



MQO

P. Thunis, D. Pernigotti, M. Gerboles (JRC)

- *A formulation of the MQO based on observation uncertainty:*

$$MQO_{\text{hourly/daily}} = \frac{RMSE}{RMS_U}$$

$$MQO_{\text{yearly}} = \frac{BIAS}{2U}$$

- *Assumptions are made to derive a simple formulation for the observation uncertainty (e.g. data reference year)*
- *MQO are currently available for NO₂ (h/y), O₃(8h) and PM₁₀ (d/y)*

Points addressed



- *Testing the robustness of the formulation*
 - **Extended datasets**
 - **Further tests on specific hypotheses**

- *Extending the formulation to new species*

"u" formulation



European
Commission

Hourly / daily

$$u^2 = u_{RV}^2 (1 - \alpha) C^2 + u_{RV}^2 \alpha RV^2$$

Yearly

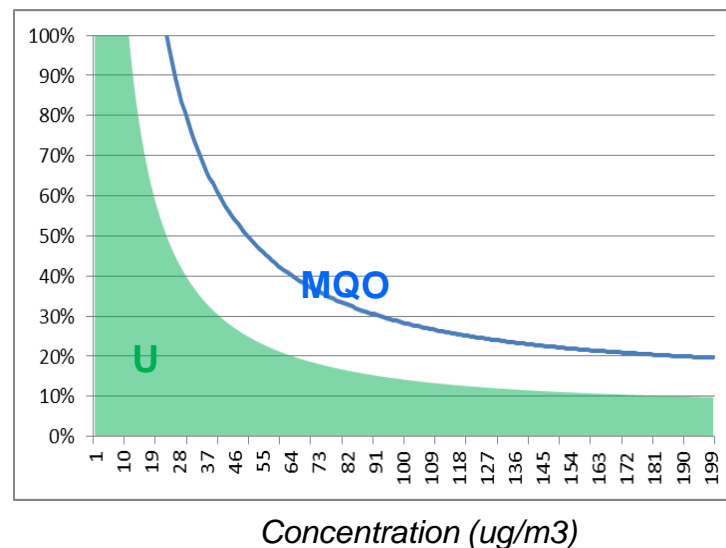
$$u^2 = \frac{u_{RV}^2 (1 - \alpha) C^2}{N_p} + \frac{u_{RV}^2 \alpha RV^2}{N_{np}}$$

u_{RV} Uncertainty at the reference value

α Degree of proportionality

RV Reference value (free user choice)

N_p, N_{np} Yearly fitting coefficients



NO2 robustness (I)

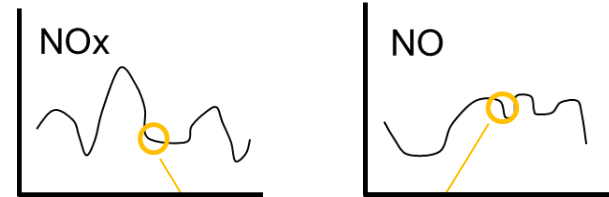


European Commission

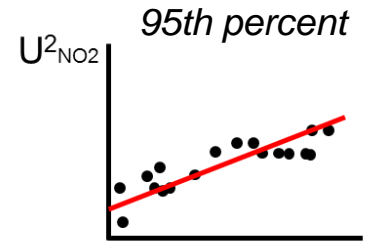
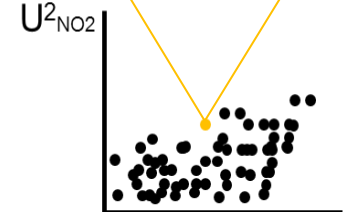
Hourly NO2: GUM approach

	Hourly values, u		Annual values, u		D,%/rand	T
	Min	Max	Min	Max		
b_{0, b_1}						
NO_x Zero(0)	$2/3^{1/2}$	$2/3^{1/2}$	$2/(0.5x4x3)^{1/2}$	$2/(0.5x2x3)^{1/2}$	R, R; R, R, 50%	pn
NO Zero(0)	$1/3^{1/2}$	$1/3^{1/2}$	$1/(0.5x4x3)^{1/2}$	$1/(0.5x2x3)^{1/2}$	R, R; R, R, 50%	pn
NO_x/NO Zero, (0)						
Repeatability at zero	0.1	$1/3^{1/2}$	$0.1/(24x3)^{1/2}$	$1/(4x3)^{1/2}$	N,R; R, R, 100%	pn
Long term zero drift	0.58	$4/3^{1/2}$	$0.58/(0.5x24)^{1/2}$	$4/(0.5x24x3)^{1/2}$	N, R; N,R, 50% ⁽ⁱ⁾	pn
% of Span (200,750)	1%	2.5%	1%	2.5%	NN; N, N, 0%	p
b_1						
% of Span _r (200,750)						
Repeatability	0.1	0.75%	$0.1/(24)^{1/2}$	$0.75\%/(24)^{1/2}$	N, N; N,N, 100%	p
Long term span drift	1.44%	$5\%/3^{1/2}$	0.29%	$5\%/(0.5x24x3)^{1/2}$	N,R; N, R, 50%	p
Repeatability	0.1	0.75%	$0.1/(N_{eff})^{1/2}$	$0.75\%/(N_{eff})^{1/2}$	N, 100%	p
Lack of Fit, linearity	$5/3^{1/2}$	$Max(5,4\%)/3^{1/2}$	0.18%	$Max(5,4\%)/N_{eff}3^{1/2}$	R, 100%	pn
$NO_{x,r}, NO_r$						
Pressure change		0.06		0.01		n
Temperature		0.7		0.18		n
Voltage change		0.02		0.0		n
Sampling ⁽ⁱⁱ⁾		$2\%/3^{1/2}$		$2\%/(0.5x2N_{eff}x3)^{1/2(iii)}$	N, 50%	p
H_2O	$2\%+2\% \cdot (14/9)/6^{1/2}$	$4\%+4\% \cdot (14/9)/6^{1/2}$	$2\%^{(iv)}$	4%	Mean Tr	p
$NO_{x,r}$						
PAN ^(v)	$1/6^{1/2}$	$7/6^{1/2}$	0.2	1		n
CO ₂		0.35		0.13		n
NH ₃ & NHO ₃	0	0	0	0		n
HNO ₂		$0.5+2.2/6^{1/2}$		0.5	Mean T	n
eff (0.95,1)	0.5%	2%	0.5%	2%	N, 0%	p
Missing data (90%)			0%	0.5%		p

