Project report

PAH in diesel: exploration

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Introduction

The purpose of this project is to determine suitable SFC×GC parameters for the quantification of PAHs in diesel. I want to use a short (2 s) collection period, to provide good resolution in the SFC dimension.

Experimental

Samples

I used the samples used by Elize Smit for her PhD research, for which I have information about aromatic content.

I performed 3 runs, with the following samples.

1. US 2D Reference Fuel
2. US 2D Reference Fuel
3. US 2D Reference Fuel
4. Swedish diesel

Conditions.

I used a 2 s modulation period. Otherwise conditions as in the parameter files.

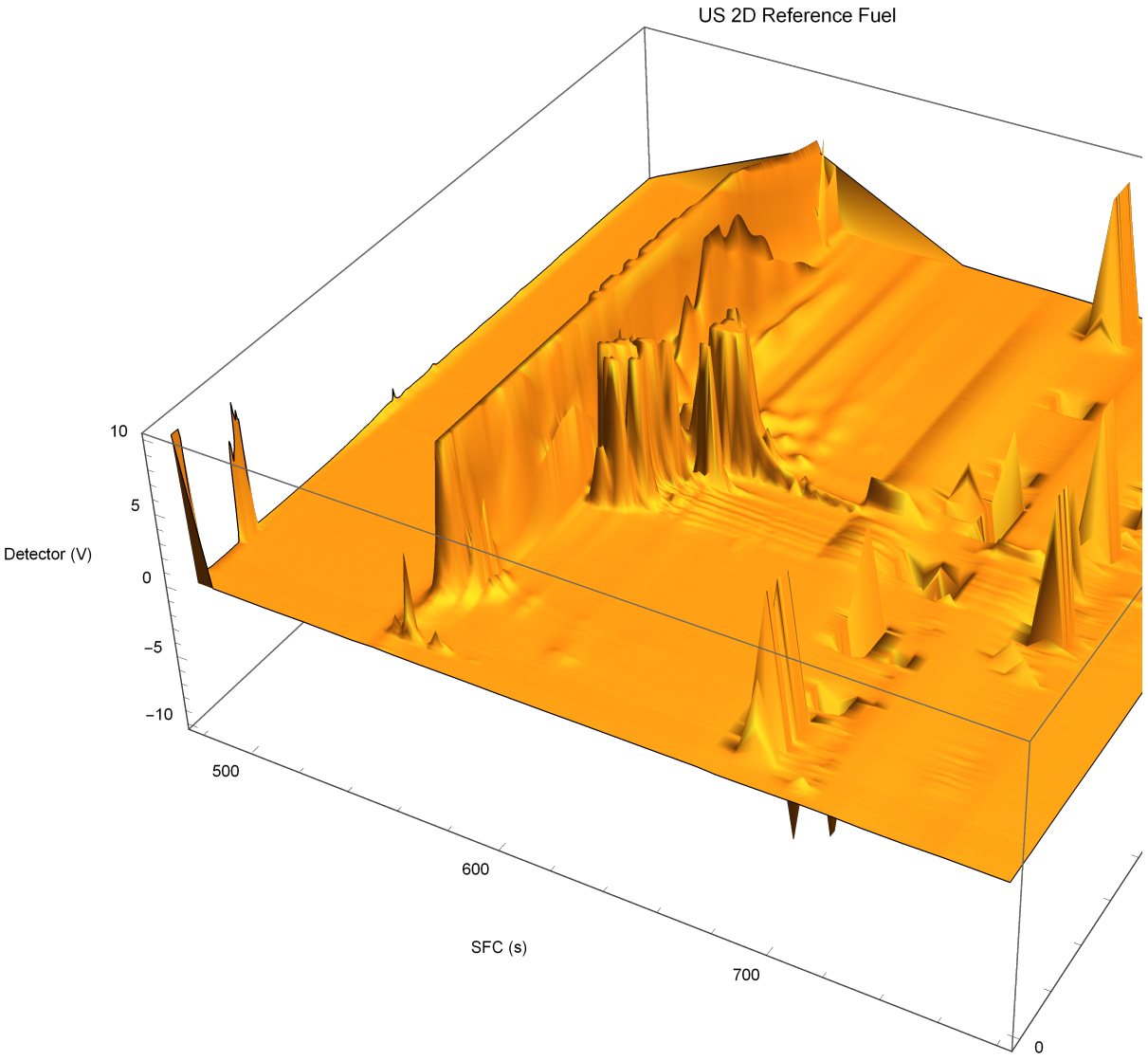
Results

Chromatograms

Run 1: US 2D reference fuel

C:\Users\fskdm\My PhD\Projects\2019_12_20_PhD_Last_Project\2019_12_23_PAH_FAMEs\Chromatograms\RawData\2020_01_20-191859.dat.prm

