

**Title:**

Application of HovaCAL Technology for Calibration of FTIR and other Multicomponent IR analyzers

**Authors:**

Edul Chikhliwala, Robert Peters and Ronald Baker – EcoChem Analytics

Martin Schmaeh, IAS GmbH

**Abstract:**

The HovaCAL technology has been used to generate hot-wet gas mixtures of various reactive compounds NH<sub>3</sub>, HCl, HF, HBr etc. These gas mixtures can be used to calibrate FTIR and other multicomponent analyzers. In addition, different water vapor compositions generated by the Hovacal can be used to formulate water interference curves and even less significant cross-interferences of other gases (NO, CO, SO<sub>2</sub>, CO<sub>2</sub>) required by the analyzers to achieve desired performance. Finally, the accurate gas-mixing capabilities of the HovaCAL enable the user to create diluted gas matrices of various compositions using one or more span gas cylinder.

In this paper we will illustrate the above described capabilities and how these activities are crucial in the initial setup and routine maintenance of FTIR and other multicomponent IR analyzer applications.

# Application of HovaCAL Technology for Calibration of FTIR and other Multicomponent IR analyzers

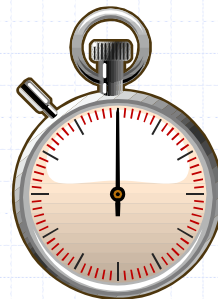
E. D. Chikhliwala, R. Baker and R. Peters, EcoChem Analytics  
M. Schmäh, IAS GmbH

EUEC 2009 – Session A5.4  
Phoenix, AZ  
Tuesday, 3<sup>rd</sup> February 2009

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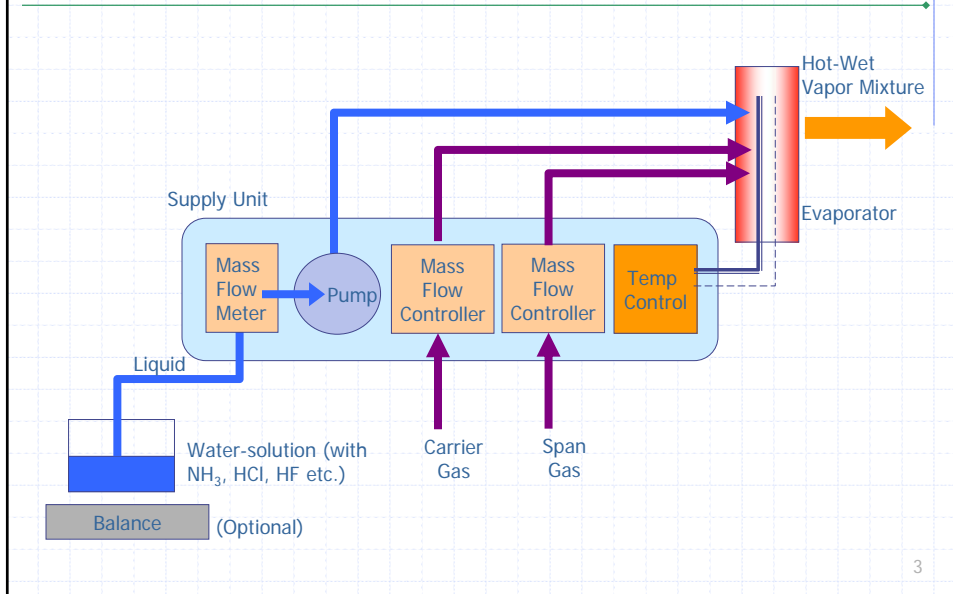
## Presentation Outline

- ◆ Technology
  - How it works
  - Instrument configuration
  
- ◆ Application
  - Water reference
  - Cross-interference
  - Reactive vapor calibration



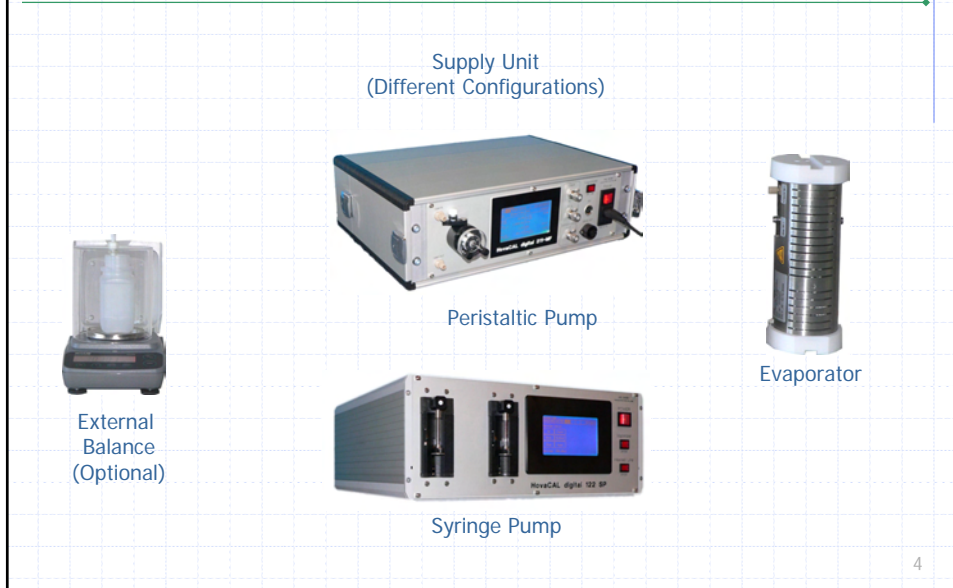
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## HovaCAL – Flow Schematic



