Results On Gas Detection and Concentration Estimation via Mid-IR-based Gas Detection System Analysis Model

Yi Xin and Joel M. Morris

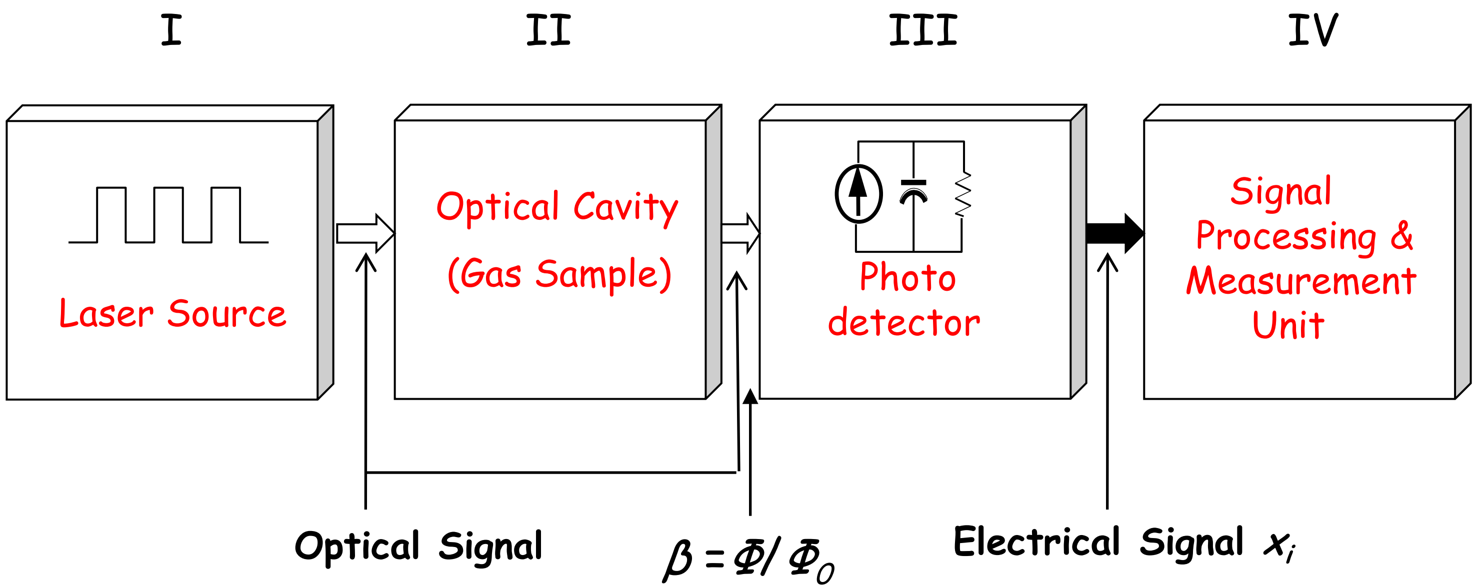
Communications and Signal Processing Laboratory
CSEE Dept/UMBC
xin1@umbc.edu, morris@umbc.edu

Motivation/Goals

For Mid-IR Gas Detection Systems

- Improve developed statistical analysis model
- Develop detection rule P_D, P_{FA}
- Detect target gas
- Estimate concentration of target gas
- Apply to 17 important trace gases
- Adapt to different photo-detectors