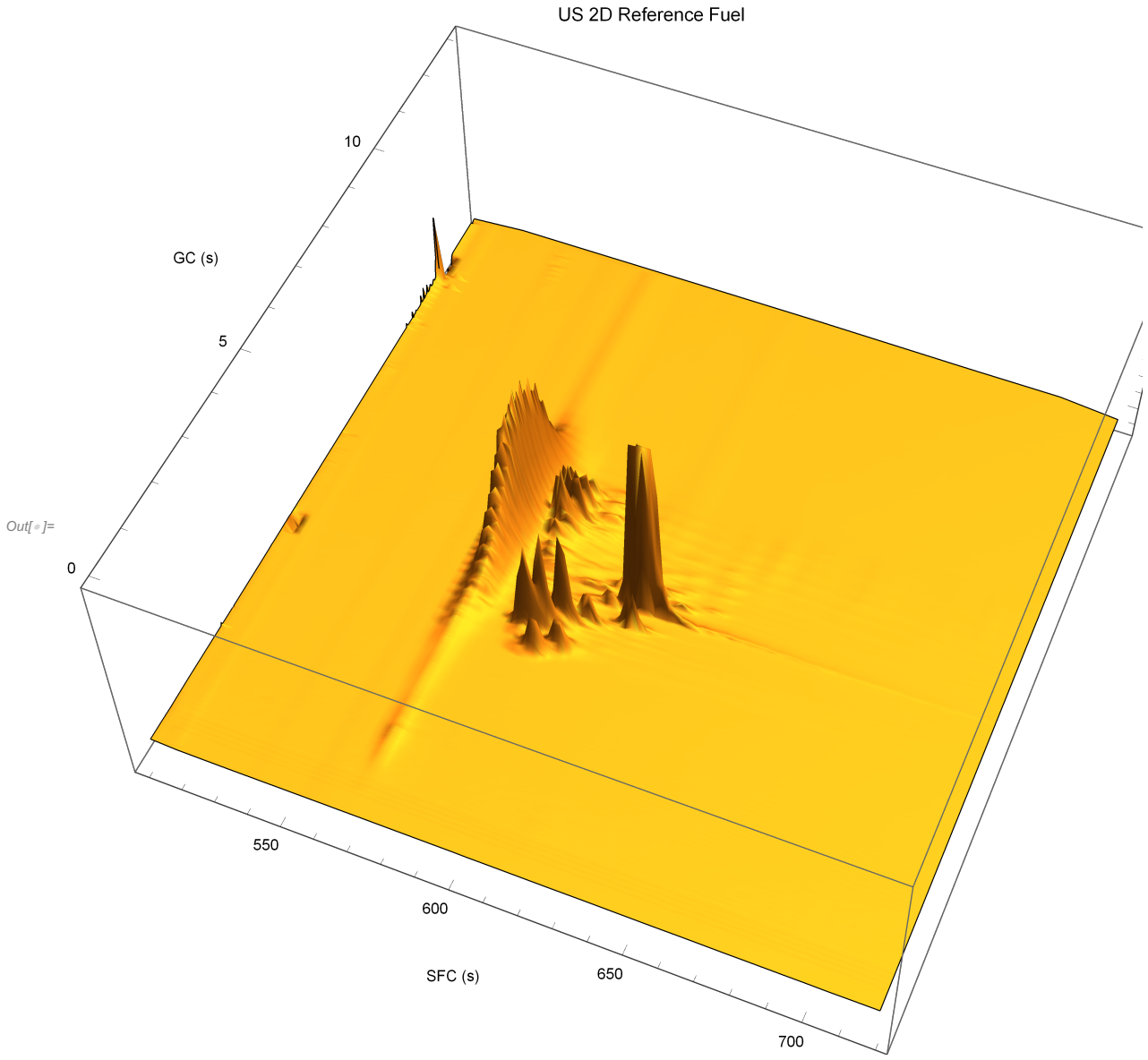
Out[ ]=



Run 3: US 2D Reference fuel

The whole chromatogram:

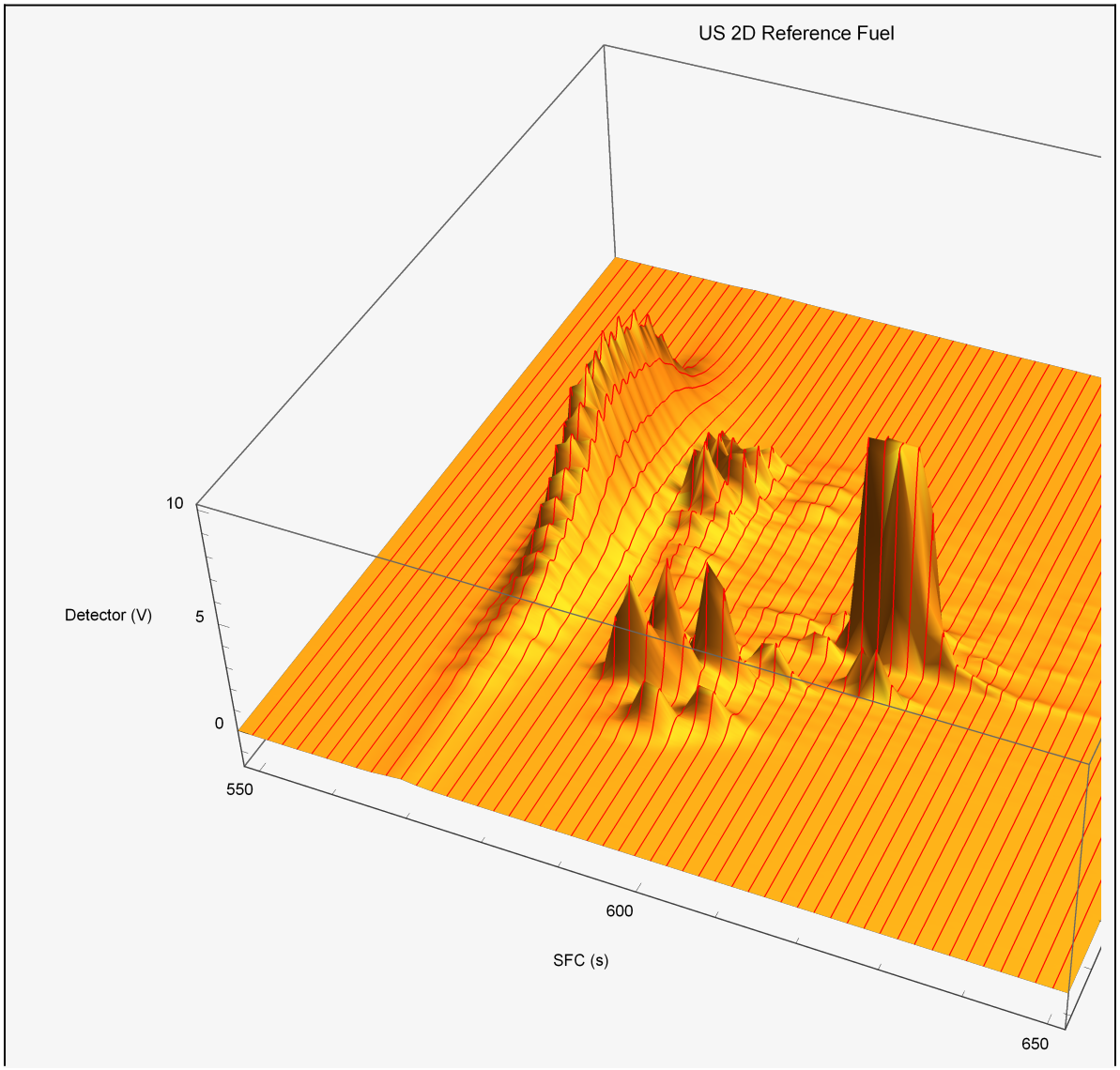
"C:\\Users\\fskdm\\My PhD\\Projects\\2019_12_20_PhD_Last_Project\\2019_12_23_PAH_-FAMEs\\Chromatograms\\RawData\\2020_01_20-173741.dat.prm"