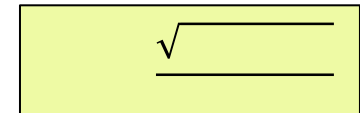
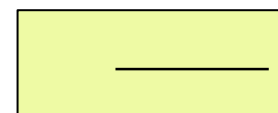
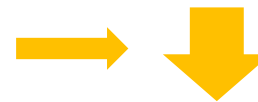
() [()]



All hours
All stations



NO₂²

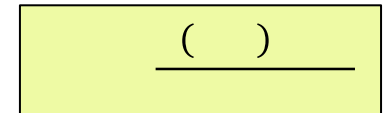
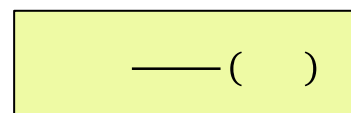
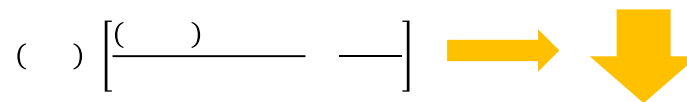
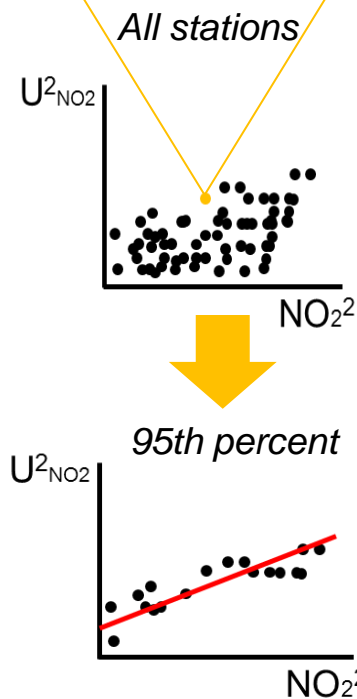
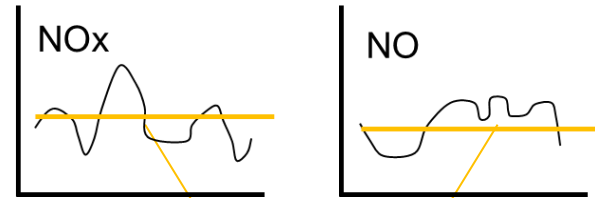


NO2 robustness (II)

European Commission

Yearly NO2: GUM approach

	Hourly values, u		Annual values, u		D,%rand	T
	Min	Max	Min	Max		
b_{0x}, b_{1x}						
NOx Zero(0)	2/3 ^{3x}	2/3 ^{3x}	2/(0.5x4x3) ^{3x}	2/(0.5x2x3) ^{3x}	R, R, R, R, 50%	pn
NO Zero(0)	1/3 ^{3x}	1/3 ^{3x}	1/(0.5x4x3) ^{3x}	1/(0.5x2x3) ^{3x}	R, R, R, R, 50%	pn
NOx/NO Zero, (0)						
Repeatability at zero	0.1	1/3 ^{3x}	0.1/(24x3) ^{3x}	1/(4x3) ^{3x}	N,R; R, R, 100%	pn
Long term zero drift	0.58	4/3 ^{3x}	0.58/(0.5x24) ^{3x}	4/(0.5x24x3) ^{3x}	N, R; N,R, 50 % ⁽ⁱ⁾	pn
% of Span, (200,750)	1%	2.5%	1%	2.5%	NN; N, N, 0%	p
b_{1y}						
% of Span, (200,750)						
Repeatability	0.1	0.75%	0.1/(24) ^{3x}	0.75%/(24) ^{3x}	N, N; N,N, 100%	p
Long term span drift	1.44%	5%/3 ^{3x}	0.29%	5%/(0.5x24x3) ^{3x}	N,R; N, R, 50%	p
Repeatability	0.1	0.75%	0.1/(N _{eff}) ^{3x}	0.75%/(N _{eff}) ^{3x}	N, 100%	p
Lack of Fit, linearity	5/3 ^{3x}	Max(5,4%)/3 ^{3x}	0.18%	Max(5,4%)/N _{eff} 3 ^{3x}	R, 100%	pn
NO_{2x}, NO_x						
Pressure change		0.06		0.01		n
Temperature		0.7		0.18		n
Voltage change		0.02		0.0		n
Sampling ⁽ⁱⁱ⁾		2%/3 ^{3x}		2%/(0.5xN _{eff} x3) ^{3x(iii)}	N, 50%	p
H ₂ O	2%+2%.(14/9)/6 ^{3x}	4%+4%.(14/9)/6 ^{3x}	2% ^(iv)	4%	Mean Tr	p
NO_{2z}						
PAN ^(v)	1/6 ^{3x}	7/6 ^{3x}	0.2	1		n
CO ₂		0.35		0.13		n
NH ₃ & NHO ₃	0	0	0	0		n
HNO ₂	0.5+2.2/6 ^{3x}		0.5	0.5	Mean T	n
eff (0.95,1)	0.5%	2%	0.5%	2%	N, 0%	p
Missing data (90%)			0%	0.5%		p