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## Typical Configuration



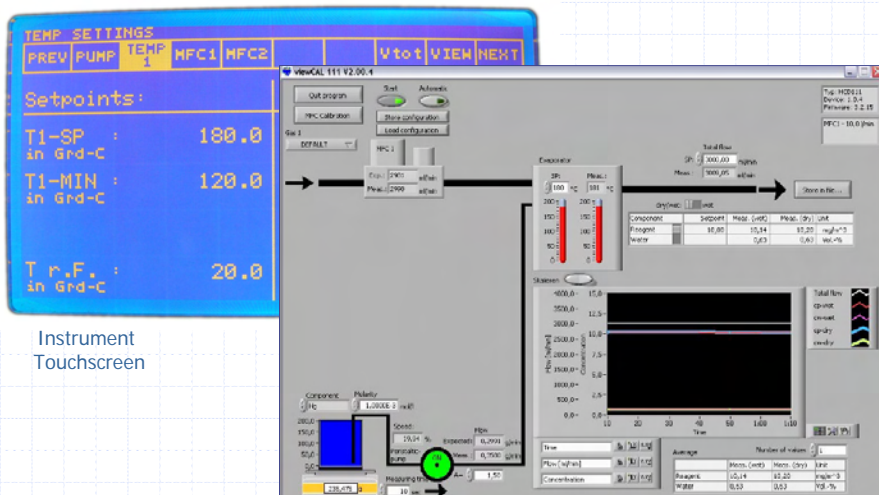
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## Typical Operating Values

- ◆ Evaporator temperature: 180 to 200 °C
- ◆ Liquid concentrations: Dependent on compound
- ◆ Liquid flow rate: 0.1 to 3 ml/min (Peristaltic Pump)  
5 to 250 µl/min (Syringe Pump)
- ◆ Carrier gas flow: 3 to 25 lit/min
- ◆ Span gas flow: 0.1 to 10 lit/min (other possible)

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## Control Software

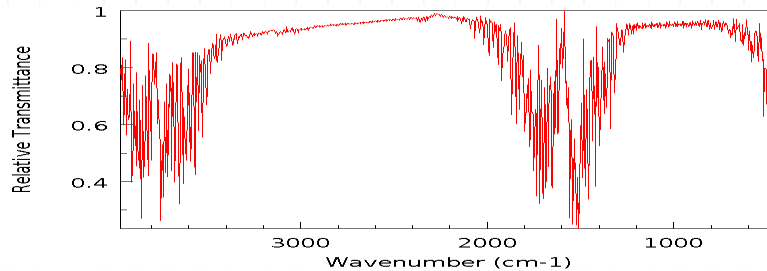


Instrument Touchscreen

PC Interface (LabView)

6

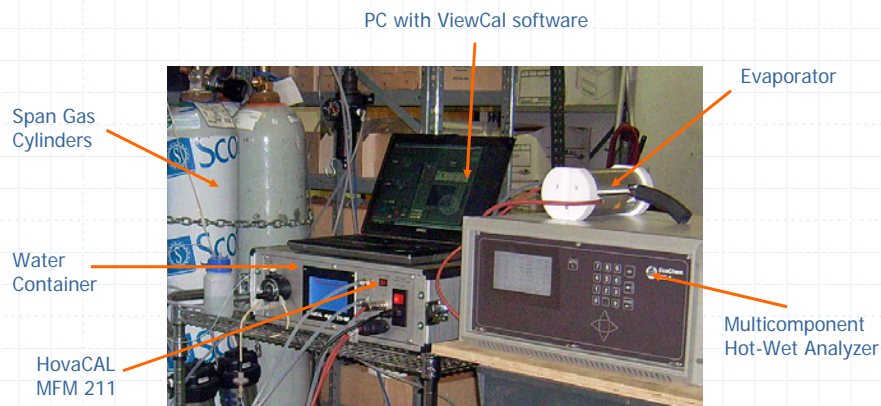
## Importance of Water Calibration



- ◆ Water has absorption lines across IR spectrum
- ◆ Water signal is typically significantly stronger than the target compounds
- ◆ A good instrument-specific water calibration greatly helps produce accurate readings
- ◆ Instrument's response to water vapor is done initially and after major maintenance

