

65th LCA Discussion Forum Zurich - May 24, 2017



Prospective LCA modelling How to deal with uncertainties ?

Part I : A new approach based on GSA Part II : The Graphene Case study

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Part I

Global sensitivity analysis in LCA of emerging technologies:

Accounting for inputs' variability





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LCA of emerging technologies: addressing high uncertainty on inputs' variability when performing global sensitivity analysis; Science of the Total Environment, 578 (2017) 268-280

LCA for emerging technologies



Emerging technologies

- Wide data gap
- No pilot/large-scale data?
- Incomplete technology development
- Unknown future applications
- Data quality concerns





How to deal with uncertainty in LCA of emerging technologies?

*Case study: Enhanced Geothermal Systems (EGS) ARMINES

EGS: an emerging technology to exploit geothermal resources where water, heat or rock permeability are not sufficient for a conventional geothermal system

- Deep wells: 2.5 − 5 km ⇒ Drilling
- Reservoir stimulation (enhancement) → Fracturing the rock (e.g. by water pumping)
- For binary systems Organic
 Rankine cycle
- Ground-water use





Image: geothermalworldwide, 2016

General modelling framework for LCA





EGS: LCA model (GHG emissions)











| Symbol | Parameters | Baseline scenario |
|------------------|----------------------------|----------------------|
| Z | Borehole depth | 4000 m |
| Nw | Number of wells | 3 wells |
| d | Fuel for drilling | 5000 MJ/m |
| LT | Lifetime | 30 y |
| f | Produced flow rate | 62.5 kg/s |
| P _{ORC} | Installed capacity ORC | 2375 kW |
| SFe | Enhancement scaling factor | 5.25 |
| LF | Load factor | 0.90 |
| P _p | Specific power of pumps | 6.1 kW/(kg/s) |
| | | |

EGS: LCA model (GHG emissions)





$$\frac{\Psi}{GHG_{EGS,A}} \left[\frac{g \ CO_2 eq}{kWh} \right] = \frac{z_A \cdot Nw_A \cdot (\boldsymbol{\alpha_1} + \boldsymbol{\alpha_2} \cdot d_A) + LT_A \cdot f_A \cdot \boldsymbol{\alpha_3} + P_{ORC,A} \cdot LT_A \cdot \boldsymbol{\alpha_4} + Nw_A \cdot Sfe_A \cdot \boldsymbol{\alpha_5}}{LF_A \cdot LT_A \cdot \left(P_{ORC,A} - f_A \cdot P_{p,A}\right) \cdot 8760}$$

With $\alpha_1 = 498761.36 \text{ gCO}_2 eq/m$; $\alpha_2 = 90.56 \text{ gCO}_2 eq/MJ$; $\alpha_3 = 487363.03 \text{ gCO}_2 eq \cdot s/(kg \cdot y)$; $\alpha_4 = 50603.13 \text{ gCO}_2 eq/(kW \cdot y)$; $\alpha_5 = 25757089.05 \text{ gCO}_2 eq$

| Symbol | Parameters | Baseline scenario | Value range |
|------------------|----------------------------|----------------------|------------------------|
| Z | Borehole depth | 4000 m | 2000 – 6000 m |
| Nw | Number of wells | 3 wells | 2 – 3 wells |
| d | Fuel for drilling | 5000 MJ/m | 3000 – 7000 MJ/m |
| LT | Lifetime | 30 y | 20 – 40 y |
| f | Produced flow rate | 62.5 kg/s | 25 – 100 kg/s |
| P _{ORC} | Installed capacity ORC | 2375 kW | 1250 – 3500 kW |
| SFe | Enhancement scaling factor | 5.25 | 0.5 – 10 |
| LF | Load factor | 0.90 | 0.85 – 0.95 |
| Pp | Specific power of pumps | 6.1 kW/(kg/s) | 3.6 – 8.6 kW/(kg/s) |



