MID-IR Gas Detection System



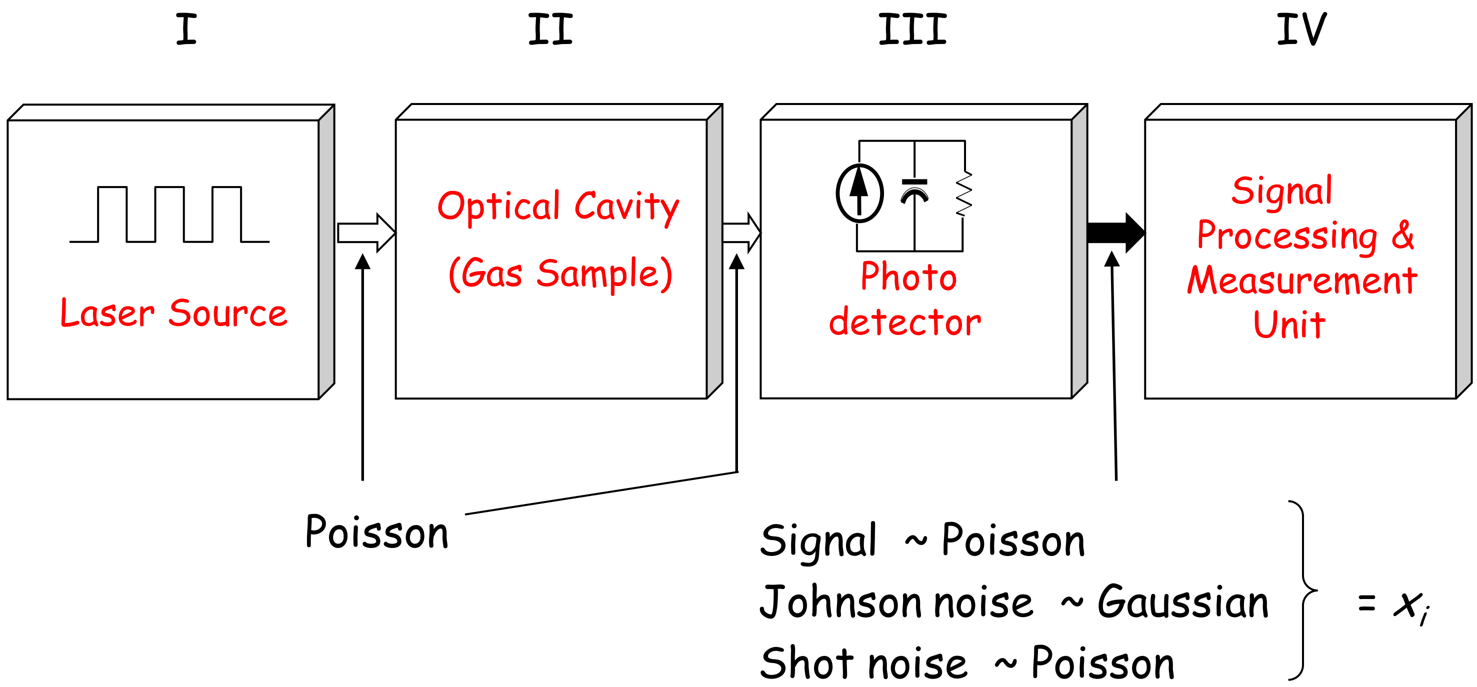
Φ =Optical intensity w/ gas

Φ_0 =Optical intensity w/o gas

System Parameters

P	~	laser power	I_{sn}	~	shot noise current
β	~	gas transmittance	I_{jn}	~	Johnson noise current
Δf	~	3dB passband ($0.35/t_r$)	a_β	~	$I_p(T_w/q)$
T_w	~	laser pulse width ($10t_r$)	μ	~	$I_d(T_w/q)$
I_p	~	photocurrent	λ_β	~	$I_p(T_w/q)+I_{sn}^2(T_w/q)$
I_d	~	dark current	σ^2	~	$I_{jn}^2(T_w/q)^2$

Statistical Model



Statistical Model

Output measurement sample-mean pdf:

$$f(x_N \mid \beta) = \sum_{k=0}^{\infty} \exp\left\{ \begin{array}{l} -N\lambda_\beta + k\ln N\lambda_\beta - \ln k! - \ln(\sqrt{2\pi\sigma^2 / N}) \\ -N(x-\mu-\alpha_\beta+\lambda_\beta-k/N)^2/2\sigma^2 \end{array} \right\}$$