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## Hot-Wet Multicomponent Analyzer Calibration



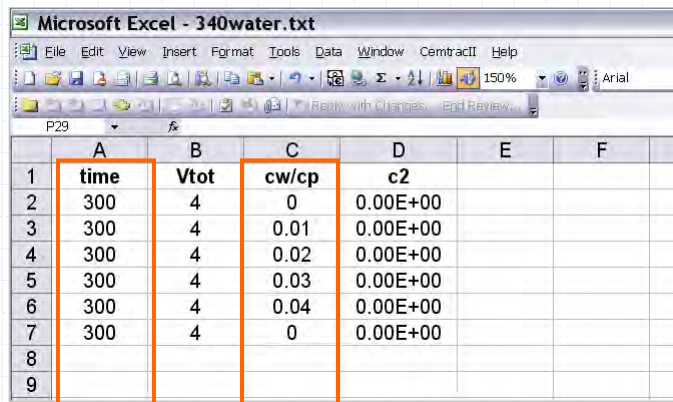
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## Calibration Procedure

- ◆ Calibration of Hot-Wet Multicomponent MC3 analyzer measuring NO, NO<sub>2</sub>, N<sub>2</sub>O, NH<sub>3</sub>, H<sub>2</sub>O, CO<sub>2</sub> and O<sub>2</sub>
- ◆ Obtain absorbance vs concentration data for linearity and cross-interference tables
- ◆ For NDIR instruments, single/dual wavelength measurements, while for FTIR entire absorbance spectrum is obtained for a particular concentration level

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## HovaCAL Input File (H<sub>2</sub>O)



	A	B	C	D	E	F
1	<b>time</b>	<b>Vtot</b>	<b>cw/cp</b>	<b>c2</b>		
2	300	4	0	0.00E+00		
3	300	4	0.01	0.00E+00		
4	300	4	0.02	0.00E+00		
5	300	4	0.03	0.00E+00		
6	300	4	0.04	0.00E+00		
7	300	4	0	0.00E+00		
8						
9						

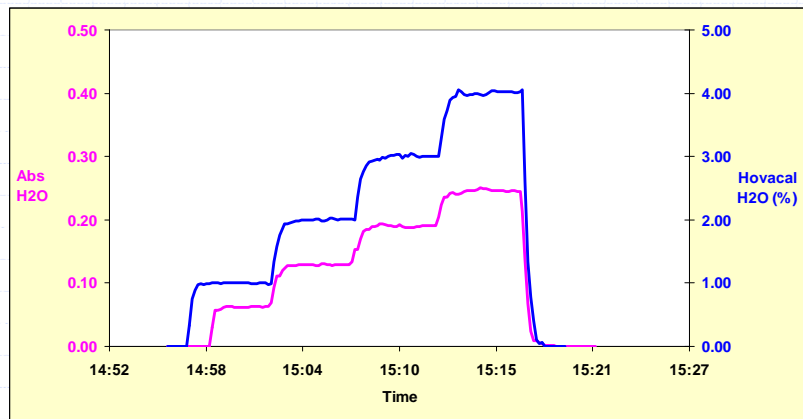
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## HovaCAL Output File