(Cucurachi et al. 2016; Lacirignola et al. 2017)

| Symbol | Parameters | Value range | Probability distribution |
|------------------|----------------------------|---------------------|---|
| z | Borehole depth | 2000 – 6000 m | Uniform |
| Nw | Number of wells | 2 – 3 wells | Uniform |
| d | Fuel for drilling | 3000 – 7000 MJ/m | Uniform |
| LT | Lifetime | 20 – 40 y | Normal distribution centered on LT=30 with σ =3.25 |
| f | Produced flow rate | 25 – 100 kg/s | Uniform |
| P _{ORC} | Installed capacity ORC | 1250 – 3500 kW | 2375 kW |
| SFe | Enhancement scaling factor | 0.5 – 10 | Lognormal distribution with σ =1, μ =0 and peak on Sfe=1 |
| LF | Load factor | 0.85 – 0.95 | Uniform |
| Pp | Specific power of pumps | 3.6 – 8.6 kW/(kg/s) | Uniform |









$$\begin{aligned} & GHG_{EGS,A}\left[\frac{g\ CO_2eq}{kWh}\right] \\ &= \frac{z_A\cdot Nw_A\cdot (\alpha_1+\alpha_2\cdot d_A) + LT_A\cdot f_A\cdot \alpha_3 + P_{ORC,A}\cdot LT_A\cdot \alpha_4 + Nw_A\cdot Sfe_A\cdot \alpha_5}{LF_A\cdot LT_A\cdot (P_{ORC,A}-f_A\cdot P_{p,A})\cdot 8760} \end{aligned}$$

Based on Sobol indices (variance decomposition method) to identify key parameters:

$$S_i = \frac{Var[E(Y|X_i)]}{Var(Y)} = \frac{V_i(Y)}{Var(Y)}$$

$$S_{ij} = \frac{V_{ij}(Y)}{Var(Y)} \qquad S_{ijk} = \frac{V_{ijk}(Y)}{Var(Y)}$$

(Cucurachi et al. 2016; Lacirignola et al. 2017)







EGS: Dependence of GSA results on PDF







For emerging technologies, characterizing inputs' probability distribution functions (PDF) may be difficult

> Which is the effect of changing PDF on inputs' ranking from GSA?

EGS: Dependence of GSA results on PDF





Global sensitivity analysis (Sobol' method)





EGS: Effect of PDFs on GSA results





Possible descriptions (probability distribution functions) for each of the 9 input parameters for EGS LCA model

(Lacirignola et al. 2017)

EGS: Effect of PDFs on GSA results



Changing the distribution function for 1 input parameter and keeps other distributions as baseline

| | - | | | | | | | | |
|-------------------------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|------------------|
| § GSA | z | SFe | f | d | LF | LT | Pp | Nw | P _{ORC} |
| §1 (Baseline) ×100 bootstraps | Baseline | Baseline |
| § 2 (×100) | TYPE 2 | Baseline | Baseline |
| § 3 (×100) | TYPE 3 | Baseline | Baseline |
| § 4 (×100) | TYPE 4 | Baseline | Baseline |
| § 5 (×100) | TYPE 5 | Baseline | Baseline |
| § 6 (×100) | Baseline | TYPE 2 | Baseline | Baseline | Baseline | Baseline | Baseline | Baseline | Baseline |
| § 7 (×100) | Baseline | TYPE 3 | Baseline | Baseline | Baseline | Baseline | Baseline | Baseline | Baseline |
| § 8 (×100) | Baseline | TYPE 4 | Baseline | Baseline | Baseline | Baseline | Baseline | Baseline | Baseline |
| § 9 (×100) | Baseline | TYPE 5 | Baseline | Baseline | Baseline | Baseline | Baseline | Baseline | Baseline |
| [] | [] | [] | [] | [] | [] | [] | [] | [] | [] |
| § 32 (×100) | Baseline | TYPE 2 |
| § 33 (×100) | Baseline | TYPE 3 |
| § 34 (×100) | Baseline | TYPE 4 |
| § 35 (×100) | Baseline | TYPE 5 |
| § 34 (×100) § 35 (×100) | Baseline Baseline | TYPE 4 TYPE 5 |

(Lacirignola et al. 2017)





For example, using the 5 possible distribution functions for **LIFETIME (LT)**:



EGS: Effect of PDF on GSA results



For each of the 9 input parameters







Considering 3500 rankings after iterative GSA:



EGS: application of GSA results



Identification of **5** key input parameters among the **9** initial ones

→ Simplified model for LCA of EGS facilities

$$GHG_{EGS_Reduced} \left[\frac{gCO_2eq}{kWh} \right] = f(P_{ORC}, N_w, z, LT, f)$$
$$= \frac{Nw \cdot (\omega_1 \cdot z + \omega_2) + LT \cdot (\omega_3 \cdot f + \omega_4 \cdot P_{ORC})}{LT \cdot (P_{ORC} - f \cdot \omega_5)} \pm 5 \ gCO_2eq/kWh$$

$$\begin{split} \omega_1 &= 120.70 \left[gCO_2 eq/(m \cdot h/y) \right]; \ \omega_2 &= 5 \ 161.87 \left[gCO_2 eq/(h/y) \right]; \\ \omega_3 &= 61.82 \left[gCO_2 eq \cdot s/(kg \cdot h) \right]; \ \omega_4 &= 6.42 \left[gCO_2 eq/(kWh) \right]; \ \omega_5 &= 6.10 \left[(kW \cdot s)/kg \right]; \end{split}$$





