MEMORANDUM

State of Alaska

Department of Environmental Conservation
Division of Air and Water Quality - Air Quality Maintenance

TO: John Stone, Chief

DATE: March 24, 1998

FILE: 74.05.02

FROM: John Kuterbach
Air Quality Maintenance

SUBJECT: Maximum SO_2 Concentration from the combustion of #2 diesel fuel

EPA in their Title V permit reviews is requiring the department to demonstrate that limiting fuel sulfur to 0.5% will ensure compliance with our 500 ppmv SO_2 limit. This memorandum sets forth engineering calculations which demonstrate that combustion of #2 diesel fuel containing up to 0.5% sulfur will always comply with the 500 ppmv SO_2 limit regardless of the engine involved. I recommend that we reference these calculations in future "statements of basis" that we send to EPA with our draft operating permits.

Summary

This engineering calculation examined the stoichiometric combustion of #2 diesel fuel and calculated the maximum sulfur dioxide content of the flue gases. Typically, combustion of #2 diesel fuel can produce up to 338 ppmv SO_2 in the flue gas. Although this figure varies proportionally with the carbon content of the diesel fuel, the figure will never exceed the 500ppm limit.

I conclude that combustion of #2 diesel fuel with air will always comply with the 500ppmv emission limit. The ASTM specification for #2 diesel fuel limits sulfur to 0.5% or less.

Assumptions

All constituents of the fuel are burned proportionally
Any excess air typical of combustion would tend to dilute the SO_2 concentration in the flue gas, therefore only theoretical air is considered.
#2 diesel fuel is composed of Carbon, Hydrogen, Sulfur, and negligible amounts of Water and ash.
Ignore the water because the standard is a dry standard and the water will drop out of any calculations.
Ignore the ash as negligible unless the study predicts an SO_2 concentration greater than 450 ppm.
Typical #2 diesel fuel is composed of 87% Carbon, 12.5% Hydrogen, and 0.5% Sulfur
Calculations.

Using normal air for combustion (79% N_2 and 21% O_2):

For each lb-mole of Oxygen in Air, there is 3.76 lb-mole Nitrogen (1 lb-mole O_2) = (0.79/0.21) = 3.76 lb-mole N_2

The stoichiometric equations are:
$C + O_2 + 3.76\ N_2 = CO_2 + 3.76\ N_2$
$2H_2 + 0_2 + 3.76\ N_2 = 2H_20 + 3.76\ N_2$
$S + 0_2 + 3.76\ N_2 = SO_2 + 3.76\ N_2$

To calculate the dry exhaust gases (CO_2, N_2, SO_2) the following equations are used:

moles CO_2 = (lb C) x (1 lb-mole C/12.01 lb C) x (l lb-mole CO_2/1 lb mole C)
moles N_2 = (lb C) x (1 lb-mole C/12.01 lb C) x (3.76 lb-mole N_2/lb-mole C)

+ (lb H_2) x (1 lb-mole H_2/2.016 lb H_2) x (3.76 lb-mole N_2/2 lb-mole H_2)
+ (lb S) x (1 lb-mole S/32.06 lb S) x (3.76 lb-mole N_2/lb-mole S)
moles SO_2 = + (lb S) x (1 lb-mole S/32.06 lb S) x (lb-mole SO_2/1 lb-mole S)

Condensing these equations leaves:

moles CO_2 = lb C/12.01
moles N_2 = 3.76 x [(lb C/12.01) + (lb H_2/4.032) + (lb S/32.06)]
moles SO_2 = lb S/32.06

Then, by Avogadro's Law and the definition of mole:

ppmv SO_2 = 1,000,000 x [moles SO_2/(moles CO_2 + moles N_2 + moles SO_2)]

Results

Using 100 pounds of fuel as a basis, we examined the following three cases:

Case	Pounds in Fuel		
	Carbon	Hydrogen	Sulfur
1	87	12.5	0.5
2	96	3.5	0.5
3	78	21.5	0.5

Case 1 is the normal case, Case 2 increases carbon by 10 percent, and Case 3 decreases carbon by 10 percent.

	Case 1	Case 2	Case 3
moles CO_2	7.24	7.99	6.49
moles N_2	38.94	33.36	44.51
moles SO_2	0.0156	0.0156	0.0156
Total Dry Moles	46.196	41.366	51.016
ppmv SO_2	338	377	306

Conclusion

The above calculations show that #2 diesel fuel combusted with air will always comply with the 500 ppmv SO_2 limit. The calculations use the conservative assumptions of complete combustion and no excess air. The real-world includes partial combustion and excess air, both of which would tend to dilute the SO_2 concentration in the exhaust effluent.

The equations above can be used as an initial screening for other petroleum fuels even with a higher sulfur content or significant ash.

If you agree this memorandum has value, please share it with the rest of the AQM staff.