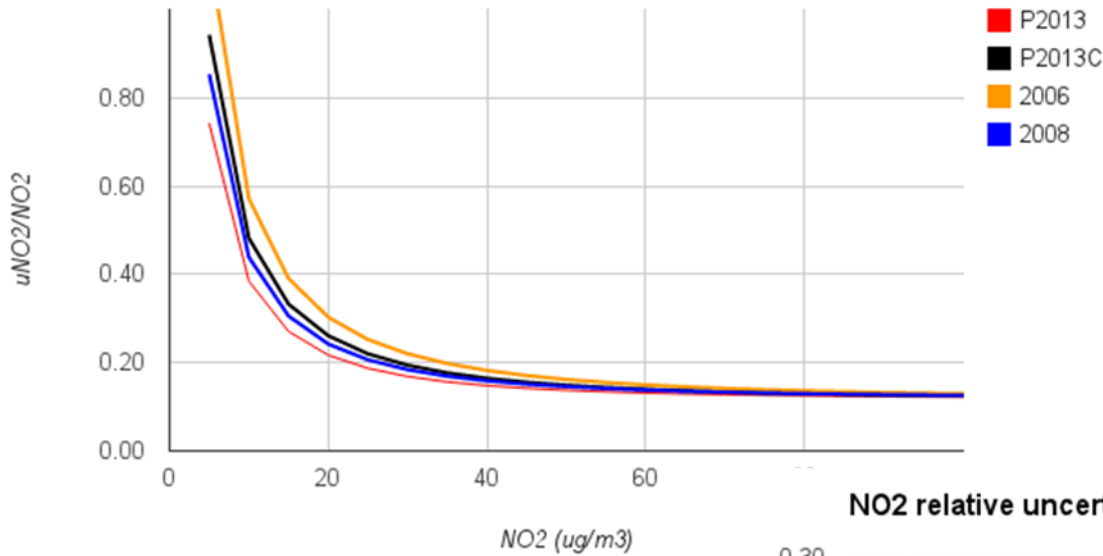


NO2 robustness (III)



European
Commission

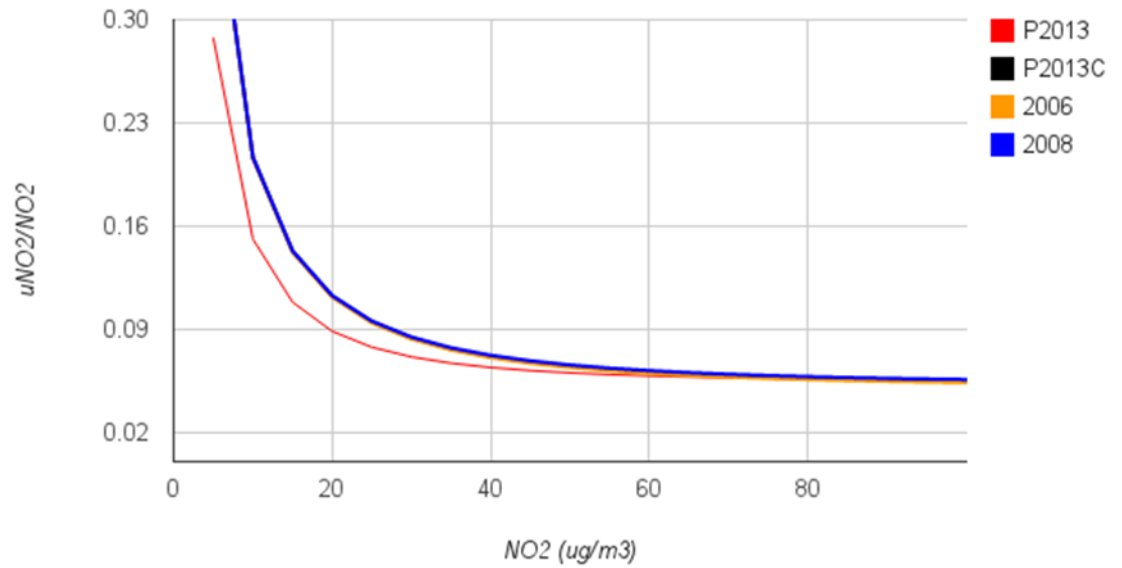
NO2 relative uncertainty



Hourly

Yearly

NO2 relative uncertainty



NO2 robustness (IV)