• From complete parametric model

$$GHG_{EGS}\left[\frac{g\ CO_2eq}{kWh}\right] = \frac{z\ \cdot Nw\ \cdot (\boldsymbol{\alpha_1} + \boldsymbol{\alpha_2} \cdot d\) + LT\ \cdot f\ \cdot \boldsymbol{\alpha_3} + P_{ORC} \cdot LT\ \cdot \boldsymbol{\alpha_4} + Nw\ \cdot Sfe\ \cdot \boldsymbol{\alpha_5}}{LF\ \cdot LT\ \cdot \left(P_{ORC} - f\ \cdot P_p\right) \cdot 8760}$$

• to simplified model

$$GHG_{EGS_Reduced}\left[\frac{gCO_2eq}{kWh}\right] = \frac{Nw \cdot (\boldsymbol{\omega_1} \cdot z + \boldsymbol{\omega_2}) + LT \cdot (\boldsymbol{\omega_3} \cdot f + \boldsymbol{\omega_4} \cdot P_{ORC})}{LT \cdot (P_{ORC} - f \cdot \boldsymbol{\omega_5})}$$

ADVANTAGES

- ✓ Reduced number of input parameters (From 9 to 5)
- ✓ For some of the least influencing parameters, data were difficult to obtain → Simplified model facilitates data gathering

Conclusions & perspectives



- Need for a specific approach to deal with large uncertainty of emerging technologies in LCA
- Global Sensitivity Analysis (GSA) based on variancedecomposition methods (e.g. Sobol) allows key parameter identification and ranking
- The protocol proposed for GSA of emerging technologies helped to evaluate the influence of **distribution functions** of input parameters in GSA results
- a simplified parametric equation to estimate GHG impact from a reduced number of parameters was obtained.
- We aim to apply the same approach to deduce a set of simplified equations for a multi-criteria LCA

Part II: GSA applied to nanomaterials

 Case study: Graphene (GR) production by chemical reduction process (Based on publication by Arvidsson et al. 2014)







| Symbols | Parameters | Baseline scenario |
|---------|---|-----------------------|
| Par 1 | Graphite + Potassium permanganate (KMnO ₄) + Hydrazine | 2.55 g / g of GR |
| Par 2 | Electricity RER medium voltage - 1 | 8.5 MJ / g of GR |
| Par 3 | Peroxide (H ₂ O ₂) | 4.675 g / g of GR |
| Par 4 | Phosphoric acid $(H_3PO_4) + Sulfuric acid (H_2SO_4)$ | 33.15 g / g of GR |
| Par 5 | Deionised water | 0.935 g / g of GR |
| Par 6 | Electricity RER medium voltage - 2 | 0.15 MJ / g of GR |
| Par 7 | Transport - lorry >32 tons class 5 | 0.259 kg·km / g of GR |

(Based on publication by Arvidsson et al. 2014)

Model for graphene production



7 independent input parameters



Graphene production: Parameters' contribution



Baseline result: 1.7 kg CO2 eq./g of GR



- Graphite + Potassium permanganate (KMnO4) + Hydrazine
- Electricity RER medium voltage 1
- Peroxyde (H2O2)
- Phosphoric acid (H3PO4) + Sulfuric acid (H2SO4)
- Deionised water
- Electricity RER medium voltage 2
- Transport lorry >32 tons class 5

Carbon footprint contribution

- 1. Electricity for Hummers' process (Par 2)
- 2. Acids (Par 4)
- 3. Graphite + $KMnO_4$ + Hydrazine (Par 1)
- 4. Electricity for chemical reduction (Par 6)
- 5. Peroxide (Par 3)
- 6. Transport (Par 7)
- 7. Deionised water (Par 5)



| Symbols | Daramatora | Pacolina cooparia | CCD ² |
|---------|---|-----------------------|-------------------|
| Symbols | Parameters | Baseline scenario | (Pedigree Matrix) |
| Par 1 | Graphite + Potassium permanganate (KMnO ₄) + Hydrazine | 2.55 g / g of GR | 1.51 |
| Par 2 | Electricity RER medium voltage - 1 | 8.5 MJ / g of GR | 1.51 |
| Par 3 | Peroxide (H ₂ O ₂) | 4.675 g / g of GR | 1.51 |
| Par 4 | Phosphoric acid (H_3PO_4) + Sulfuric acid (H_2SO_4) | 33.15 g / g of GR | 1.51 |
| Par 5 | Deionised water | 0.935 g / g of GR | 1.51 |
| Par 6 | Electricity RER medium voltage - 2 | 0.15 MJ / g of GR | 1.50 |
| Par 7 | Transport - lorry >32 tons class 5 | 0.259 kg∙km / g of GR | 1.72 |