where α_β & λ_β are functions of β and photon-detector parameters

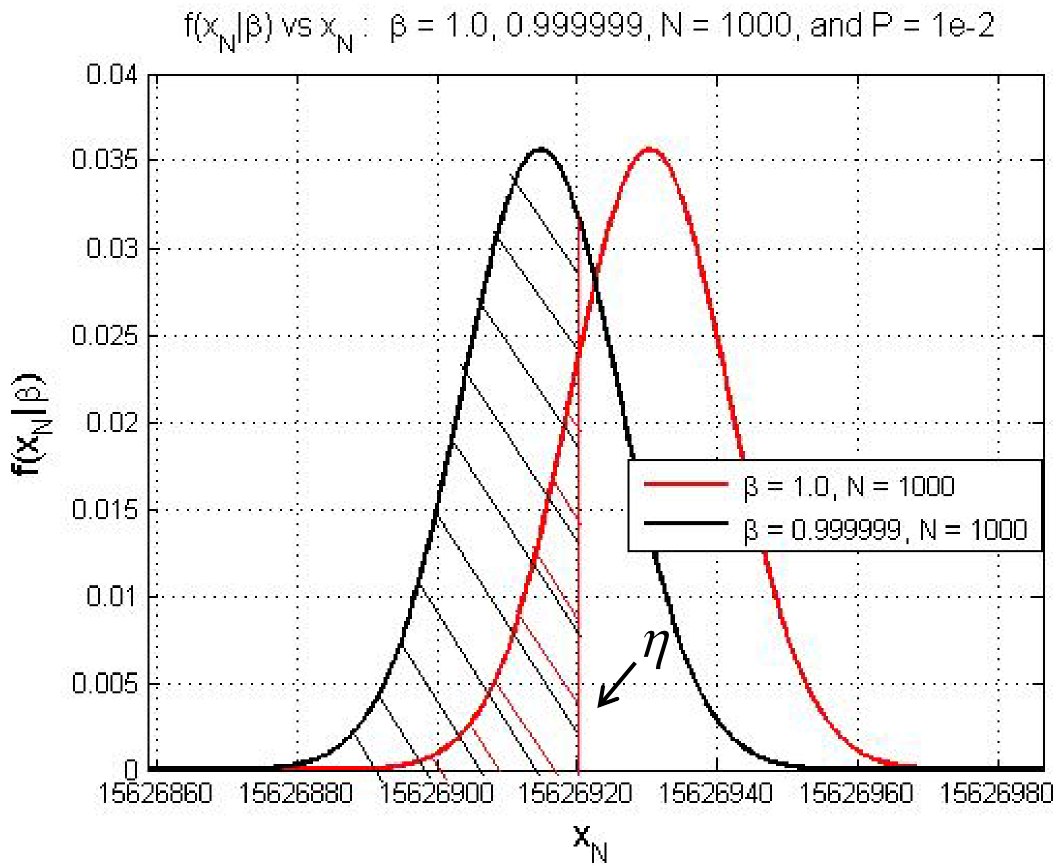
We use central limit theorem (CLT) to approximate $f(x_N|\beta)$ as a Gaussian pdf for $N \geq 100$:

$$f(x_N|\beta) = \frac{1}{\sqrt{2\pi(\lambda_\beta+\sigma^2)/N}} \exp\left\{ \frac{-(x_N-(\alpha_\beta+\mu))^2 N}{2(\lambda_\beta+\sigma^2)} \right\}$$

$E\{x_N\} = \alpha_\beta + \mu$

$\mathrm{var}\{x_N\} = (\lambda_\beta + \sigma^2)/N$

Neyman-Pearson Decision Rule: Single-Peak



Single-Peak Detection

$$P_D = \int_{-\infty}^{\eta} f(x_N|\beta < 1)dx_N$$

$$P_{FA} = \int_{-\infty}^{\eta} f(x_N|\beta = 1)dx_N$$

ESNR

Essential *SNR* (*ESNR*) is defined as the ratio of signal power to the averaged (over the 2 hypotheses) noise power corrupting the signal.

$$ESNR = \frac{2N(1-\beta)^2 I_p^2}{qI_p(1+\beta)/T_w + 4q(I_p + I_d)\Delta f + \frac{8kT_o}{R}\Delta f}$$

$$= \frac{2N(\alpha_{\beta=1} - \alpha_{\beta<1})^2}{(\lambda_{\beta=1} + \lambda_{\beta<1}) + 2\sigma^2}$$

Differential of ESNR

We can analyze the sensitivity of *ESNR* to system parameters by computing the differential of *ESNR* defined by

$$dESNR = \frac{\partial ESNR}{\partial \alpha_{\beta=1}} d\alpha_{\beta=1} + \frac{\partial ESNR}{\partial \lambda_{\beta=1}} d\lambda_{\beta=1} + \frac{\partial ESNR}{\partial \sigma^2} d\sigma^2 + \frac{\partial ESNR}{\partial N} dN$$