European
Commission

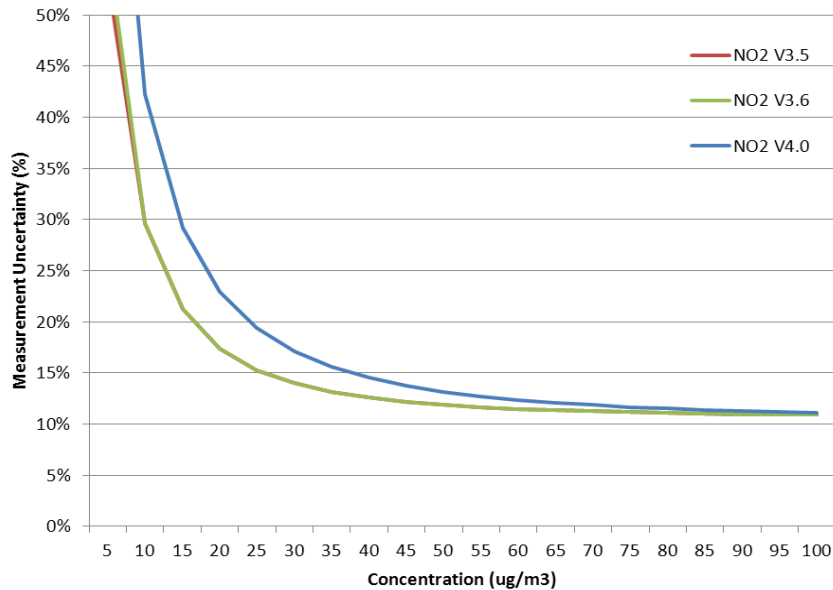
Yearly

	k	UrLV	alpha	LV	Np	Nnp
NO2 V3.5	2	0.12	0.02	200	4.7	6.7
NO2 V3.6	2	0.12	0.04	200	5	12
NO2 V4.0	2	0.12	0.04	200	5.2	5.5

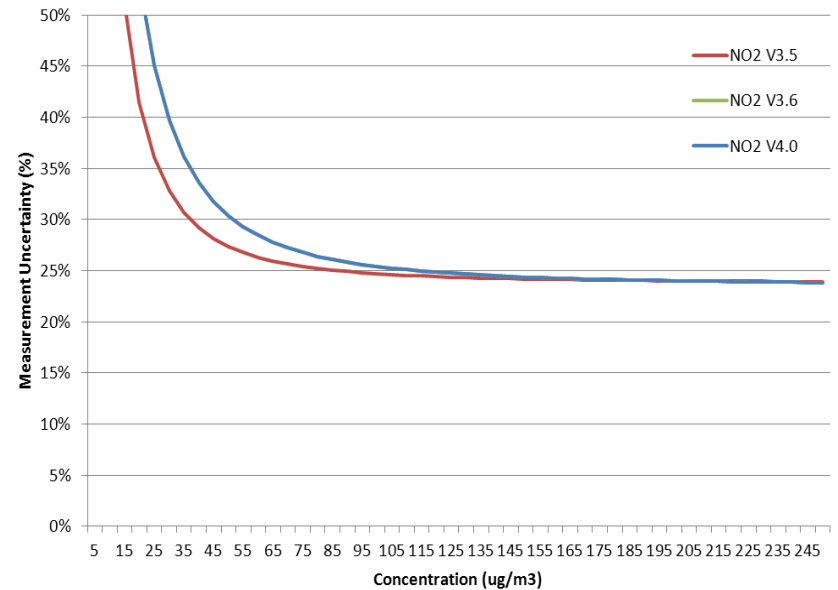
Hourly

	k	UrLV	alpha	LV
NO2 V3.5	2	0.12	0.02	200
NO2 V3.6	2	0.12	0.04	200
NO2 V4.0	2	0.12	0.04	200

Relative uncertainties for yearly averages



Relative uncertainties for hourly values



PM10 robustness



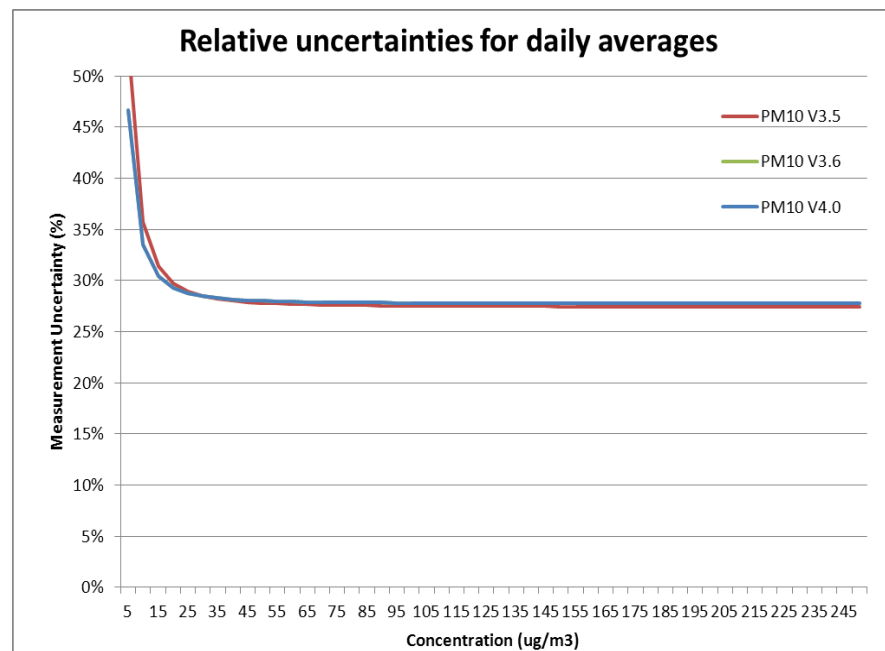
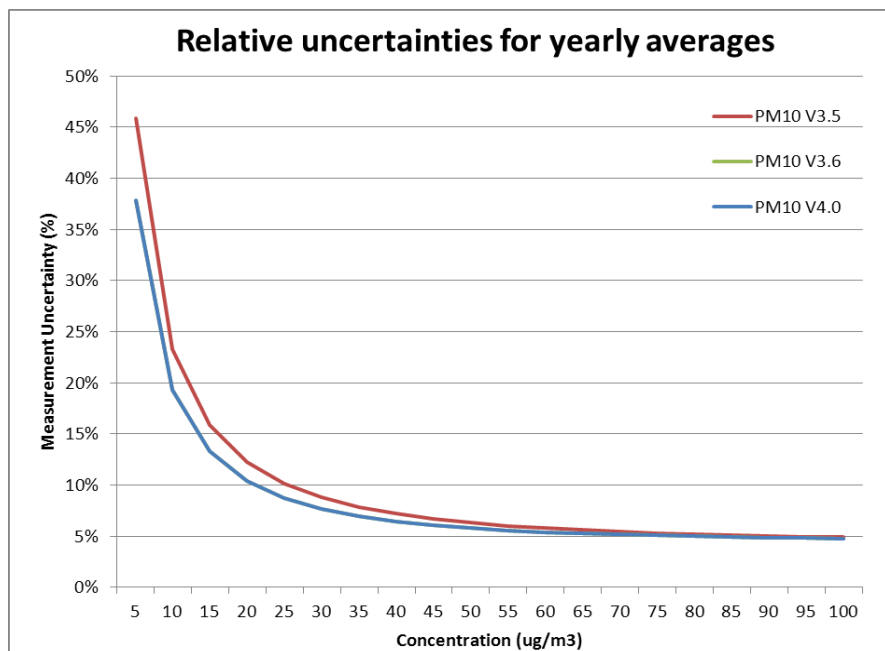
European
Commission