(Based on publication by Arvidsson et al. 2014)

Equivalent relative uncertainty

Sobol results- Only lognormal & equivalent uncertainties



| | | Par 2 | Par 6 | Par 4 | Par 1 | Par 3 | Par 7 | Par 5 |
|---------------------------------------|---|-----------------|-----------------|---------|------------------------------------|----------|-----------|---------|
| | | Electricity - 1 | Electricity - 2 | Acids | Graphite + KMnO4 + Hydrazine | Peroxide | Transport | Water |
| | 1 | 100 000 | | | | | | |
| | 2 | | | 100 000 | | | | |
| 00 | 3 | | | | 100 000 | | | |
| ankin | 4 | | 100 000 | | | | | |
| E E E E E E E E E E E E E E E E E E E | 5 | | | | | 100 000 | | |
| | 6 | | | | | | 100 000 | |
| | 7 | | | | | | | 100 000 |

Graphene production: Prospective LCA model

| / | | | | |
|---|---|----|----|----|
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| R | Μ | 11 | ٩I | ES |

| Symbols | Parameters | Baseline scenario | Value range |
|---------|---|-----------------------|--------------------|
| Par 1 | Graphite + Potassium permanganate (KMnO ₄) + Hydrazine | 2.55 g / g of GR | 0.85 – 4.25 g |
| Par 2 | Electricity RER medium voltage - 1 | 8.5 MJ / g of GR | 3.4 – 1133 MJ |
| Par 3 | Peroxide (H ₂ O ₂) | 4.675 g / g of GR | 0.85 – 8.5 g |
| Par 4 | Phosphoric acid (H_3PO_4) + Sulfuric acid (H_2SO_4) | 33.15 g / g of GR | 22.1 – 44.2 g |
| Par 5 | Deionised water | 0.935 g / g of GR | 25 – 100 kg |
| Par 6 | Electricity RER medium voltage - 2 | 0.15 MJ / g of GR | 0.06 – 6 MJ |
| Par 7 | Transport - lorry >32 tons class 5 | 0.259 kg∙km / g of GR | 0.013 – 5.18 kg·km |

(Based on publication by Arvidsson et al. 2014 and its references)

Inputs for the GSA – All distributions



| Parameters | Value range | Baseline distribution | Alternative distributions | | | |
|------------|--------------------|--------------------------|---------------------------|------------|--|--|
| | | Type 1 | Type 2 | Туре 3 | | |
| Par 1 | 0.85 – 4.25 g | lognormal | Uniform | Triangular | | |
| Par 2 | 3.4 – 1133 MJ | lognormal | Uniform | Triangular | | |
| Par 3 | 0.85 – 8.5 g | lognormal | Uniform | Triangular | | |
| Par 4 | 22.1 – 44.2 g | lognormal | Uniform | Triangular | | |
| Par 5 | 25 – 100 kg | lognormal | Uniform | Triangular | | |
| Par 6 | 0.06 – 6 MJ | lognormal | Uniform | Triangular | | |
| Par 7 | 0.013 – 5.18 kg∙km | lognormal | Uniform | Triangular | | |





Difference between lognormal and uniform distribution for electricity used in Hummers' process



Pedigree approach propose much lower uncertainty than the value range found in the reference

Results for the GSA – lognormal + uniform



| | | Par 2 | Par 6 | Par 4 | Par 1 | Par 3 | Par 7 | Par 5 |
|-------|---|-----------------|-----------------|---------|------------------------------------|----------|-----------|---------|
| | | Electricity - 1 | Electricity - 2 | Acids | Graphite + KMnO4 + Hydrazine | Peroxide | Transport | Water |
| | 1 | 200 000 | | | | | | |
| | 2 | | 100 273 | 99 727 | | | | |
| ۵۵ | 3 | | | 100 273 | 99 727 | | | |
| ankin | 4 | | 99 727 | 1 | 100 273 | | | |
| E E E | 5 | | | | | 200 000 | | |
| | 6 | | | | | | 200 000 | |
| | 7 | | | | | | | 200 000 |

