AQUAnews

The Newsletter for *AQUAlibrium* Users

Volume 2 Number 2 **Winter 1998**

Welcome to another issue of ***AQUAnews***. As with the previous issues, you can make additional copies for your colleagues provided they are distributed *free of charge*.

In this edition:

- a practical application of the ***AQUAlibrium*** flash
- how to import ***AQUAlibrium*** output into a word processor
- ***AQUAlibrium*** and Y2K

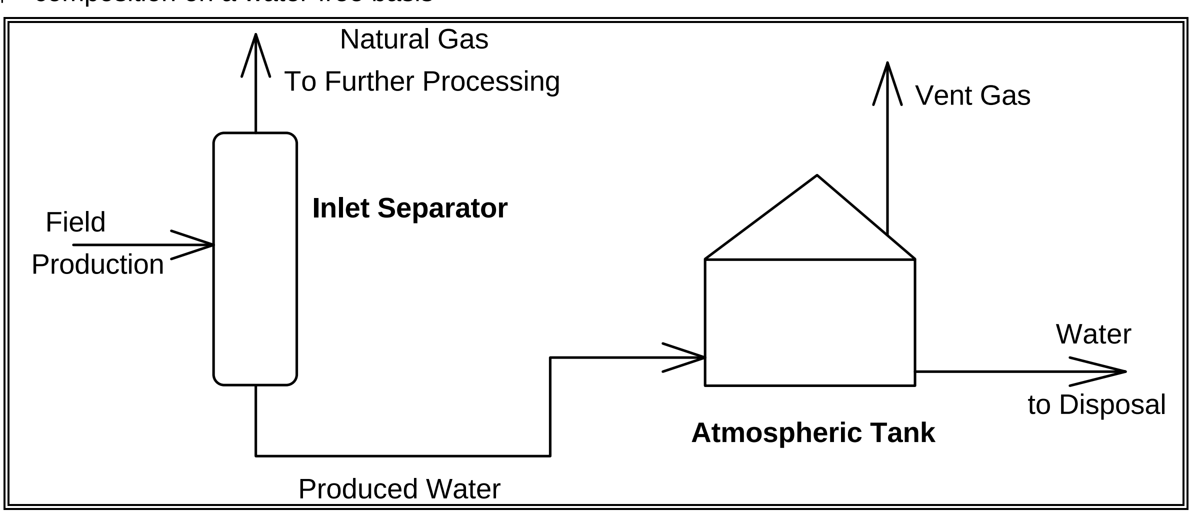
AQUAlibrium Flash Calculations

A gas field produces sour natural gas and water. These are pipelined from the field to an inlet separator at gas plant. The inlet separator operates at 50°C and 7 MPa. Following the separator, the produced water is sent to an atmospheric storage tank and the gas is sent for further treatment. The compositions and flow rates are given in the table below. The problem is to calculate the hydrogen sulfide content of the gas in the storage tank. Assume the storage tank is at 20°C.

Table 1 Feed to Gas Plant

Natural Gas	10 MMCFD
H_2S	0.25 mol%†
CO_2	2.49 mol%
CH_4	88.23 mol%
C_2H_6	7.84 mol%
C_3H_8	1.07 mol%
C_4H_{10}	0.12 mol%
Produced Water	10 bpd

† - composition on a water-free basis



The first step in the solution is to calculate the water content of the natural gas (since the composition is given on a water-free basis). This is done using Module 4, to calculate the water content of a gas. These results are given in output on the pages that follow.

Now the gas and produced water are blended to obtain the feed for the flash calculation. This calculation is summarized in Table 2. Note the following conversions:

10 bpd = 1590 L/d
= 1580 kg/d
= 87.70 kmol/d

From the ideal gas law, we have Pv = nRT, so we have the following conversion:

$$n = (10\times10^6)(14.696)/(10.73)/(60+460)$$
$$= 26{,}338.8 \text{ lbmol/d}$$
$$= 11\,947 \text{ kmol/d}$$

Table 2 Modified Feed to Plant

	kmol/d
Water	
Free Water	87.70
With Gas	27.30
Total Water	115.00
H_2S	29.80
CO_2	296.76
CH_4	10 516.94
C_2H_6	920.65
C_3H_8	127.59
C_4H_{10}	14.30
Total	12 034.70

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VAPOR-LIQUID DEW POINT CALCULATION IN A NATURAL GAS-WATER SYSTEM
Equilibrium Water Content of Vapor - FEED ON WATER-FREE BASIS

User Input - Temperature: 50 c   Pressure: 7 mpa
Temperature 50.00 deg C   Pressure   7000.0 kPa