Yearly

Daily

	k	UrLV	alpha	LV	Np	Nnp
PM10 V3.5	2	0.139	0.027	50	40	1
PM10 V3.6	2	0.14	0.018	50	40	1
PM10 V4.0	2	0.14	0.018	50	40	1

	k	UrLV	alpha	LV
PM10 V3.5	2	0.139	0.027	50
PM10 V3.6	2	0.14	0.018	50
PM10 V4.0	2	0.14	0.018	50



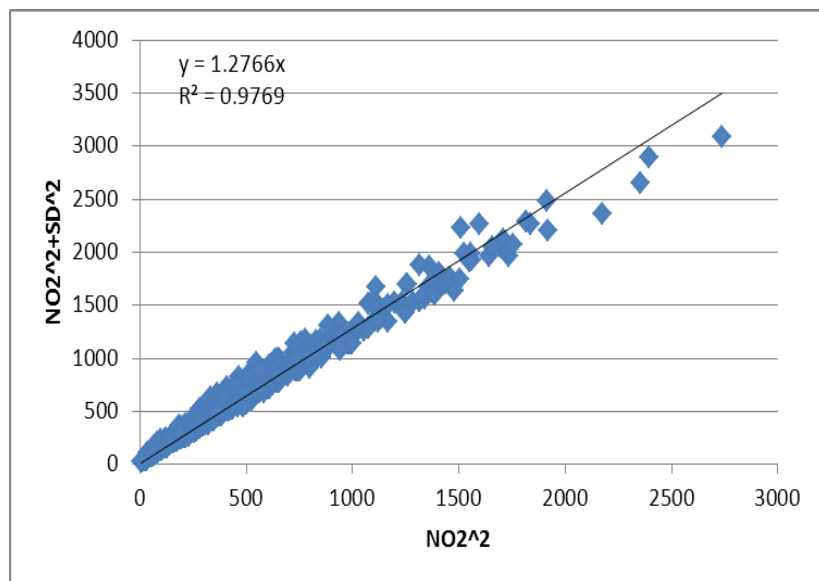
Robustness of the assumptions (I)



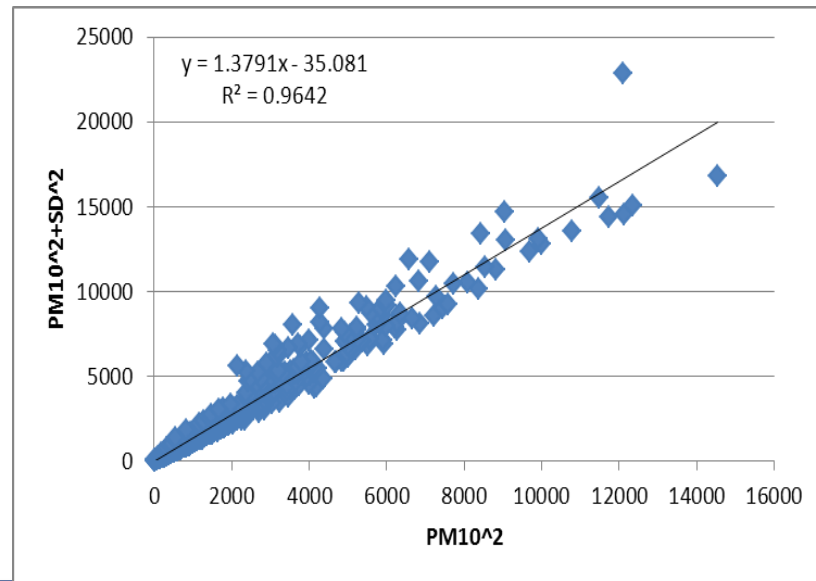
► Linearization of the standard deviation term