Results for the GSA – lognormal + triangular



| | | Par 2 | Par 6 | Par 4 | Par 1 | Par 3 | Par 7 | Par 5 |
|-------|---|-----------------|-----------------|---------|------------------------------------|----------|-----------|---------|
| | | Electricity - 1 | Electricity - 2 | Acids | Graphite + KMnO4 + Hydrazine | Peroxide | Transport | Water |
| | 1 | 200 000 | | | | | | |
| | 2 | | 100 383 | 99 617 | | | | |
| ۵۵ | 3 | | | 100 383 | 99 617 | | | |
| ankin | 4 | | 99 617 | | 100 383 | | | |
| E E | 5 | | | | | 200 000 | | |
| | 6 | | | | | | 200 000 | |
| | 7 | | | | | | | 200 000 |

Results for the GSA – uniform + triangular



| | | Par 2 | Par 6 | Par 4 | Par 1 | Par 3 | Par 7 | Par 5 |
|---------|---|-----------------|-----------------|---------|------------------------------------|----------|-----------|---------|
| | | Electricity - 1 | Electricity - 2 | Acids | Graphite + KMnO4 + Hydrazine | Peroxide | Transport | Water |
| Ranking | 1 | 200 000 | | | | | | |
| | 2 | | 200 000 | | | | | |
| | 3 | | | 150 119 | 49 881 | | | |
| | 4 | | | 49 881 | 150 119 | | | |
| | 5 | | | · | | 200 000 | | |
| | 6 | | | | | | 200 000 | |
| | 7 | | | | | | | 200 000 |

Results for the GSA – All distributions



| | | Par 2 | Par 6 | Par 4 | Par 1 | Par 3 | Par 7 | Par 5 |
|---------|---|-----------------|-----------------|---------|------------------------------------|----------|-----------|---------|
| | | Electricity - 1 | Electricity - 2 | Acids | Graphite + KMnO4 + Hydrazine | Peroxide | Transport | Water |
| Ranking | 1 | 300 000 | | | | | | |
| | 2 | | 199 867 | 89 137 | 10 996 | | | |
| | 3 | | | 188 894 | 111 106 | | | |
| | 4 | | 100 133 | 21 969 | 177 898 | | | |
| | 5 | • | | | | 300 000 | | |
| | 6 | | | | | | 300 000 | |
| | 7 | | | | | | | 300 000 |

Graphene production: Parameters' ranking



Baseline result: 1.7 kg CO2 eq./g of GR



- Graphite + Potassium permanganate (KMnO4) + Hydrazine
- Electricity RER medium voltage 1
- Peroxyde (H2O2)
- Phosphoric acid (H3PO4) + Sulfuric acid (H2SO4)
- Deionised water
- Electricity RER medium voltage 2
- Transport lorry >32 tons class 5

Global sensitivity Analysis / Ranking

- 1. Electricity for Hummers' process (Par 2)
- 2. Acids (Par 4)
- 3. Graphite + $KMnO_4$ + Hydrazine (Par 1)
- 4. Electricity for chemical reduction (Par 6)
- 5. Peroxide (Par 3)
- 6. Transport (Par 7)
- 7. Deionised water (Par 5)



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Thank you for your attention

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EGS: LCA model (GHG emissions)





EGS: LCA model (GHG emissions)



A) General modeling framework for LCA



 $\begin{cases} \Psi \\ GHG_{EGS,A} \left[\frac{g \ CO_2 eq}{kWh} \right] = \frac{z_A \cdot Nw_A \cdot (\boldsymbol{\alpha_1} + \boldsymbol{\alpha_2} \cdot d_A) + LT_A \cdot f_A \cdot \boldsymbol{\alpha_3} + P_{ORC,A} \cdot LT_A \cdot \boldsymbol{\alpha_4} + Nw_A \cdot Sfe_A \cdot \boldsymbol{\alpha_5}}{LF_A \cdot LT_A \cdot \left(P_{ORC,A} - f_A \cdot P_{p,A} \right) \cdot 8760} \end{cases}$

With $\alpha_1 = 498761.36 \text{ gCO}_2 eq/m$; $\alpha_2 = 90.56 \text{ gCO}_2 eq/MJ$; $\alpha_3 = 487363.03 \text{ gCO}_2 eq \cdot s/(kg \cdot y)$; $\alpha_4 = 50603.13 \text{ gCO}_2 eq/(kW \cdot y)$; $\alpha_5 = 25757089.05 \text{ gCO}_2 eq$