Component	Mole Fraction Feed	Mole Fraction Vapor	Mole Fraction Aqueous	K-factor	Fugacity (kPa)
Water	0.0000E+00	0.2285E-02	0.9984E+00	0.2289E-02	0.1293E+02
H2S	0.2500E-02	0.2494E-02	0.1497E-03	0.1666E+02	0.1256E+02
CO2	0.2490E-01	0.2484E-01	0.4515E-03	0.5502E+02	0.1386E+03
Methane	0.8823E+00	0.8803E+00	0.8914E-03	0.9875E+03	0.5526E+04
Ethane	0.7840E-01	0.7822E-01	0.6334E-04	0.1235E+04	0.3762E+03
Propane	0.1070E-01	0.1068E-01	0.5523E-05	0.1933E+04	0.4182E+02
Butane	0.1200E-02	0.1197E-02	0.4184E-06	0.2862E+04	0.3793E+01

PHASE PROPERTIES

	Vapor	Aqueous
Mole Per Cent	100.00	.00
Weight Per Cent	100.00	.00
Volume Per Cent	100.00	.00
Molecular Weight (g/mol)	18.23	18.03
z-factor (z=Pv/RT)	.9167	.0474
Density (kg/m**3)	51.825	990.0
Density (lb/ft**3)	3.2352	61.80

```
Water content of gas = 1.837E-03 kg/m**3 (STP)
                     = 1.738E-03 kg/m**3 (std)
                     = 1.068E+02 lb/MMSCF
                     = 2.285E+03 ppm

Total hydrocarbon in aqueous liquid = 9.607E-04 mole frac
                                    = 9.607E+02 ppm
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VAPOR-LIQUID FLASH CALCULATION IN A NATURAL GAS-WATER SYSTEM

User Input - Temperature: 50 c   Pressure: 7 mpa
Temperature 50.00 deg C   Pressure   7000.0 kPa

Component	Mole Fraction Feed	Mole Fraction Vapor	Mole Fraction Aqueous	K-factor	Fugacity (kPa)
Water	0.9567E-02	0.2285E-02	0.9984E+00	0.2289E-02	0.1293E+02
H2S	0.2479E-02	0.2496E-02	0.1498E-03	0.1666E+02	0.1257E+02
CO2	0.2469E-01	0.2487E-01	0.4519E-03	0.5502E+02	0.1387E+03
Methane	0.8749E+00	0.8813E+00	0.8924E-03	0.9876E+03	0.5532E+04
Ethane	0.7659E-01	0.7715E-01	0.6249E-04	0.1235E+04	0.3711E+03
Propane	0.1061E-01	0.1069E-01	0.5534E-05	0.1932E+04	0.4191E+02
Butane	0.1190E-02	0.1198E-02	0.4190E-06	0.2860E+04	0.3799E+01

PHASE PROPERTIES

	Vapor	Aqueous
Mole Per Cent	99.27	.73
Weight Per Cent	99.28	.72
Volume Per Cent	99.96	.04
Molecular Weight (g/mol)	18.22	18.03
z-factor (z=Pv/RT)	.9170	.0474
Density (kg/m**3)	51.767	990.0
Density (lb/ft**3)	3.2317	61.80

```
Water content of gas = 1.837E-03 kg/m**3 (STP)
                     = 1.738E-03 kg/m**3 (std)
                     = 1.068E+02 lb/MMSCF
                     = 2.285E+03 ppm

Total hydrocarbon in aqueous liquid = 9.609E-04 mole frac
                                    = 9.609E+02 ppm
```

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VAPOR-LIQUID FLASH CALCULATION IN A NATURAL GAS-WATER SYSTEM

User Input - Temperature: 20 c   Pressure: 1 atm
Temperature 20.00 deg C   Pressure   101.3 kPa

Component	Mole Fraction Feed	Mole Fraction Vapor	Mole Fraction Aqueous	K-factor	Fugacity (kPa)
Water	0.9984E+00	0.2324E-01	0.9997E+00	0.2324E-01	0.2340E+01
H2S	0.1496E-03	0.4386E-01	0.9166E-04	0.4785E+03	0.4414E+01
CO2	0.4519E-03	0.2221E+00	0.1581E-03	0.1404E+04	0.2239E+02
Methane	0.8924E-03	0.6605E+00	0.1797E-04	0.3675E+05	0.6678E+02
Ethane	0.6249E-04	0.4591E-01	0.1720E-05	0.2670E+05	0.4618E+01
Propane	0.5534E-05	0.4079E-02	0.1348E-06	0.3026E+05	0.4085E+00
Butane	0.4190E-06	0.3102E-03	0.8340E-08	0.3720E+05	0.3094E-01

PHASE PROPERTIES

	Vapor	Aqueous
Mole Per Cent	.13	99.87
Weight Per Cent	.18	99.82
Volume Per Cent	63.78	36.22
Molecular Weight (g/mol)	23.86	18.02
z-factor (z=Pv/RT)	.9971	.0008
Density (kg/m**3)	.995	998.2
Density (lb/ft**3)	.0621	62.32

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Water content of gas = 1.868E-02 kg/m**3 (STP)
                     = 1.767E-02 kg/m**3 (std)
                     = 1.086E+03 lb/MMSCF
                     = 2.324E+04 ppm

Total hydrocarbon in aqueous liquid = 1.984E-05 mole frac
                                    = 1.984E+01 ppm
```

