

DEVELOPMENT OF INTERACTIVE SOFTWARE FOR MODELING AND OPTIMIZING ENERGY PROCESSES USING MACHINE LEARNING AND AI

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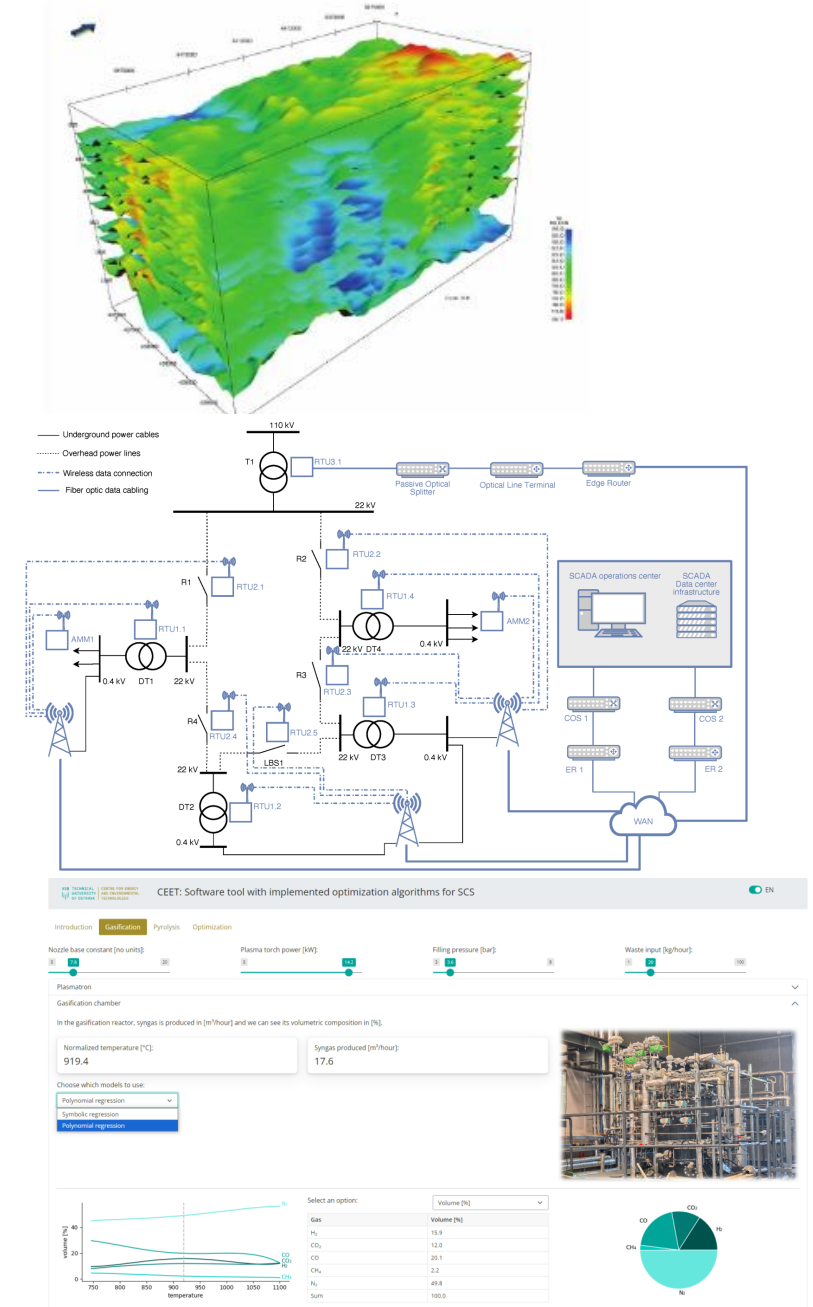


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the European Union

OUTLINE

- Development of interactive software for modeling and optimizing energy processes using machine learning (ML) and AI
- **Use cases:**
 - **Carbon sequestration using OPM Flow** (research cooperation IT4Innovations VSB TUO with SINTEF Digital, Oslo, Norway)
 - **Interconnected infrastructures** (electricity and communication networks – research cooperation with Brno University of Technology, Brno, CZ)
 - **Shinyenet software** for selected waste-to-energy processes at innovation polygon CEETe VSB TUO

Machine learning and sensitivity analysis on



SELECTED PAPERS FOR USE CASES

Carbon sequestration using OPM Flow

- Praks, P., Rasmussen, A., Lye, K. O., Martinovič, J., Praksová, R., Watson, F., & Brkić, D. (2024). Sensitivity analysis of parameters for carbon sequestration: Symbolic regression models based on open porous media reservoir simulators predictions. In Heliyon (Vol. 10, Issue 22, p. e40044). Elsevier BV.
<https://doi.org/10.1016/j.heliyon.2024.e40044>

Interconnected infrastructures (electricity and communication networks)

- Krpelik, D., Vrtal, M., Bris, R., Praks, P., Fujdiak, R., & Toman, P. (2026). Multi-objective optimization of smart grid operations via preventive maintenance scheduling using time-dependent unavailability. Reliability Engineering & System Safety, 265, 111567. <https://doi.org/10.1016/j.ress.2025.111567>
- **ZEUS project papers:**
 - Běloch M., Praks P.; Praksová R.; Fujdiak R.; Vrtal M.; Briš R.; Brkić D. (2025). Evaluating the unavailability of interconnected power and communication networks with open-source tools on a petascale cluster. Energy Exploration & Exploitation. 2025;0(0). <https://doi.org/10.1177/01445987251377791>
 - Briš, R., Praks, P., Fujdiak, R., Vrtal, M., & Brkić, D. (2025). Maintenance optimization for unavailability enhancement of representative interconnected infrastructure based on minimum cost. Science Progress, 108(3) 1–23. <https://doi.org/10.1177/00368504251366357>

