# A global sensitivity study of sulphur chemistry in a premixed methane flame model using HDMR

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2 HDMR - High Dimensional Model Representation

- 3 Application and Results
- 4 HDMR Software

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2 HDMR - High Dimensional Model Representation

3 Application and Results

### HDMR Software

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- 3 Application and Results
- 4 HDMR Software

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### Need for new methods in sensitivity analysis

- Complex chemical mechanisms are increasingly used in models describing a range of important chemical processes (e.g. combustion)
- Models contain a large number of parameters and are often highly non-linear
- Large uncertainty ranges for the parameters
- Models are computationally expensive to run
- Traditional methods for global uncertainty and sensitivity analysis not suitable due to their computational expense and the difficulty in interpreting the results
- Aim: method that can cope with large parameter numbers
- Do we need a screening method, which identifies unimportant parameters beforehand?

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# High Dimensional Model Representation (HDMR)

### HDMR basics

 Output f(x) of a model can be expressed as finite hierarchical function expansion in terms of the input parameters x

$$f(\mathbf{x}) = f_0 + \sum_{i=1}^n f_i(x_i) + \sum_{1 \le i < j \le n} f_{ij}(x_i, x_j) + \ldots + f_{12\dots n}(x_1, x_2, \ldots, x_n)$$

- Usually HDMR expansion to second order provides satisfactory results and a good description of f(x)
- Provides detailed input-output mapping suitable to create a model replacement and for global SA
- Several decomposition methods: e.g. cut-HDMR, RS-HDMR

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# Random Samping (RS)-HDMR

### Principles

- Only one set of random samples necessary to estimate all component functions
- Component functions can be approximated by analytical basis functions such as polynomials or splines

$$f_{i}(x_{i}) \approx \sum_{r=1}^{k} \alpha_{r}^{i} \varphi_{r}(x_{i})$$
  
$$f_{ij}(x_{i}, x_{j}) \approx \sum_{p=1}^{l} \sum_{q=1}^{l'} \beta_{pq}^{ij} \varphi_{p}(x_{i}) \varphi_{q}(x_{j})$$

• Here: $\varphi_r(x_i)$ ,  $\varphi_p(x_i)$  and  $\varphi_q(x_j)$  orthonormal polynomials

# Random Samping (RS)-HDMR extension

#### Optimisation of the polynomial expansion order (1)

- Usually the same polynomial order is used for all first-order and second-order component functions respectively
- Order of the polynomial approximation should be chosen separately for each component function
- Optimisation algorithm is based on least square method
- Sum of square errors is calculated using the results of the full model runs and the approximation of the component functions by various orders (e.g. 0th to 5th order)
- Smallest sum of square errors indicates the best approximation order for the corresponding component function

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# Random Samping (RS)-HDMR extension

### Optimisation of the polynomial expansion order (2)

- Exclude component functions which do not contribute (identified as 0th order by optimisation)
- Threshold to exclude unimportant component functions (not identified as 0th order, but only very small contribution to overall value)
- Idea: avoid the need for screening methods
- Low computational effort to calculate optimal order for all polynomials
- Improvement in the accuracy of the final model replacement

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# Global sensitivity analysis

### Sensitivity Indices

- Sensitivity Indices measure the effect of one or more input parameters on the output
- S<sub>i</sub> measures the effect of x<sub>i</sub> (fractional contribution)
- S<sub>ii</sub> measures the interactive effect of x<sub>i</sub> and x<sub>i</sub>

#### Computation

• Easily calculated from the HDMR expansion (no additional full model runs required), e.g.

$$D_i pprox \sum_{r=1}^{k_i} (lpha_r^i)^2 \qquad S_i = rac{D_i}{D_i}$$

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# Application

#### Modelling in combustion

- Aim: development of combustion applications with low emissions of pollutants such as nitrogen and sulphur oxides
- Design of low emission technologies depends on accurate computational models describing combustion processes
- Trace amounts of sulphur in fuel can have an impact on the extent of nitrogen oxide emissions
- Models required which describe the interaction of sulphur containing compounds with other species within flames

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# Application

#### Methane flame model

- Premixed methane flame model describing the influence of sulphur containing compounds on the formation of nitrogen oxides
- Assessment of the resulting uncertainty in predictions of nitrogen oxide emissions is important to improve the confidence in the design process
- Modelling using CHEMKIN and simulation using PREMIX
- Model contains large number of parameters (with large uncertainty ranges)
- 177 uncertain parameters: 153 reactions rates and 24 heats of formation (calculated by NASA polynomials)