$$u(\bar{C}) = u^{RV} \sqrt{\frac{1-\alpha}{N_p^*} |\bar{C}^2 + \sigma^2| + \frac{\alpha RV^2}{N_{np}}} \cong u^{RV} \sqrt{\frac{1-\alpha}{N_p^*} k\bar{C}^2 + \frac{\alpha RV^2}{N_{np}}} \cong u^{RV} \sqrt{\frac{1-\alpha}{N_p} \bar{C}^2 + \frac{\alpha RV^2}{N_{np}}}$$

$$|NO_2|^2 = k \left(|NO_2|^2 + \sigma_{NO_2}^2 \right)$$



$$|PM_{10}|^2 = k \left(|PM_{10}|^2 + \sigma_{PM_{10}}^2 \right)$$

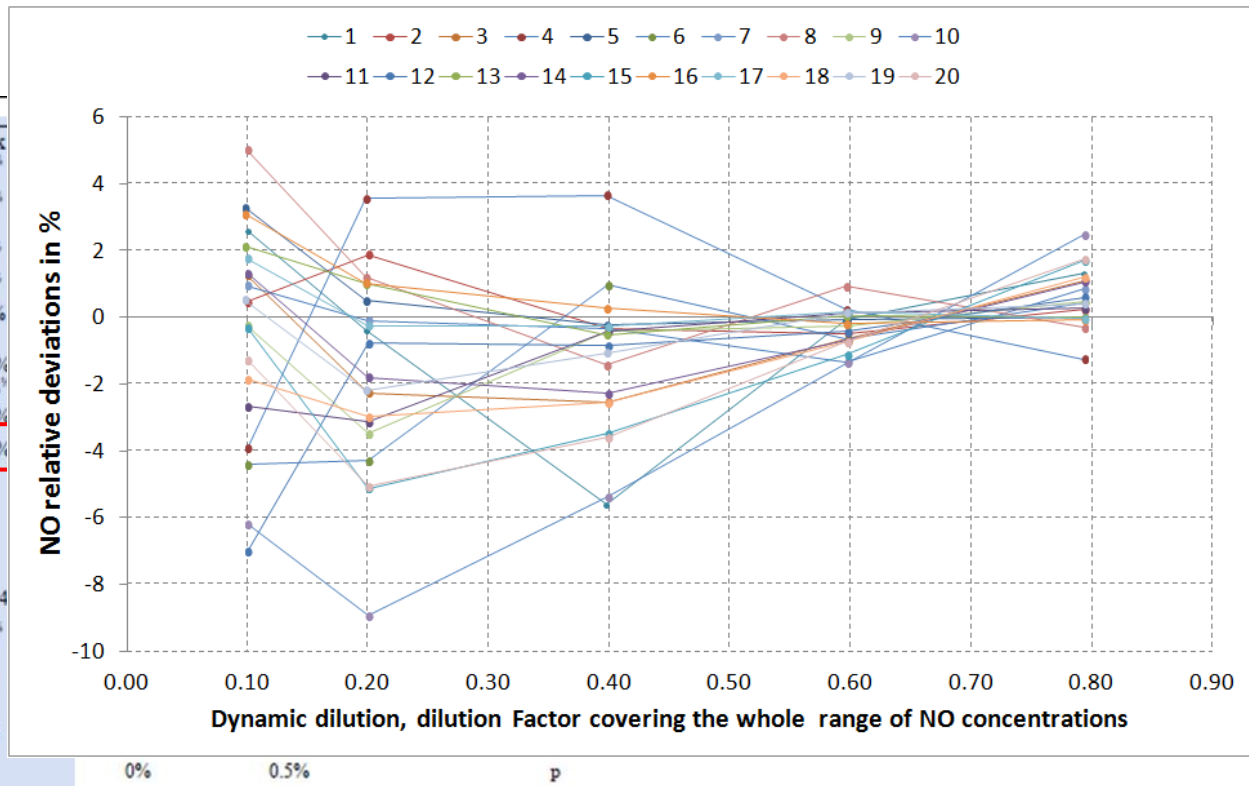


Robustness of the assumptions (II)



➤ Linearity of NO₂ automatic analysers - check of the randomness of the linearity deviations

		Hourly values, u	
		Min	Max
b_0, b_1	NO _x Zero(0)	2/3 ^{1/2}	2/3 ^{1/2}
	NO Zero(0)	1/3 ^{1/2}	1/3 ^{1/2}
	NO _x /NO Zero _r (0)		
	Repeatability at zero	0.1	1/3 ^{1/2}
	Long term zero drift	0.58	4/3 ^{1/2}
b_1	% of Span _r (200,750)	1%	2.5%
	% of Span _r (200,750)		
	Repeatability	0.1	0.75%
	Long term span drift	1.44%	5%/3 ^{1/2}
	Repeatability	0.1	0.75%
NO _{x,r} , NO _r	Lack of Fit, linearity	5/3 ^{1/2}	Max(5,4%)
	Pressure change		0.06
	Temperature		0.7
	Voltage change		0.02
	Sampling ⁽¹⁰⁾		2%/3 ^{1/2}
	H ₂ O	2%+2%.(14/9)/6 ^{1/2}	
NO _{x,r}	PAN ⁽¹⁷⁾	1/6 ^{1/2}	7/6 ^{1/2}
	CO ₂		0.35
	NH ₃ & NHO ₃	0	0
	HNO ₂		0.5+2.2/6 ^{1/2}
eff (0.95,1)		0.5%	2%
Missing data (90%)			

