SSA 3

Model adjustments

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Goal

- In the previous assignment, Dolf and Thomas made a theoretical pressure volume diagram and a thermodynamic model to accompany it. In this model, they worked with mass ratios of fuels were they should have been volume ratios. Furthermore, they did not manage to find the correct fuel stoichiometric ratio. The goal of this assignment is to correct these two issues.

Conclusion

- The fixes have been made with satisfactory results. The problem pointed out by Dolf has also been solved.

Problems

- Dolf correctly pointed out that in the first version of this SSA, the amount of oxygen needed to combust the fuel was determined by making an arbitrary 'average molecule' of fuel. This method is inconsistent with reality and is not allowed to be used. The combustion reactions need to be treated separately and combined afterwards.

Follow up Steps

- The best course of action is to start working on how to present our findings in the interim presentation and in the report.
- In case we have not yet completed everything we should have done before the interim presentation, we should do so as well (think of the gathering of the data for the experimental analysis or further emission research).

Work Division

- It was the collective responsibility of Alexandra, Lars and I to fix some issues with the model. We divided it as such that I had to fix the problem of volume and mass ratios. Whilst I was working on this problem, I saw that the air to fuel ratio had not yet been determined properly and considering that my SSA would otherwise be quite short, I opted to do it. Needless to say, before I did this, I counselled the WhatsApp group.

Time Division

- Fixing the volume and mass ratios: two hours (This could have been done faster)
- Fixing the stoichiometric ratio and the air to fuel ratio: one hour.
- Writing the SSA: fifteen minutes
- Resolving issues pointed out by Dolf: thirty minutes
- Total: 3,75 hours.

Overleaf Link

1 Explanation fixes

1.1 Volume and mass ratios

Initially, all calculations were done using mass ratios. However, it was later discovered that the literature presents all ratios in the form of volume ratios. This means the volume ratios had to be recomputed into mass ratios in order to make the model function properly again. Furthermore, for the combustion computations it is also important to know the molar ratios of the fuel, air and combustion products.

Multiplying the volume ratios with the densities yields the mass ratios.

$$V \cdot \rho = m_{nonunity}$$

However, these ratios do not add up to unity. In order to do so, every element in the matrix has to be divided by the sum of each element.

$$\frac{m_{nonunity}}{\sum m} = m$$

This results in the proper mass ratio.

In order to compute the molar ratios, the mass ratio needs to be divided by the molar mass.

$$\frac{m}{M} = N_{nonunity}$$

Similarly as before, these ratios do not add up to unity. Therefore, each element in this matrix is - once again - divided by the sum of all elements.

$$\frac{N_{nonunity}}{\sum N} = N$$

This leaves the correct molar ratio.

1.2 AF ratio

In order to find the stoichiometric air to fuel ratio, in the following chemical reactions are used. For octane

$$2C_8H_18_{(l)} + 25O_{2(g)} \rightarrow 16CO_{2(g)} + 18H_2O_{(g)}$$

And for ethanol

$$C_2H_5OH_{(l)} + 3O_{2(g)} \rightarrow 2CO_{2(g)} + 3H_2O_{(g)}$$

The total amount of oxygen - and therefore air - needed depends on the molar ratios of the fuel molecules. The amount of moles of oxygen needed to combust one mole of fuel mixture can then be computed using the molar ratios in the fuel.

$$N_{O2/fuel} = \frac{25}{2}N_{oct} + 3N_{eth}$$

The molar mass of the combined fuel can also be computed in a very similar way, using the molar masses of octane and ethanol.

$$M_{fuel} = 114.232N_{oct} + 30.07N_{eth}$$

The fuel consumption can be found in the data sheet in kilogrammes per second.

By using the molar ratio of oxygen to fuel, followed by the mass ratios of nitrogen to oxygen in the air and carbon dioxide to oxygen in the air, the stoichiometric air to fuel ratio can be computed using the following formula.

$$AF_{stoi} = N_{O2/fuel}(M_{O2} + m_{N2/O2}M_{N2} + m_{CO2/O2}M_{CO2})M_{fuel}^{-1}$$

The stoichiometric ratio has been found to be 14,8946.