#### Investigated scenarios

- Output of interest: NO concentration
- Uncertainty ranges for all parameters according to min and max value with equal probability
- Ranges for the 153 reaction rates according to Tomlin (2006)
- 3 different sets of ranges for the 24 heats of formation:
- **①**  $\Delta$ **Hf** = ±10**KJ** for all 24 parameters (assume equal uncertainties)
- Ranges according to Burcat table if available (ΔHf SN = ±105KJ) (http://technicon.ac.il/~aer0201)
- ③ Ranges according to Burcat table, but △Hf SN = +13KJ (based on updated value for heats of formations for SN according to Peebles and Marshal (2002) with smaller uncertainty range)

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### HDMR set up

- Second order RS-HDMR expansion
- Approximation of the component function by orthonormal polynomials
- Quasi-random sampling (N=1024)
- Optimisation of the polynomial order:
  - Maximum order for approximation of first-order component functions: 10
  - Maximum order for approximation of second-order component functions: 3
- Excluding component functions via threshold
- Correlation method for variance reduction (Li et. al 2002)
- HDMR method including all 177 parameters

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- Sample size: N=1024
- Threshold to exclude component functions: 1 %

### Optimal polynomial order

#### 5 of 177 first-order component functions are non-zero

- 2 have been approximated by 1st-order polynomials
- 2 have been approximated by 2nd-order polynomials
- 1 has been approximated by 8th-order polynomial

• 0 of 15576 second-order component functions are non-zero

- Sample size: N=1024
- Threshold to exclude component functions: 0.001 %

### Optimal polynomial order

• 51 of 177 first-order component functions are non-zero

- 25 have been approximated by 1st-order polynomials
- 17 have been approximated by 2nd-order polynomials
- 6 have been approximated by 3rd-order polynomials
- 1 has been approximated by 4th-order polynomial
- 1 has been approximated by 5th-order polynomial
- 1 has been approximated by 9th-order polynomial
- 4 of 15576 second-order component functions are non-zero
  - 4 have been approximated by 1st-order polynomials

#### Accuracy - variance

- No additional full model runs required
- Variance full model runs (N=1024):  $D = 1.7367 \cdot 10^{-8}$
- Variance 1st-order model replacement:  $\hat{D}_{1st} = 1.7002 \cdot 10^{-8} \rightarrow 97.89\%$
- Variance 2nd-order model replacement:  $\hat{D}_{2nd} = 1.7043 \cdot 10^{-8} \rightarrow 98.13\%$

#### Accuracy - Relative Error (RE)

- Additional set of full model runs required (N=2000)
- Ist-order model replacement 5 % RE: 99.50 %
- 2nd-order model replacement 5 % RE: 99.65 %

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### Results - Scenario 3 (Burcat table, $\Delta$ Hf SN = +13KJ)

#### Scatter plots



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### Scatter plots + first-order RS-HDMR component function



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### Results - Scenario 3 (Burcat table, $\Delta$ Hf SN = +13KJ)

### Scatter plots + first-order RS-HDMR component functions



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### First and second-order sensitivity indices (N=1024)

Parameter	Rank	$S_i$
SO + NH = NO + SH	1	0.5956
SO + N = NO + S	2	0.2758
$\mathrm{SO} + \mathrm{OH} = \mathrm{SO}_2 + \mathrm{H}$	3	0.0735
ΔHf SO	4	0.0140
$\mathrm{SH} + \mathrm{NH} = \mathrm{NS} + \mathrm{H}_2$	5	0.0111
$\sum S_i$		0.9784
Parameter 1	Parameter 2	$S_{ij}$
$SO + OH = SO_2 + H$	SO + NH = NO + SH	0.0018
SH + H = H2 + S	$\mathrm{SH} + \mathrm{NH} = \mathrm{NS} + \mathrm{H}_2$	0.0015
$\mathbf{S} + \mathbf{C}\mathbf{S}_2 = \mathbf{C}\mathbf{S} + \mathbf{S}_2$	$\mathrm{HS}_2 + \mathrm{H} + \mathrm{M} = \mathrm{H}_2 \mathrm{S}_2 + \mathrm{M}$	0.0005
$H_2S+M=H_2+S+M$	$S + NO_2 = NO + SO$	0.0004
$\sum S_{ij}$		0.0042
		0.0000

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# Results - comparison of all scenarios