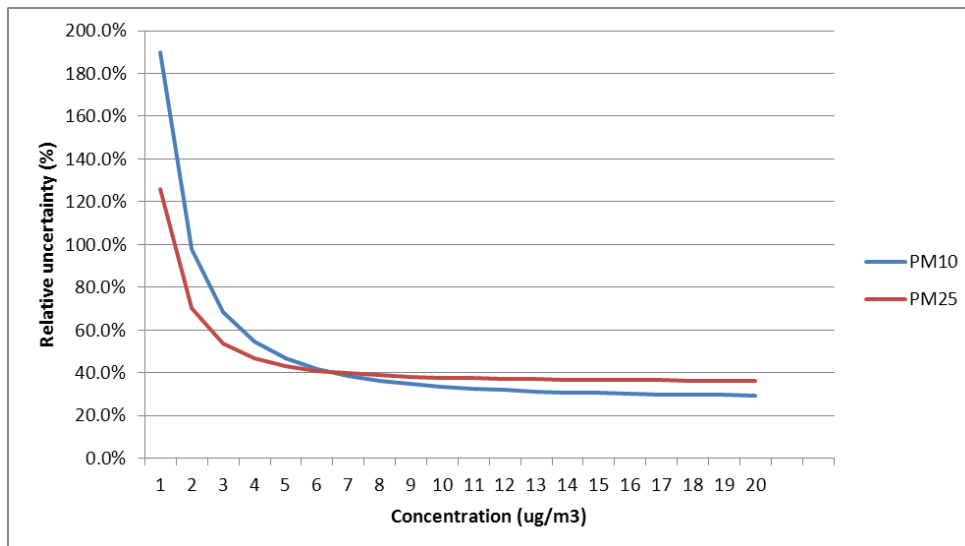


Extension to new species (I)

European
Commission

PM2.5

- *Based on 140 days of gravimetric measurements (JRC inter-comparison exercise)*
- *No significant results for TEOM and beta-ray (not enough measurements!)*



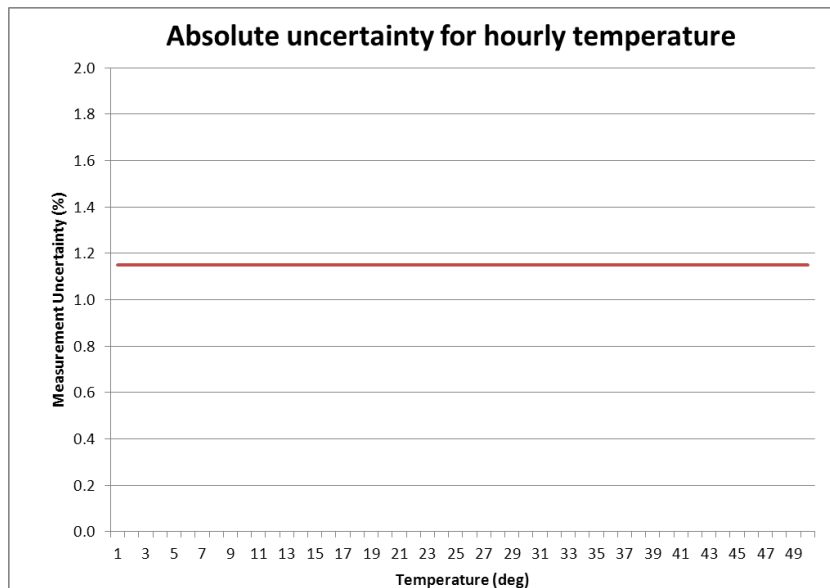
	RV	UrRV	alpha
PM10	50	0.14	0.018
PM2.5	25	0.18	0.018

Extension to new species (II)



Temperature

- Instrument uncertainty is extremely low (0.1 degree)
- Shield structure leads to larger error around one degree (Leroy 2002)
- Assumption made: equi-probable uncertainty (rectangular distribution) leading to $u=0.57\text{ C}$



	RV	UrRV	alpha
TEMP	25	0.023	1

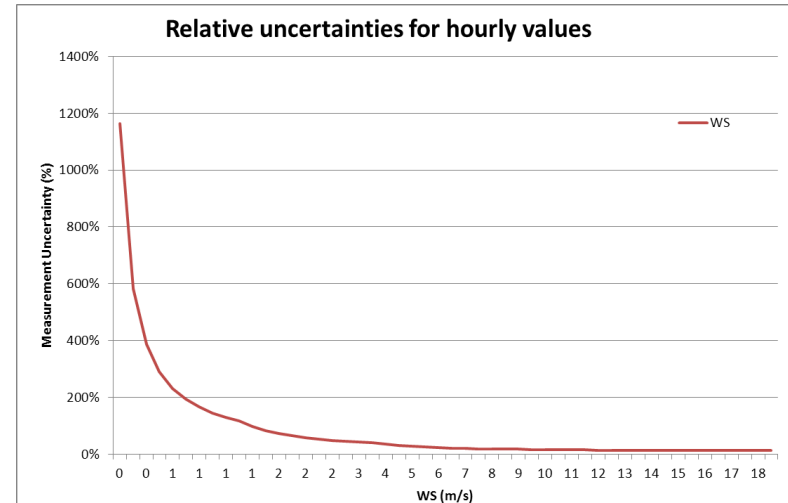
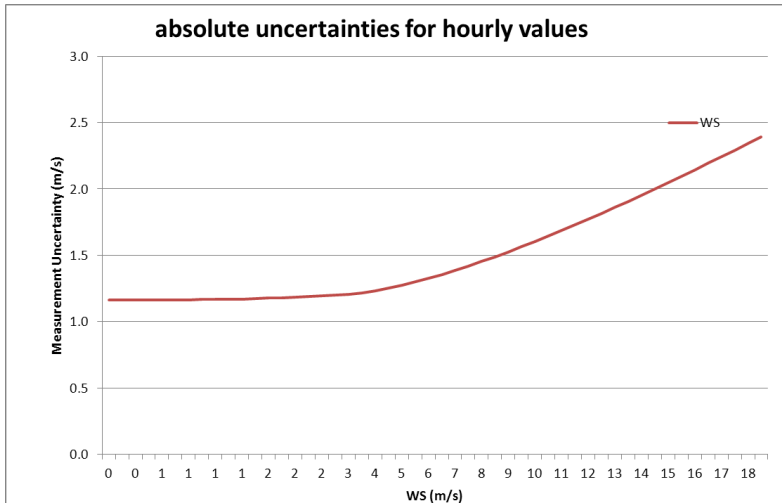
Extension to new species (III)