The molar flow rate for each component is the product of the mole fraction and the total molar flow.

It is interesting to note that in this case almost ¼ of the water in the total feed is from water in the gas.

There is no need to convert the modified feed to mole fraction. With recent modifications to the ***AQUAlibrium*** you can input the molar flow rate and convert to mole fraction when prompted by the program.

The flash calculation is performed using Module 1 and the results are given in the previous pages.

The aqueous phase from this calculation is used as the feed for the final flash calculation. Again this calculation is performed using Module 1. From the output given it can be seen that the hydrogen sulfide concentration in the gas is about 4.4 mol% or 44,000 ppm. This compares with only 2500 ppm in the natural gas entering the plant.

Also note that at atmospheeric pressure the gas appears to be small - only 0.12 mol%. However, this converts to 64% by volume.

Hydrogen sulfide is a very toxic gas, even at relatively low concentrations. Thus, the gas in the storage tank is very dangerous. The engineer should be aware of this when proposing such a design.

The separator sizing procedure outlined in the previous edition of ***AQUAnews*** (v.2 no. 1) can be used to size the inlet separator in this example.

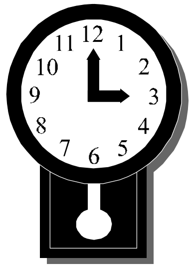
Importing *AQUAlibrium* Results

AQUAlibrium gives the user the option of writing the results to a file (`AQUA.PRN`). This file is an ASCII file (plain text). It is a simple matter to import this file into the word processor of your choice (as I do with my reports and with ***AQUAnews*** - for example the previous two pages). When you tell your word processor to open a file, tell it to open `AQUA.PRN` (make sure that it is directed to the correct subdirectory).

When formatting the ***AQUAlibrium*** output within your word processor, you should use a non-proportional font (such as Courier). This will ensure that the columns in the output line up properly. If you chose a proportional (such as Times Roman), then you will have to line up the columns yourself. However, we suggest that you use tabs to facilitate the process. See the instructions for your word process on how to use tabs.

Y2K and *AQUAlibrium*

The Y2K bug is upon us. The good news is that ***AQUAlibrium*** is Y2K compliant.



1. ***AQUAlibrium*** does not use the clock or the calendar for any of its main routines. They are not used to generate initial conditions (i.e., random numbers) and they are not used for security purposes (passwords or version expiration, etc.).

2. The only place that the date occurs in ***AQUAlibrium*** is when information is printed to a file.

   The software reads the year in four digit format from the computer. Therefore if the computer supplies a four digit year then ***AQUAlibrium*** has no trouble.

   The date is also read from the computer. Once again, if the date is supplied in the proper manner then there is no problem with ***AQUAlibrium***.

3. Finally the date is printed in an unambiguous format. The month is given a four-character symbol. In the case of four-letter month names, then entire name is used. Otherwise the month is abbreviated using three letters followed by a period. The exception is the month of May, which is formatted using only three characters. For single digit day numbers, neither a space nor a leading zero is printed.

   Examples of the date format are:

```
June 1, 1999
Sep. 23, 2001
May 6, 1981
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We hope this addresses any and all concerns with ***AQUAlibrium*** and the millennium bug. And the bottom line is that there is no Y2K problem with ***AQUAlibrium***.

AQUAlibrium on the World Wide Web

AQUAlibrium is wired! Please visit the ***AQUAlibrium*** web page at:

http://www.telusplanet.net/public/jcarroll/AQUA.HTM

We try to continually add material to the site. We are always looking for new ideas and for links. Please let us know. And we thank those who had made suggestions in the past.

Previous problems with the case in the URL of the web site have now be rectified. In other words, lower case aqua.htm will also work.

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