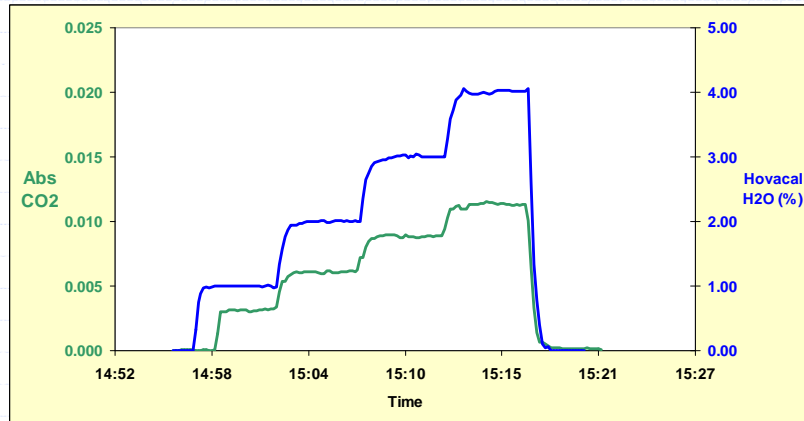
Microsoft Excel - 16012009\_145059.xls

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
	Date	Time	molarity/ molmass	pump flow	Vtot	cp-wet	cw-wet	c1-wet	c2-wet	cp-dry	cw-dry	c1-dry	c2-dry	cp unit	cw unit
76	16.01.2009	15:03:30	1.00E-12	6.43E-02	3.99E+03	0.00E+00	2.00E+00	9.80E-04	0.00E+00	0.00E+00	2.05E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
77	16.01.2009	15:03:40	1.00E-12	6.44E-02	3.99E+03	0.00E+00	2.01E+00	9.80E-04	0.00E+00	0.00E+00	2.05E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
78	16.01.2009	15:03:49	1.00E-12	6.44E-02	3.99E+03	0.00E+00	2.01E+00	9.80E-04	0.00E+00	0.00E+00	2.05E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
79	16.01.2009	15:03:59	1.00E-12	6.38E-02	3.99E+03	0.00E+00	1.99E+00	9.80E-04	0.00E+00	0.00E+00	2.03E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
80	16.01.2009	15:04:09	1.00E-12	6.36E-02	3.99E+03	0.00E+00	1.99E+00	9.80E-04	0.00E+00	0.00E+00	2.03E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
81	16.01.2009	15:04:19	1.00E-12	6.41E-02	3.99E+03	0.00E+00	2.00E+00	9.80E-04	0.00E+00	0.00E+00	2.04E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
82	16.01.2009	15:04:30	1.00E-12	6.48E-02	3.99E+03	0.00E+00	2.02E+00	9.80E-04	0.00E+00	0.00E+00	2.06E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
83	16.01.2009	15:04:40	1.00E-12	6.48E-02	3.99E+03	0.00E+00	2.02E+00	9.80E-04	0.00E+00	0.00E+00	2.06E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
84	16.01.2009	15:04:50	1.00E-12	6.45E-02	3.99E+03	0.00E+00	2.01E+00	9.80E-04	0.00E+00	0.00E+00	2.05E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
85	16.01.2009	15:04:59	1.00E-12	6.42E-02	3.99E+03	0.00E+00	2.00E+00	9.80E-04	0.00E+00	0.00E+00	2.04E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
86	16.01.2009	15:05:10	1.00E-12	6.44E-02	3.99E+03	0.00E+00	2.01E+00	9.80E-04	0.00E+00	0.00E+00	2.05E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
87	16.01.2009	15:05:19	1.00E-12	6.43E-02	3.99E+03	0.00E+00	2.01E+00	9.80E-04	0.00E+00	0.00E+00	2.05E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
88	16.01.2009	15:05:29	1.00E-12	6.43E-02	3.99E+03	0.00E+00	2.01E+00	9.80E-04	0.00E+00	0.00E+00	2.05E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
89	16.01.2009	15:05:39	1.00E-12	6.45E-02	3.99E+03	0.00E+00	2.01E+00	9.80E-04	0.00E+00	0.00E+00	2.05E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
90	16.01.2009	15:05:49	1.00E-12	6.43E-02	3.99E+03	0.00E+00	2.01E+00	9.80E-04	0.00E+00	0.00E+00	2.05E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
91	16.01.2009	15:05:59	1.00E-12	6.42E-02	3.99E+03	0.00E+00	2.00E+00	9.80E-04	0.00E+00	0.00E+00	2.04E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
92	16.01.2009	15:06:09	1.00E-12	7.58E-02	4.00E+03	0.00E+00	2.36E+00	9.76E-04	0.00E+00	0.00E+00	2.42E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
93	16.01.2009	15:06:19	1.00E-12	8.51E-02	4.00E+03	0.00E+00	2.65E+00	9.74E-04	0.00E+00	0.00E+00	2.72E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
94	16.01.2009	15:06:29	1.00E-12	8.66E-02	4.00E+03	0.00E+00	2.76E+00	9.72E-04	0.00E+00	0.00E+00	2.83E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
95	16.01.2009	15:06:39	1.00E-12	9.17E-02	4.00E+03	0.00E+00	2.95E+00	9.71E-04	0.00E+00	0.00E+00	2.94E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
96	16.01.2009	15:06:49	1.00E-12	9.36E-02	4.00E+03	0.00E+00	2.91E+00	9.71E-04	0.00E+00	0.00E+00	3.00E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
97	16.01.2009	15:06:59	1.00E-12	9.40E-02	4.00E+03	0.00E+00	2.92E+00	9.71E-04	0.00E+00	0.00E+00	3.02E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
98	16.01.2009	15:07:10	1.00E-12	9.47E-02	4.00E+03	0.00E+00	2.95E+00	9.71E-04	0.00E+00	0.00E+00	3.04E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
99	16.01.2009	15:07:19	1.00E-12	9.52E-02	4.00E+03	0.00E+00	2.96E+00	9.70E-04	0.00E+00	0.00E+00	3.05E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
100	16.01.2009	15:07:29	1.00E-12	9.47E-02	3.99E+03	0.00E+00	2.95E+00	9.70E-04	0.00E+00	0.00E+00	3.04E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
101	16.01.2009	15:07:39	1.00E-12	9.56E-02	3.99E+03	0.00E+00	2.96E+00	9.70E-04	0.00E+00	0.00E+00	3.06E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
102	16.01.2009	15:07:49	1.00E-12	9.56E-02	3.99E+03	0.00E+00	2.98E+00	9.70E-04	0.00E+00	0.00E+00	3.07E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
103	16.01.2009	15:07:59	1.00E-12	9.65E-02	3.99E+03	0.00E+00	3.01E+00	9.70E-04	0.00E+00	0.00E+00	3.10E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%
104	16.01.2009	15:08:09	1.00E-12	9.65E-02	3.99E+03	0.00E+00	3.03E+00	9.70E-04	0.00E+00	0.00E+00	3.13E+00	0.00E-03	0.00E+00	Vol.-%	Vol.-%