European
Commission

Wind-speed

	RV	UrRV	alpha
TEMP	5	0.13	0.8

- *Difficulty to use real datasets*
- *Assumption WMO taken as basis (0.5 fixed below 5 m/s and proportional 10% above).*
- *In addition: equi-probable 0.5 m/s due to integer rounding*

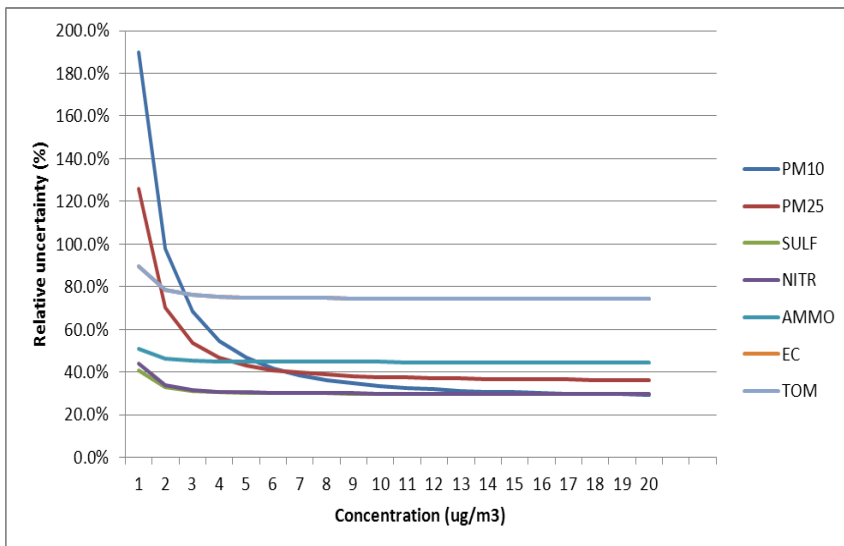


Extension to new species (IV)



PM components

- *RV and urRV from expert judgments*
- *Alpha, Np and Nnp similar to PM10 and PM2.5*



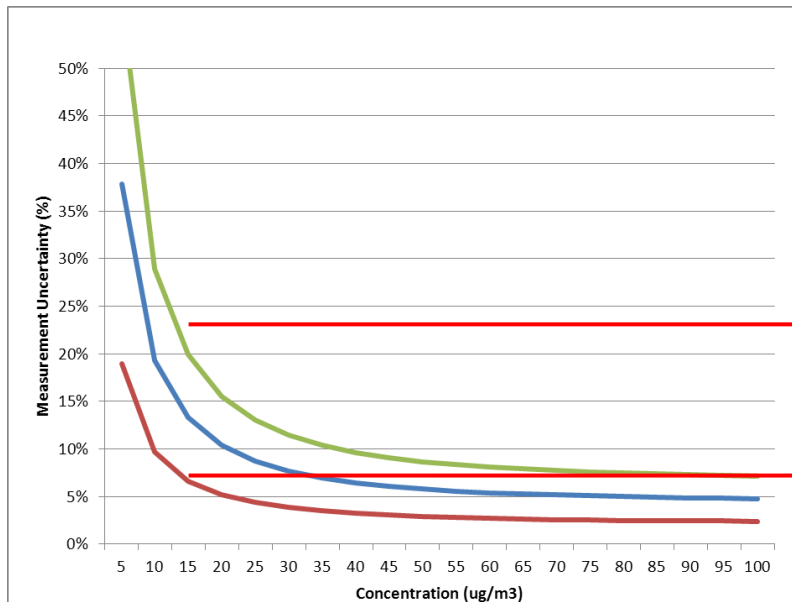
	RV	UrRV	α	Np	Nnp
SO4	7	0.15	0.018	40	1
NO3	8	0.15			
NH4	4	0.225			
EC	5	0.375			
TOM	10	0.375			

Conclusions (I)



- *NO₂ and PM₁₀ MQO seem to be robust as well as underlying assumptions*
- *A new MQO is available for testing (PM_{2.5})*
- *Other MQO (WS, TEMP, PM components) have been derived for other projects. Of interest to FAIRMODE?*

Conclusions (II)



MQO is not ambitious enough
Everybody succeeds – Useless

MQO is too ambitious
Nobody succeeds – Useless

- *What is important is to relate the model error to the observation uncertainty and assume a realistic functional relationship (U)*
- *Ways exist to tune the MQO to an adequate compromise in terms of stringency (coverage factor (K), max. vs. mean uncertainty...)*