mol] and the mass m in [g] of a substance (mixture or constituent of a mixture) are linked by

$$n = \frac{m}{M}$$

where M in [$g \cdot mol^{-1}$] is the molar mass, a physical property of the substance. Table 2 provides the molar mass of all the constituents needed throughout the project.

Substance	Molar mass	Substance	Molar mass
C	$12.0107\,g \cdot mol^{-1}$	CH_4	$16.042\,46\,g \cdot mol^{-1}$
H	$1.007\,94\,g \cdot mol^{-1}$	C_2H_6	$30.069\,04\,g \cdot mol^{-1}$
O	$15.9994\,g \cdot mol^{-1}$	C_3H_8	$44.095\,62\,g \cdot mol^{-1}$
N	$14.0067\,g \cdot mol^{-1}$	Air	$28.850\,334\,g \cdot mol^{-1}$
O_2	$31.9988\,g \cdot mol^{-1}$	CO_2	$44.0095\,g \cdot mol^{-1}$
N_2	$28.0134\,g \cdot mol^{-1}$	H_2O	$18.015\,28\,g \cdot mol^{-1}$

Table 2: Molar masses

There are several ways to describe the relative quantities of constituents in a mixture (e.g. hydrocarbons in the natural gas mixture, or all the products in the hot fumes mixture):

- the mass fraction w_i in [wt%] is the ratio of one constituent with mass m_i in [g] to the mass of the total mixture m in [g], defined as $w_i = \frac{m_i}{m}$, with $\sum_i m_i = m$ and $\sum_i w_i = 1$;

- the mole fraction or molar fraction $x_i = \frac{n_i}{n}$ in [mol%], where n_i in [mol] is the amount of moles of the constituent and n in [mol] is the amount of moles of the total mixture, with $\sum_i n_i = n$ and $\sum_i x_i = 1$;

- the volume fraction $\phi_i = \frac{V_i}{V}$ in [vol%], where V_i in [m^3] is the volume of the constituent and V in [m^3] is the volume of the total mixture, with $\sum_i V_i = V$ (for ideal gases and ideal solutions) and $\sum_i \phi_i = 1$.

For ideal gases and ideal solutions, we have the following properties:

- the volumes of the constituents are additive (the volume of the mixture is equal to the sum of the volumes of its constituents);

- the volume fraction ϕ_i is equal to the molar fraction x_i.

Conversions between mass and molar fractions:

$$x_i = w_i \frac{M}{M_i} = \frac{\frac{w_i}{M_i}}{\sum_i \frac{w_i}{M_i}}$$

$$w_i = x_i \frac{M_i}{M} = \frac{x_i M_i}{\sum_i x_i M_i}$$

where M_i is the molar mass of the constituent and M is the average molar mass of the mixture, defined as

$$M = \sum_i x_i M_i \quad \text{or} \quad \frac{1}{M} = \sum_i \frac{w_i}{M_i}.$$

Volumetric flow meters measure the volumetric flow rate in $[\text{m}^3\cdot\text{s}^{-1}]$ of all mixtures at every time period t. Non-dispersive infrared spectrometers measure the mass fraction of all constituents of the natural gas and hot fumes at the same time periods t.

To help gradually build the model, two simplifications are proposed:

 (i) the infrared spectrometers perform an exact measurement of all mass fractions and the measurement value is the same at all t, hence they need not be reconciled;

 (ii) the natural gas mixture is only composed of methane.

All models must be written in JuMP.

1. Assume (i) and (ii). Write a linear reconciliation model to fulfill the material conservation law of the burner. Solve it with the `q1.jld` dataset.

2. Assume (i) but not (ii), i.e. the natural gas is composed of all three hydrocarbons. Write a linear reconciliation model to fulfill the material conservation law of the burner. Solve it with the `q2.jld` dataset.

3. Make neither the (i) nor the (ii) simplification. Write a linear reconciliation model to fulfill the material conservation law of the burner. Solve it with the `q3.jld` dataset.

4. Plot the corrections and interpret.

5. Use an Euclidean norm for the reconciliation objective function. Convert your model to a conic program.

6. Volumes are additive for ideal gases and ideal solutions. Use sensitivity information to figure out whether the natural gas or the exhaust is most impacted if volume additivity does not hold.