## Calibration – H2O

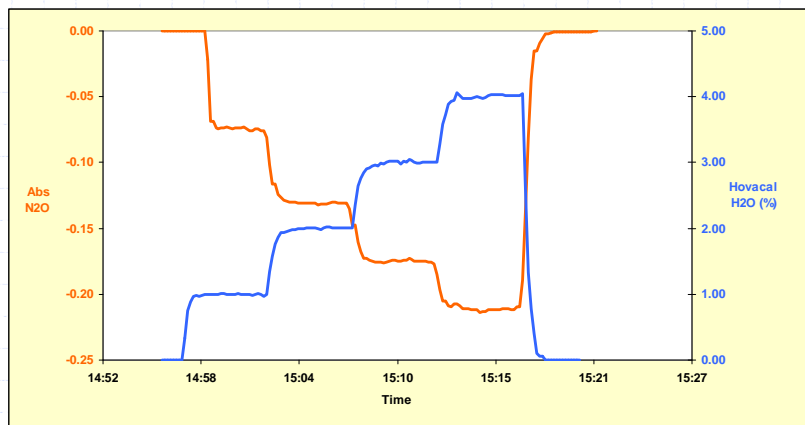


## Cross Interference H<sub>2</sub>O – CO<sub>2</sub>



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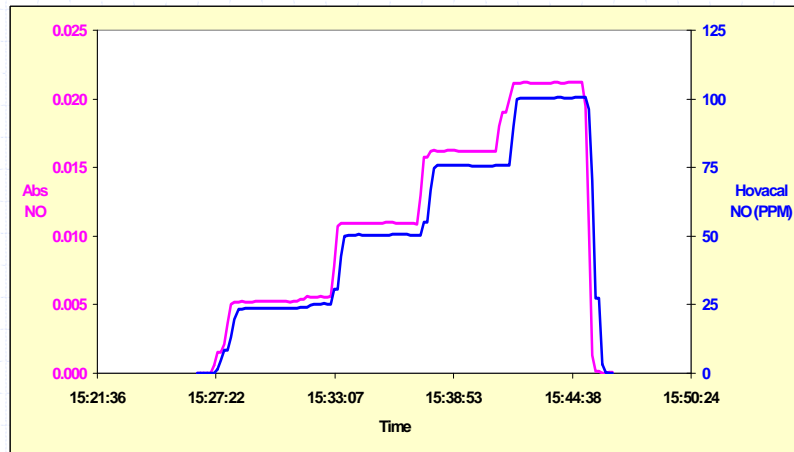
## Cross Interference H<sub>2</sub>O & N<sub>2</sub>O



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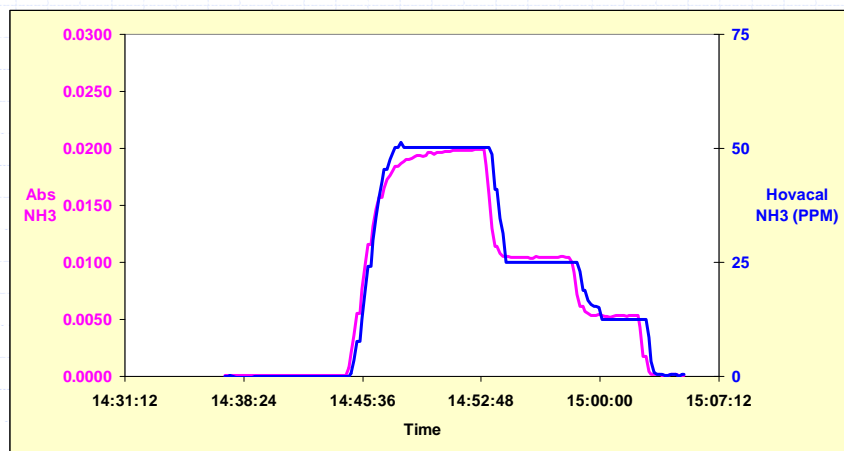


## Gas Mixing – NO Calibration



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## Reactive Vapor – NH<sub>3</sub> Calibration



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## Evaluation -- H<sub>2</sub>O Linearity