where

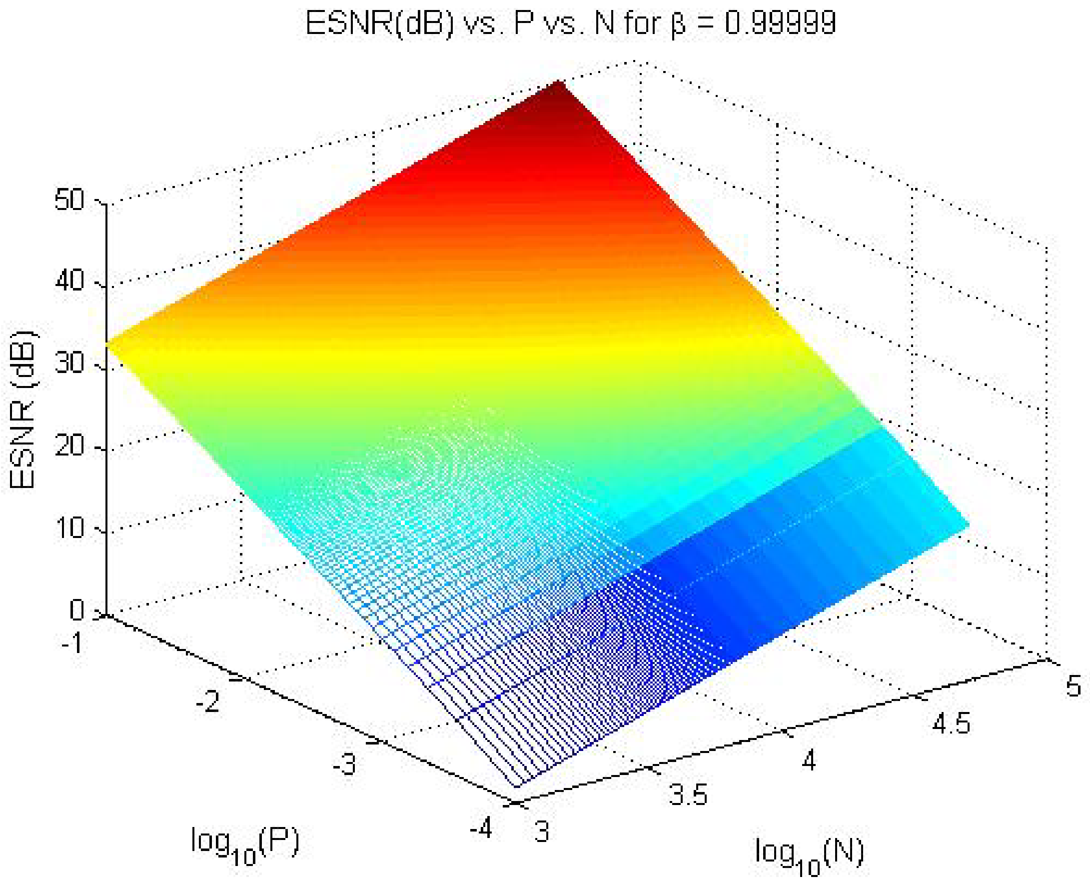
$$\frac{\partial ESNR}{\partial \alpha_{\beta=1}} = \frac{4N\alpha_{\beta=1}(1-\beta)^2(2(\lambda_{\beta=1}+\sigma^2)-\alpha_{\beta=1}(1-\beta)) - 2N\alpha_{\beta=1}^2(1-\beta)^2(\beta-1)}{(2(\lambda_{\beta=1}+\sigma^2)-\alpha_{\beta=1}(1-\beta))^2}$$

$$\frac{\partial ESNR}{\partial \lambda_{\beta=1}} = \frac{\partial ESNR}{\partial \sigma^2} = \frac{-4N\alpha_{\beta=1}^2(1-\beta)^2}{(2(\lambda_{\beta=1}+\sigma^2)-\alpha_{\beta=1}(1-\beta))^2}$$