### First-order sensitivity indices (N=1024)

	Scenario 1		Scenario 2		Scenario 3	
	$(\Delta Hf = \pm 10 KJ)$		$(\Delta Hf SN = \pm 105 KJ)$		$(\Delta Hf SN = +13KJ)$	
Parameter	S <sub>i</sub> (Rank)		<i>S<sub>i</sub></i> (Rank)		<i>S<sub>i</sub></i> (Rank)	
SO + NH = NO + SH	0.2297	(3)	0.3631	(1)	0.5956	(1)
SO + N = NO + S	0.1007	(4)	0.1219	(3)	0.2758	(2)
$SO + OH = SO_2 + H$	0.0255	(5)	0.0316	(4)	0.0735	(3)
$\Delta$ Hf SO	0.3082	(1)	0.0101	(5)	0.0140	(4)
$SH + NH = NS + H_2$	0.0035		0.0019		0.0111	(5)
$\Delta$ Hf SO <sub>2</sub>	0.2874	(2)	0		0	
$\Delta$ Hf SN	0.0001		0.3479	(2)	0.0001	
$\sum S_i$	0.9771		0.8904		0.9784	
S	0.9842		0.9055		0.9826	

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#### Improvement of the accuracy

- RS-HDMR method using 177 inputs (N=4096)
- Morris Method to identify unimportant parameters first (N=1780) + RS-HDMR method using 47 inputs (N=1024)

	RS-HDMR	<b>RS-HDMR</b>	Screening + RS-HDMR
	(N=1024)	(N=4096)	(N=1780+1024)
1st-order 5 % RE	85.85 %	90.40%	89.90 %
2nd-order 5 % RE	86.25 %	94.80 %	95.30 %

### First-order sensitivity indices

- RS-HDMR method using 177 inputs (N=4096)
- Morris Method to identify unimportant parameters first (N=1780) + RS-HDMR method using 47 inputs (N=1024)

	RS-HDMR		Screening + RS-HDMR		
Parameter	$S_i$	(Rank)	$S_i$	(Rank)	
ΔHf SN	0.3815	(1)	0.3855	(1)	
SO + NH = NO + SH	0.3700	(2)	0.3719	(2)	
SO + N = NO + S	0.1344	(3)	0.1365	(3)	
$SO + OH = SO_2 + H$	0.0410	(4)	0.0386	(4)	
ΔHf SO	0.0086	(5)	0.0087	(5)	
$\sum S_i$	0.9524		0.9590		
S	0.9695		0.9755		

### Results - Scenario 2 (Burcat table, $\Delta$ Hf SN = $\pm$ 105KJ)

### First-order RS-HDMR component functions and scatter plot



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### First-order RS-HDMR component functions and scatter plot



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### Graphical User Interface for RS-HDMR

🛃 <student version=""> : RS-HDMR GUI Ver</student>	s. 0.1 - Setup	_ = ×
File Help		r
_ Sample files		
Sample input-file (for HDMR): Sample output-file (for HDMR):	177 Inputs and 10000 Samples 1 Output and 4096 Samples	
Sample input–file (for accuracy test): Sample output–file (for accuracy test):	177 Inputs and 2000 Samples 1 Output and 2000 Samples	
Settings		
Number of samples to use for HDMR: Number of samples to use for accuracy test + Max order for approximation of 1st-order cor Max order for approximation of 2nd-order co	- scatter plots: mponent functions : mponent functions :	1024 1000 9 3
Variance reduction method : Number of iterations for 1st-order componen Number of iterations for 2nd-order componen	correlation 100 10	
Do you want to use a threshold? Value of threshold for 1st–order component f Value of threshold for 2nd–order component	iunctions (in %): functions (in %):	yes • 0.001 0.001
Default		ОК