TUV Report 2007 for  
 H<sub>2</sub>O, HCl, NH<sub>3</sub>, HF and Mercury

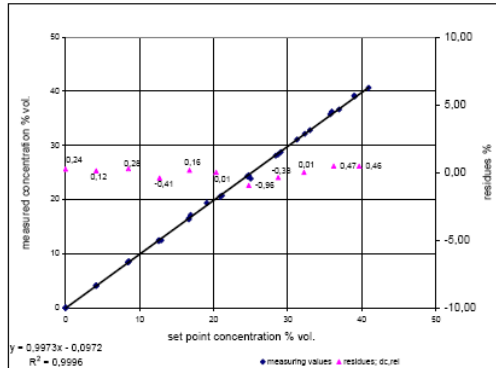
TÜV IMMISSIONSSCHUTZ  
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DAP-PL-3856.99

Bericht über die die Prüfung der  
 Leistungseigenschaften  
 und der Einsatzbereiche des Prüfgasgenerators  
 HovaCAL digital 211 MF

TÜV-Bericht Nr.: 936/21205306 A  
 Köln. 15. März 2007



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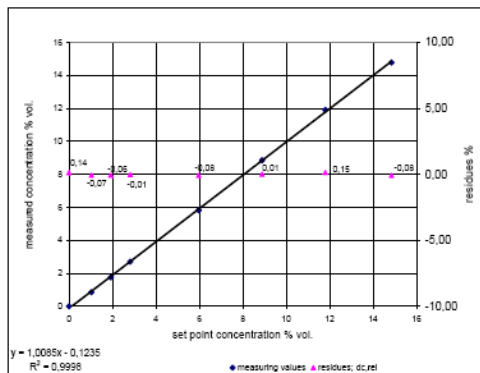
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## HovaCAL Applications Summary

- ◆ New analyzers – create linearity and cross-interference curves
- ◆ Field maintenance activities on a routine basis (semi-annual, annual)
  - Check the calibration of water channel and interference curves with HovaCAL
  - Span gas checks for NH<sub>3</sub>, HCl, HF etc
- ◆ Repair of analyzer in factory and field – sample cell rebuild, source replacement, optical bench repairs require re-calibration with HovaCAL
- ◆ Eliminate or minimize use of calibration gas cylinders
- ◆ Compact & flexible – delivered concentrations can be optimized at point of use

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## Questions & Answers ?

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By Edul Chikhliwala, Robert Peters, Ronald Baker & Martin Schmaeh

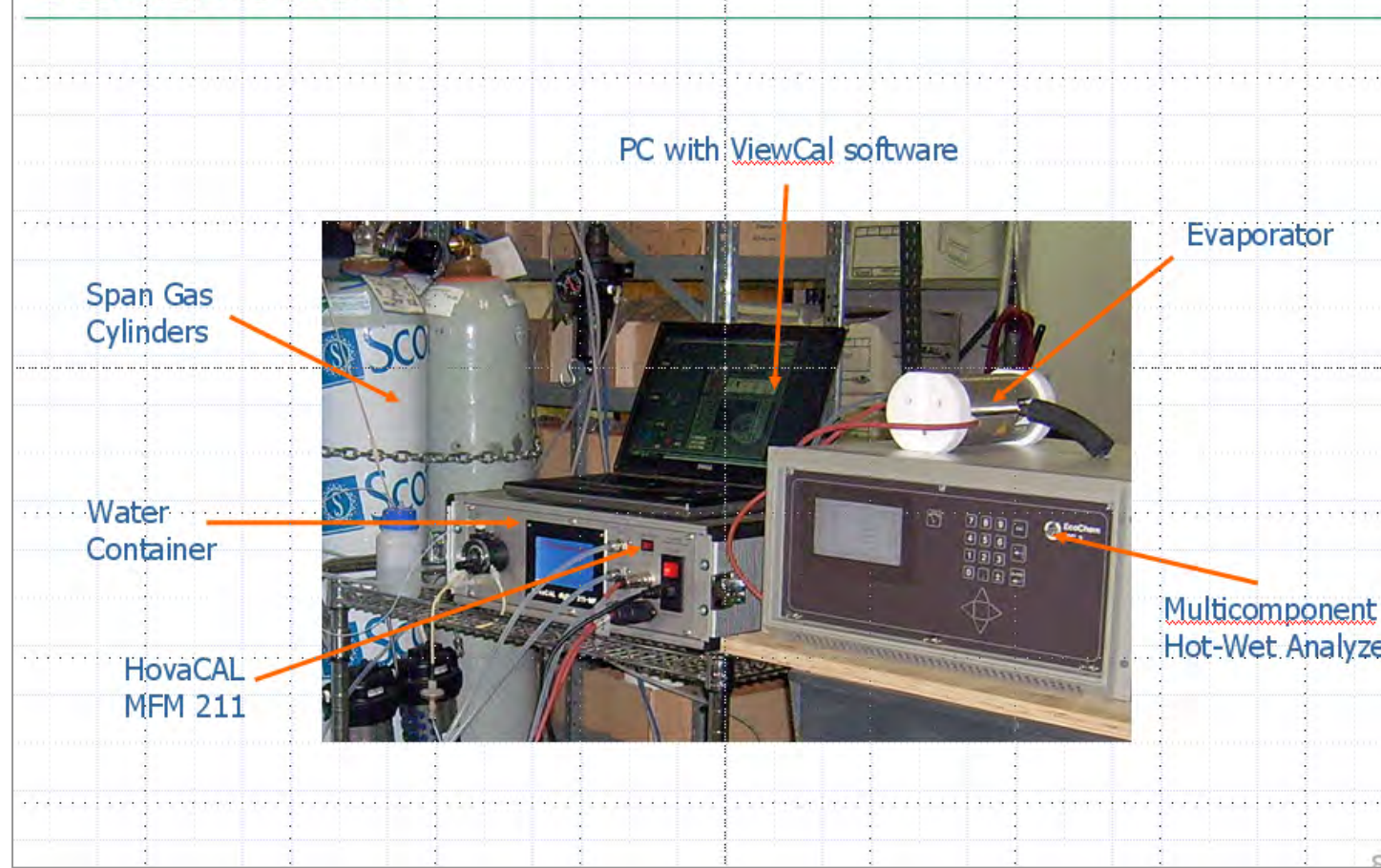
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The HovaCAL technology has been used to generate hot-wet gas mixtures of various reactive compounds NH<sub>3</sub>, HCl, HF, HBr etc. These gas mixtures can be used to calibrate FTIR and other multicomponent analyzers. In addition, different water vapor compositions generated by the Hovacal can be used to generate water interference curves required by the analyzers. Finally, the gas-mixing capabilities of the HovaCAL enable the user to create diluted gas mixtures of various compositions using one or more span gas cylinder. In this paper we will illustrate the above described capabilities and how these activities are crucial in the initial setup and routine maintenance of these analyzer applications.