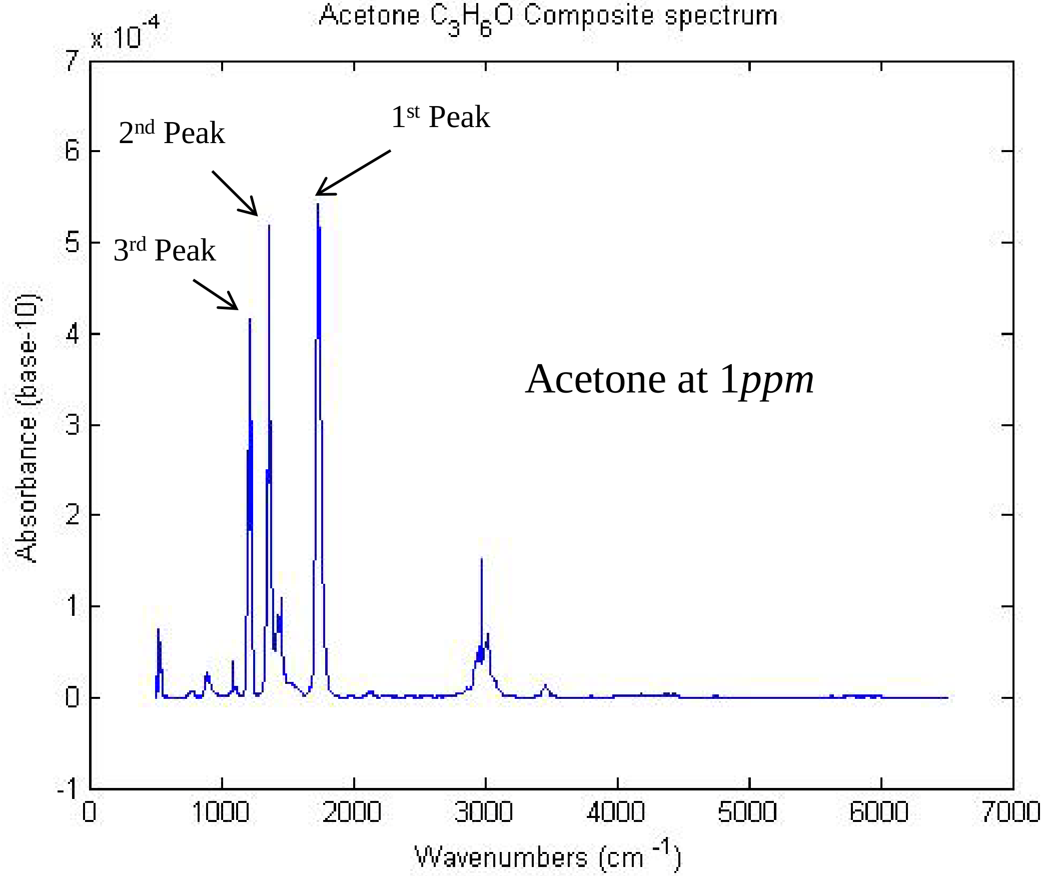
$$\frac{\partial ESNR}{\partial N} = \frac{2\alpha_{\beta=1}^2(1-\beta)^2}{2(\lambda_{\beta=1}+\sigma^2)-\alpha_{\beta=1}(1-\beta)}$$

ESNR

ESNR(dB) vs. *P* vs. *N* for β = 0.9999



Example Gas Spectrum (PNNL Data)



From PNNL data, ε = - 24.15 (log β)/(1*ppm*·1m) at 296° K.

PNNL ~ Pacific Northwest National Laboratory

Beer-Lambert Law

$$A = -\log T = -\log \beta = \varepsilon bc$$

$$\varepsilon = \frac{-24.15(L/mol) \cdot \log \beta}{1\,ppm \cdot 1m} = 24.15 \cdot \Delta$$

where A ~ absorbance

$\beta = T$ ~ transmittance

ε ~ molar absorptivity ($L \cdot mol^{-1} \cdot m^{-1}$)