Out[ ]=

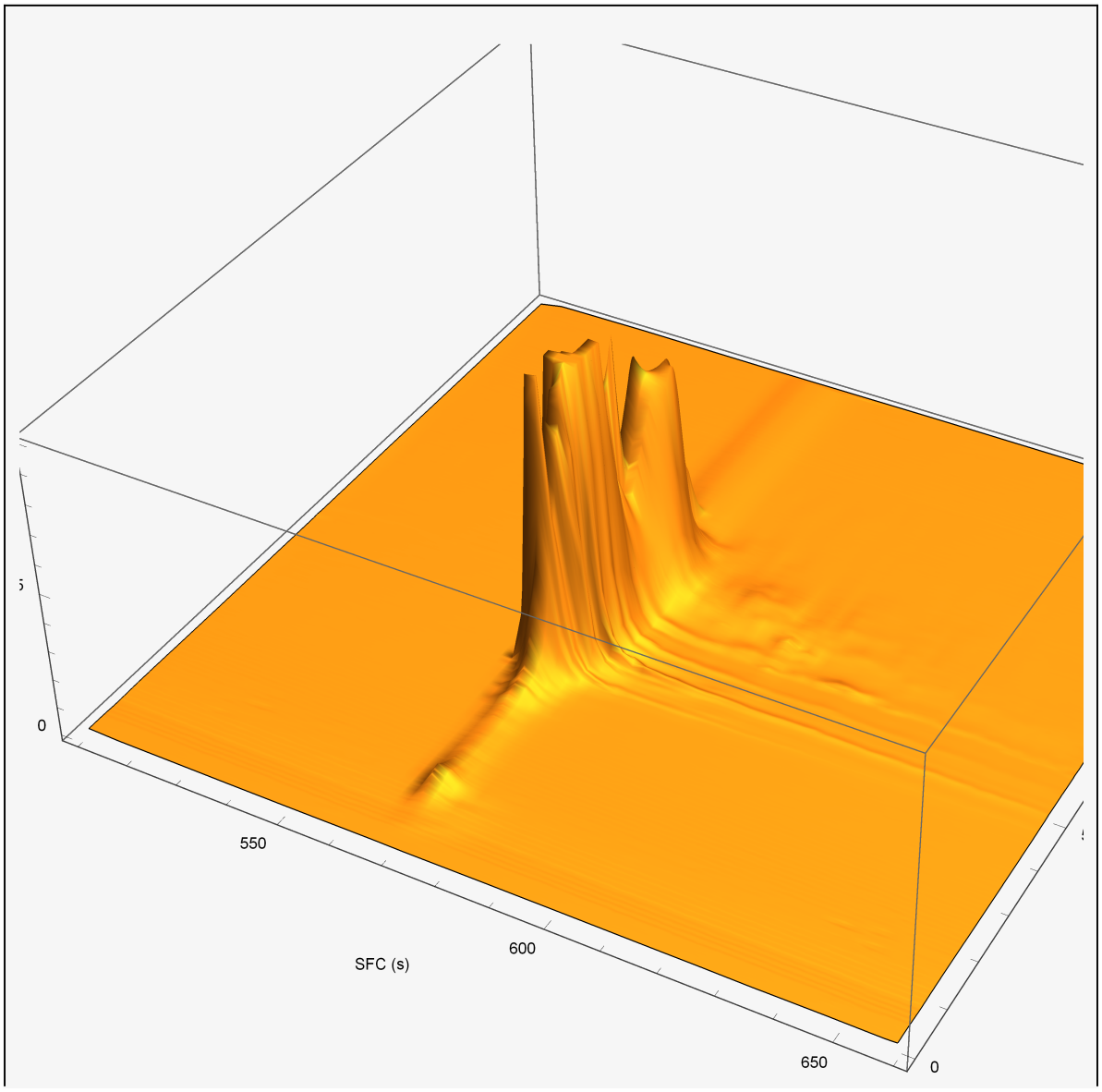
Zoomed in a bit:

Out[ ]=



Sample 4: Swedish diesel

Out[ ]=



Discussion

Samples

Run 1: US 2D reference fuel

This run shows that the amplifier gain should be less, but it does suggest that the chromatography is good. Plenty of flameouts and overtemperature events.