B. Heat exchanger

In this Section, the temperature of the hot fumes T_{HF} must be an unknown variable.

Reactant	Heat of combustion
CH_4	$802.34\,\text{kJ}\cdot\text{mol}^{-1}$
C_2H_6	$1437.2\,\text{kJ}\cdot\text{mol}^{-1}$
C_3H_8	$2044.2\,\text{kJ}\cdot\text{mol}^{-1}$

Table 3: Amounts of heat released

We consider the energy conservation law. Table 3 provides the amount of heat released by the combustion of one mole of CH_4, C_2H_6 and C_3H_8 respectively, cf. the reactions (4), (5) and (6). We assume that there is no heat loss, so the total heat Z in [kJ] is absorbed by the products CO_2, H_2O and N_2 to raise their temperature to T_{HF} according to

$$Z = n_{CO_2} \Delta H_{CO_2}(T_{HF}) + n_{H_2O} \Delta H_{H_2O}(T_{HF}) + n_{N_2} \Delta H_{N_2}(T_{HF})$$

where n_i is the amount of moles of product, and $\Delta H_i(T_{HF})$ in [kJ·mol^{-1}] is the amount of heat per mole of product which must be absorbed to reach a temperature of T_{HF}. The expression of $\Delta H_i(t)$ is

$$\Delta H_i(t) = At + Bt^2/2 + Ct^3/3 + Dt^4/4 - E/t + F - H \tag{7}$$

where t is the absolute temperature in [10^3 K] and the coefficients[1, 2, 3] are defined in Table 4.

	CO$_2$	H$_2$O	N$_2$
A	58.166 39	41.964 26	19.505 83
B	2.720 074	8.622 05	19.887 05
C	−0.492 289	−1.499 780	−8.598 535
D	0.038 844	0.098 119	1.369 784
E	−6.447 293	−11.157 64	0.527 601
F	−425.9186	−272.1797	−4.935 202
G	263.6125	219.7809	212.3900
H	−393.5224	−241.8264	0.0

Table 4: Coefficients of the polynomials

7. Add the energy conservation laws of T_{HF} to the model and solve it. What is the type of the problem? You may want to try to provide a starting value for certain variables[4].

8. Write an appropriate linearization of your previous model and discuss.
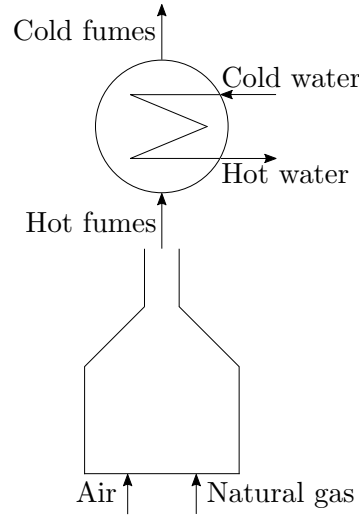

Figure 2: Burner and heat exchanger

On Figure 2 a heat exchanger uses the hot exhausts from the burner to heat water. As they go through the heat exchanger, the hot fumes transfer energy to the water which heats and vaporizes into water vapor (steam). We assume that the temperature of the fumes decrease by 600 °C. The pressure remains at 1 atm. Since the composition of the 'cold' fumes is the same as the hot fumes', (7) can be reused, for the temperature $T_{HF} - 600$.

9. Implement in the model the balances of the cold fumes. Give the energy transfered to the water.

References

[1] CO$_2$. https://webbook.nist.gov/cgi/cbook.cgi?ID=C124389&Units=SI&Mask=1#Thermo-Gas.

[2] H$_2$O. https://webbook.nist.gov/cgi/cbook.cgi?ID=C7732185&Units=SI&Mask=1#Thermo-Gas.

[3] N$_2$. https://webbook.nist.gov/cgi/cbook.cgi?ID=C7727379&Units=SI&Mask=1#Thermo-Gas.

[4] Starting value. http://www.juliaopt.org/JuMP.jl/stable/refvariable.html?highlight=start.