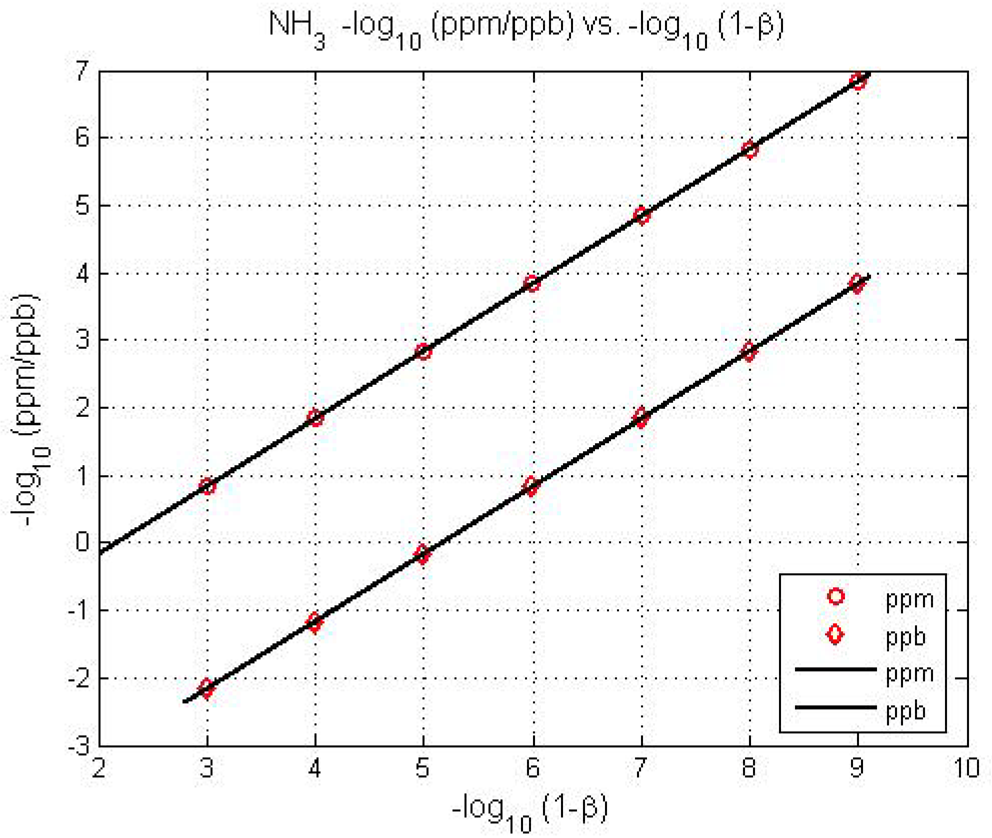
b ~ optical cavity length (m)

c ~ concentration (mol/L)

Δ = - (log β)/(1ppm.1m)

Concentration (*ppm/ ppb*) vs β

Concentration (*ppm/ ppb*) vs β at peak-1 of Ammonia (NH_3)



3-Peaks Joint Detection

For gas detection:

- Perform *independent* absorption-spectral-peak detection on each of the 3 *largest spectral peaks* of the gas.
- Obtain P_{Di}, $i = 1, 2, 3$, for the same P_{FA} defined by η_i

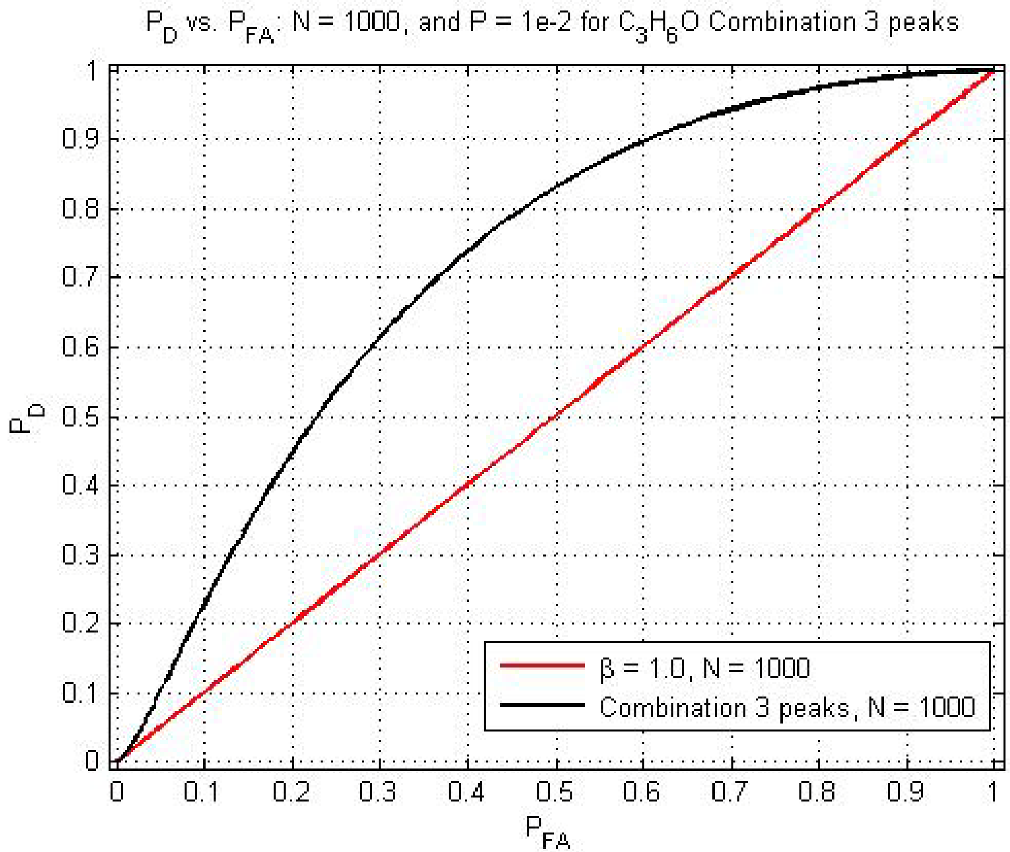
$$P_{Di} = \int_{-\infty}^{\eta_i} f(x_N \mid \beta_i < 1) dx_N$$