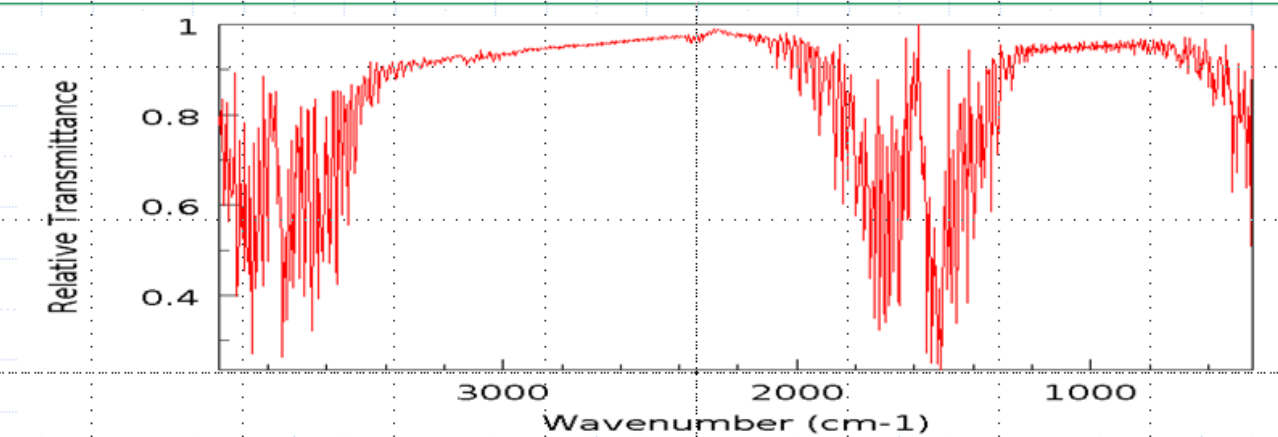
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## Hot-Wet Multicomponent Analyzer Calibration