HDMR Software

### Graphical User Interface for RS-HDMR

File    Help    •      Results    Ist-order    51 out of 177 first-order component functions are computed to be non-zero      Ist-order    S1 out of 177 first-order component functions are computed to be non-zero      Component functions approximated by    Ist-order polynomials: 25      Ist-order polynomials:    17      3rd-order polynomials:    17      Ist-order polynomials:    1      Sth-order polynomials:    1      Output:    0      Output:    1      Output:    1      Accuracy    Relative Error	🛃 <student th="" v<=""><th>'ersion&gt; : RS-HDMR GUI Vers.</th><th>0.1 - Results</th><th></th></student>	'ersion> : RS-HDMR GUI Vers.	0.1 - Results	
Results    First-order component functions for output: 1      S1 out of 177 first-order component functions are computed to be non-zero      Ist-order    Component functions approximated by      Ind-order    1st-order polynomials: 25      Accuracy    3rd-order polynomials: 17      3rd-order polynomials: 6    4th-order polynomials: 1      Sth-order polynomials: 0    5th-order polynomials: 0      2nd-order    7th-order polynomials: 0      9th-order polynomials: 1    1      Output:    10th-order polynomials: 0      4    9th-order polynomials: 0	File Help			ы
Results    51 out of 177 first-order component functions are computed to be non-zero      Ist-order    Component functions approximated by      Ind-order    1st-order polynomials: 25      Accuracy    Ist-order polynomials: 17      Sth-order polynomials: 17    3rd-order polynomials: 6      Accuracy    4th-order polynomials: 1      Ist-order    5th-order polynomials: 0      Ist-order    7th-order polynomials: 0      Sth-order polynomials: 1    0      Output:    10th-order polynomials: 0      I		First-order component function	ons for output: 1	
1st-order    Component functions approximated by      2nd-order    1st-order polynomials:    25      2nd-order polynomials:    17      Accuracy    3rd-order polynomials:    17      1st-order    Sth-order polynomials:    1      2nd-order polynomials:    1    1      2nd-order    Sth-order polynomials:    0      2nd-order    Sth-order polynomials:    0      2nd-order    Sth-order polynomials:    0      2nd-order    Sth-order polynomials:    0      3th-order polynomials:    1    0      Output:    10th-order polynomials:    0      1    Accuracy - Relative Fror	Results	51 out of 177 first-order cor	nponent functions are computed to be non-zero	
2nd-order  1st-order polynomials:  25    2nd-order polynomials:  17    Accuracy  3rd-order polynomials:  17    1st-order  5th-order polynomials:  1    2nd-order  5th-order polynomials:  1    2nd-order  7th-order polynomials:  0    2nd-order  7th-order polynomials:  0    3th-order polynomials:  1  0    2nd-order  7th-order polynomials:  0    3th-order polynomials:  1  0    0utput:  10th-order polynomials:  0    1  - Accuracy - Belative Fror  -	1st-order	Component functions approximated by		
Accuracy  2nd-order polynomials:  17    Accuracy  3rd-order polynomials:  6    1st-order  4th-order polynomials:  1    2nd-order  5th-order polynomials:  1    2nd-order  5th-order polynomials:  0    2nd-order  7th-order polynomials:  0    3th-order  9th-order polynomials:  1    Output:  10th-order polynomials:  0    1  - Accuracy - Belative Fror  -	2nd-order	1st-order polynomials:	25	
Accuracy    3rd-order polynomials:    6      1st-order    4th-order polynomials:    1      1st-order    5th-order polynomials:    1      2nd-order    7th-order polynomials:    0      8th-order polynomials:    0    3th-order polynomials:      0utput:    10th-order polynomials:    1      - Accuracy - Belative Frror    -		2nd-order polynomials:	17	
Accuracy  4th-order polynomials:  1    1st-order  5th-order polynomials:  1    2nd-order  7th-order polynomials:  0    3th-order polynomials:  0    9th-order polynomials:  1    0utput:  10th-order polynomials:    1  - Accuracy - Belative Fror	A	3rd–order polynomials:	6	
1st-order    5th-order polynomials:    1      2nd-order    6th-order polynomials:    0      2nd-order    7th-order polynomials:    0      9th-order polynomials:    1    0      Output:    10th-order polynomials:    0      1    - Accuracy - Relative Fror    -	Accuracy	4th-order polynomials:	1	
2nd-order      6th-order polynomials:      0        2nd-order      7th-order polynomials:      0        8th-order polynomials:      0        9th-order polynomials:      1        0utput:      10th-order polynomials:      0        1      - Accuracy - Relative Fror      -	1st–order	5th-order polynomials:	1	
2nd-order  7th-order polynomials:  0    8th-order polynomials:  0    9th-order polynomials:  1    Output:  10th-order polynomials:  0    1		6th-order polynomials:	0	
8th-order polynomials:  0    9th-order polynomials:  1    Output:  10th-order polynomials:  0    1  - Accuracy - Belative From	2nd-order	7th–order polynomials:	0	
Output:      9th-order polynomials:      1        1      10th-order polynomials:      0        1      - Accuracy - Relative Error		8th-order polynomials:	0	
Output: 10th-order polynomials: 0		9th-order polynomials:	1	
Accuracy - Relative Fron	Output:	10th-order polynomials:	0	
		Accuracy – Relative Error		
1% RE: 68.5 % 10% RE: 100 %	Exit	1% RE: 68.5 %	10% RE: 100 %	
5% RE: 99.8 % 20% RE: 100 %		5% RE: 99.8 %	20% RE: 100 %	

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HDMR Software

### Graphical User Interface for RS-HDMR



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### Conclusions

- RS-HDMR method provides straightforeward approach for global sensitivity analysis
- However, extension to existing HDMR tools necessary to explore large number of input parameters
- Optimisation method in combination with excluding component functions via a threshold is one useful extension
- Variance reduction method (correlation method, Li et. al 2003) useful to further improve accuracy
- Generally no screening method necessary in order to reduce the number of parameters, but using one can in certain cases reduce the computational effort
- Final ranking of the important parameters is critically dependent on the input ranges chosen

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