$$P_{FA} = \int_{-\infty}^{\eta_i} f(x_N \mid \beta_i = 1) dx_N$$

- Overall gas detection achieved with $P_D = P_{D1} \times P_{D2} \times P_{D3}$, corresponding to the joint detection of all 3 peaks of the gas.

3-Peaks Joint Detection

3-Peak P_D vs P_{FA} corresponding to Acetone @ 1*ppb*



β Estimation and Reliability

For each peak the independent β-estimate, $\hat{\beta}_i$, $i = 1, 2, 3$, is

$$\hat{\beta}_i = (x_{Ni} - \mu)/\alpha_{\beta=1}$$

where $E\{x_{Ni}\} = \beta_i \alpha_{\beta=1} + \mu$ and $x_{N\,i} = \hat{\beta}_i\, \alpha_{\beta=1} + \mu$ for $\beta_i < 1$.

We can obtain the corresponding confidence-interval upper and lower limits, β_{max} and β_{min}, for each peak are obtained from

$$\beta = 0.5\left[C(\hat{\beta}) \pm \sqrt{C^2(\hat{\beta}) - 4D(\hat{\beta})} \right]$$

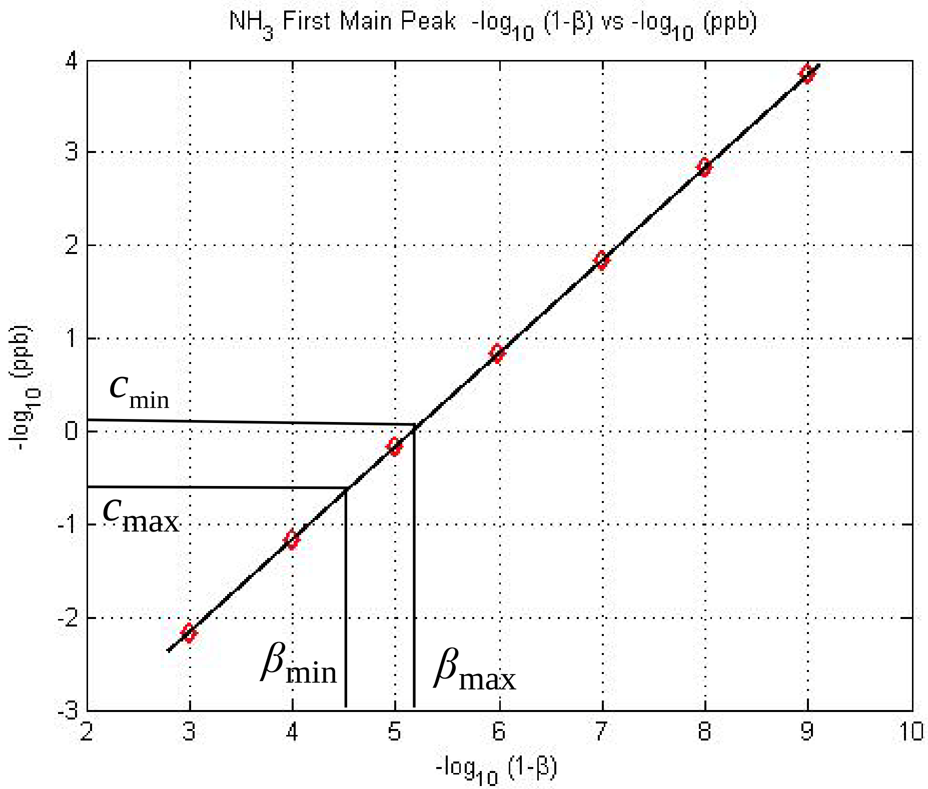
where

$$C(\hat{\beta}) = 2\hat{\beta} + \left(\frac{t}{\alpha_{\beta=1}}\right)^2 \left(\frac{\lambda_{\beta=1} - \varphi}{N}\right) \qquad \varphi = \lambda_{\beta=1} - \alpha_{\beta=1}$$

$$D(\hat{\beta}) = \hat{\beta}^2 + \left(\frac{t}{\alpha_{\beta=1}}\right)^2 \left(\frac{\sigma^2 + \varphi}{N}\right)$$