Run 2: US 2D reference fuel

This run had to be stopped due to a short circuit between the coaxial heater and the cryo shut-off

valve. See “2020_ 01_ 20_Valve _Short.nb”.

Run 3: US 2D reference fuel

This shows that an amplifier gain of AMPS FULL SCALE = 10^{-8} is suitable for the PAHs, even though one peak is cut off.

The comparison with an SFC-FID chromatogram from literature shows great similarity.

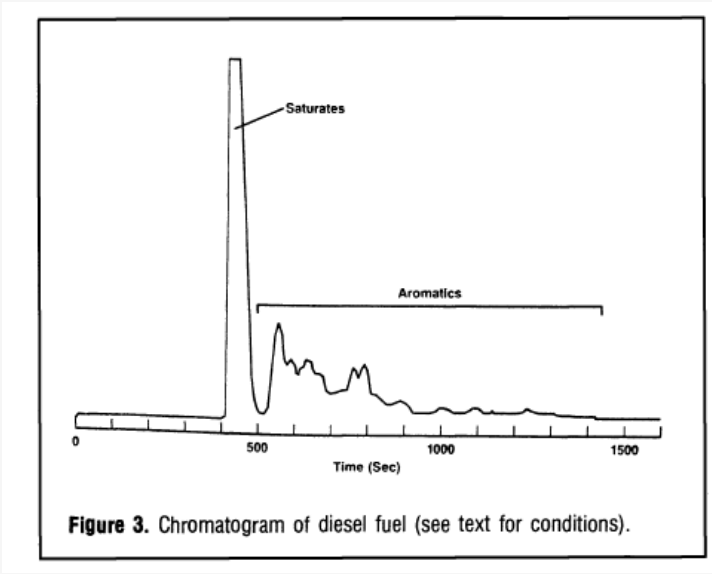
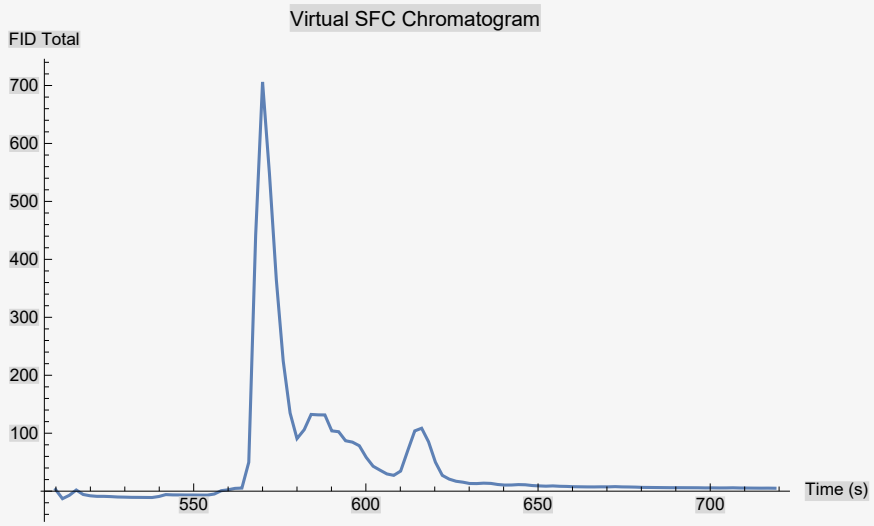


Figure 3. Chromatogram of diesel fuel (see text for conditions).



Sample 4: Swedish diesel

There is a clear difference between this sample and the previous one, which seems to show that the idea of separating aromatics by SFC×GC is sound. The concentration of olefins in this sample is higher than in the Reference Fuel, but it has no (0.5 %) aromatics. There are no peaks

Sampling time/modulation period

In this project I used a modulation period/sampling time of 2 s, and it tempting to want to see if this can be reduced, for higher resolution in the SFC dimension. This number must be treated with some caution. It is the time that elapses between commanding the valve on and commanding it off, and not the actual period of flow. The SFC stop valve is a rotary valve, with a fairly slow rotation rate, which means that there is a dead period which is counted as sampling time. I would

Conclusion

SFC×GC can create highly structured chromatograms of the aromatic compounds in diesel fuels.

Recommendations

1. Do not reduced modulation period without learning more about valve timings.
2. Use these settings for further work.