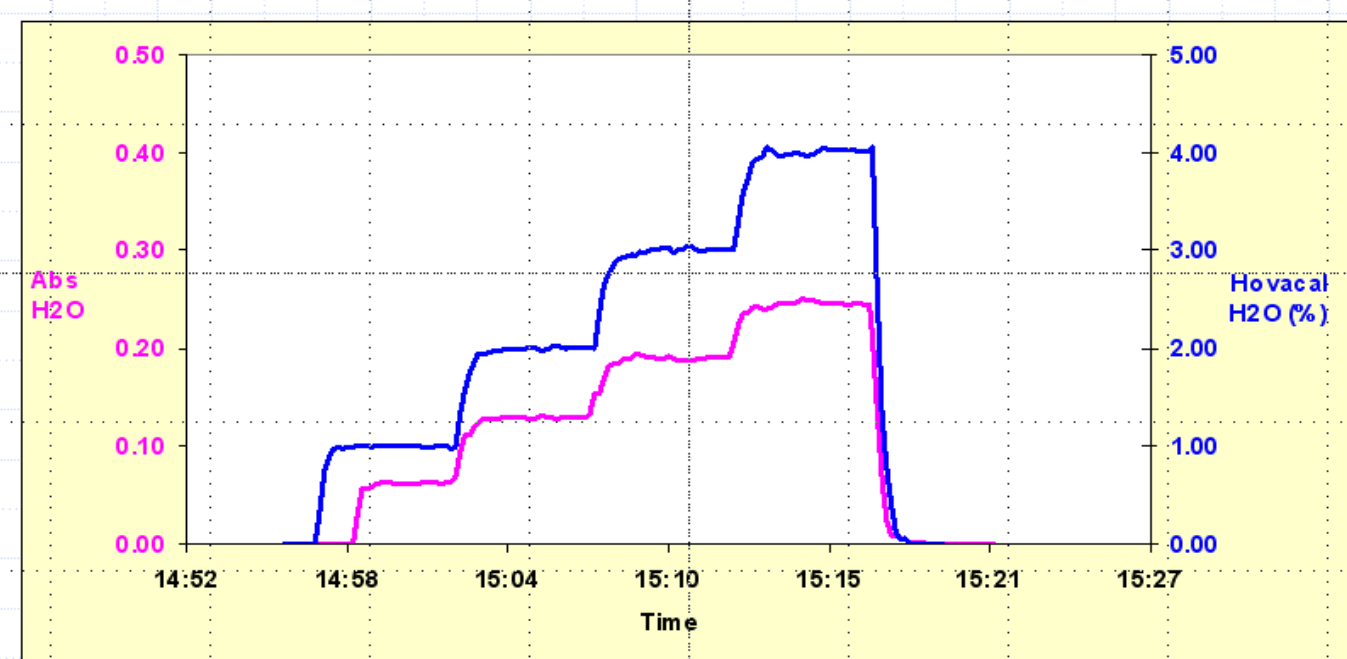


## Importance of Water Calibration

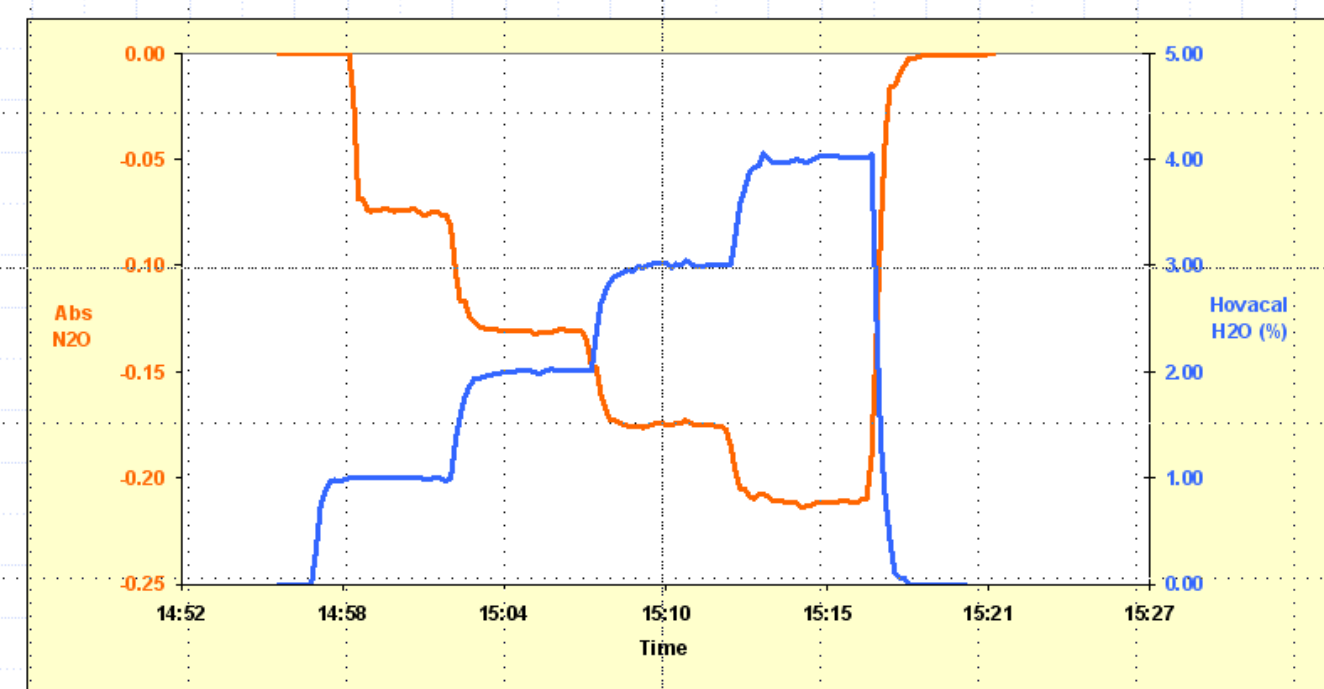


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- ◆ Water signal is typically significantly stronger than the target compounds
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## Calibration – H<sub>2</sub>O



## Cross Interference H<sub>2</sub>O & N<sub>2</sub>O



## Reactive Vapor – NH<sub>3</sub> Calibration