Concentration-Estimate Reliability

Concentration error bounds, c_{min} and c_{max}, can be obtained from corresponding β_{max} and β_{min}. Concentration-estimate error ~ $(c_{max} - c_{min})/\ \hat{c}$



Concentration-Estimate Results

17 trace gases at 1*ppb*, *P* = 1e-2w, *N* = 1000, and P_{FA} = 0.1 for photodetector DET 10D

Gas	P_D	1st Peak c-error (ppb)	1st Peak ESNR (dB)
C_3H_6O	0.23	288.78%	4.825
NO	0.065	246.01%	7.059
C_5H_{12}	0.02	204.37%	9.975
H_2O	0.11	203.32%	10.062
C_5H_8	0.23	141.48%	13.353
CH_2O	0.17	122.53%	14.602
C_2H_4	0.1	101.07%	16.275
CH_4	0.1	99.98%	16.369
CO	0.11	93.69%	16.934
C_2H_6	0.028	87.19%	17.558
NH_3	0.085	68.64%	19.636
HNO	0.91	48.68%	22.62
N_2O	0.93	47.77%	22.784
COS	0.31	32.39%	26.159
CS_2	0.2	31.39%	26.43
C_2H_2	0.7	15.33%	32.659
CO_2	1	13.01%	34.085

Concentration-Estimate Results

17 trace gases at 1*ppb*, *P* = 1e-1w, *N* = 50k, and P_{FA} = 0.1 for photodetector DET 10D

Gas	P_D	1st Peak *c*-error (*ppb*)	1st Peak *ESNR* (dB)
C_3H_6O	1	16.86%	31.826
NO	0.353	13.04%	34.060
C_5H_{12}	0.477	9.32%	36.976
H_2O	1	9.23%	37.063
C_5H_8	1	6.32%	40.354
CH_2O	1	5.47%	41.603
C_2H_4	1	4.51%	43.276
CH_4	0.912	4.46%	43.370
CO	0.408	4.18%	43.934
C_2H_6	1	3.89%	44.559
NH_3	1	3.07%	46.637
HNO	1	2.17%	49.620
N_2O	1	2.13%	49.785
COS	1	1.45%	53.160
CS_2	1	1.40%	53.431
C_2H_2	1	0.68%	59.660
CO_2	1	0.58%	61.086

Concentration-Estimate Results

17 trace gases at 1*ppb*, P = 1e-1w, N = 50k, and P_{FA} = 0.1 for photodetector G8422-03

Gas	P_D	1st Peak c-error (*ppb*)	1st Peak *ESNR* (dB)
C_3H_6O	1	42.99%	23.702
NO	0.177	33.24%	25.936
C_5H_{12}	0.209	23.76%	28.852
H_2O	0.812	23.53%	28.940
C_5H_8	1	16.11%	32.231
CH_2O	0.961	13.95%	33.479
C_2H_4	1	11.51%	35.152
CH_4	0.403	11.38%	35.246
CO	0.193	10.67%	35.811
C_2H_6	0.86	9.93%	36.435
NH_3	0.991	7.81%	38.513
HNO	1	5.54%	41.497
N_2O	1	5.44%	41.661
COS	1	3.69%	45.036
CS_2	1	3.57%	45.308
C_2H_2	1	1.75%	51.536
CO_2	1	1.48%	52.962

Summary and Conclusions

Summary & Conclusions

- Simplified the statistical analysis model to simulate the results efficiently, based on the CLT.
- Used the model to simulate the performance of detecting 3-main peaks of a trace gas using parameters from PNNL data.
- Investigated the accuracy of gas concentration estimation through confidence interval method.
- Better gas detection and concentration estimation performance obtained through increasing N and P and by appropriate choice of device.
- The statistical analysis model adaptable to other system components via specifying their parameter values.

Thank You

Questions ?