ML-ACCELERATED GLOBAL SENSITIVITY ANALYSIS

Sobol method:

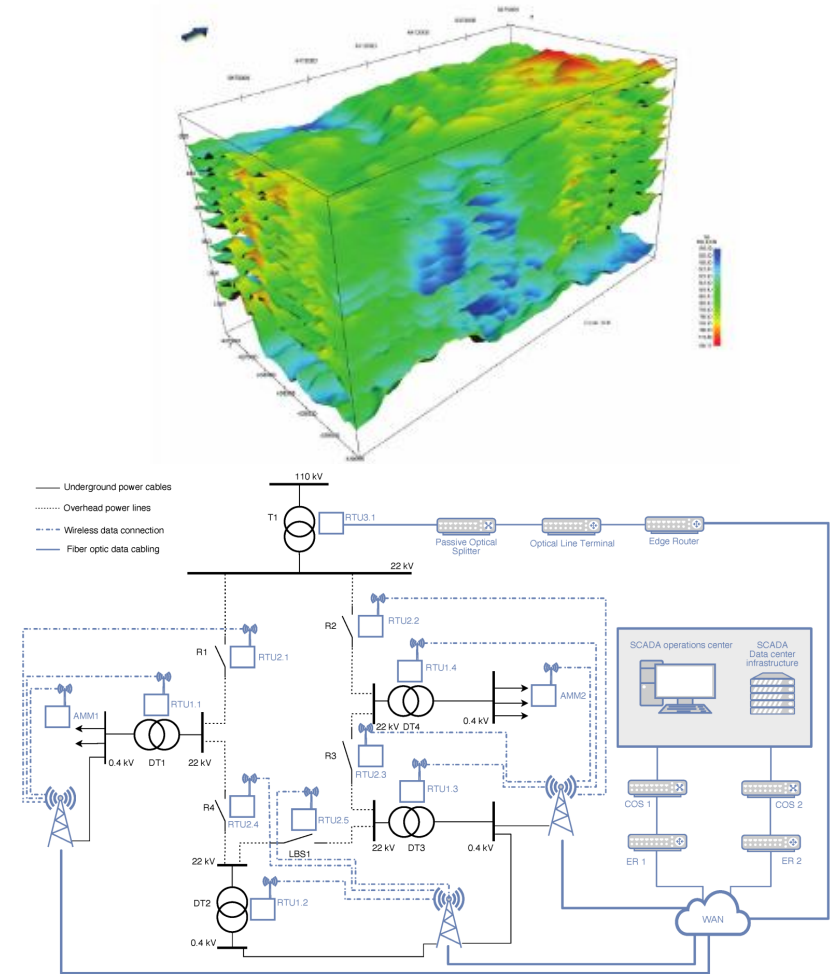
- Probabilistic, global, handles uncertainty
- Works with nonlinear responses & interactions
- Sensitivity indices indicate feature importance

Challenge:

- Requires thousands of simulations → costly

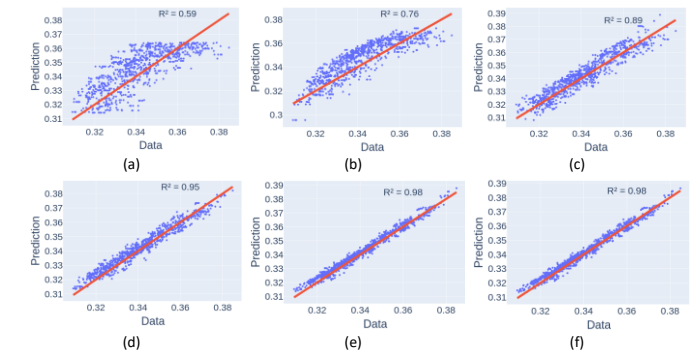
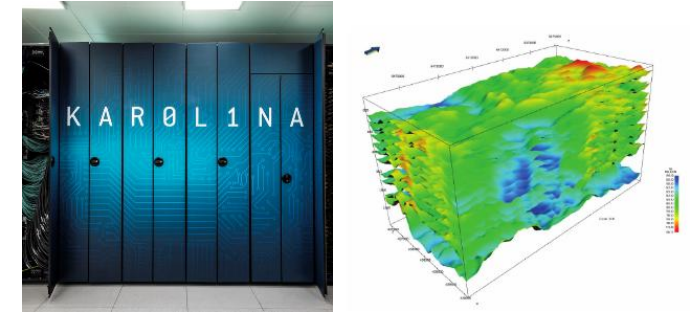
Our aim:

- Use machine learning (ML) to predict sensitivity indices
- Reduce simulation cost while preserving accuracy



ACCELERATING SENSITIVITY ANALYSIS OF OPM FLOW WITH ML

- **OPM Flow:** Open-source reservoir simulator for carbon sequestration
 - Industry-standard formats (ECLIPSE)
 - Easy integration with pre/post-processing tools
- **Approach:** Model uncertain input parameters to quantify impact on outcomes
- **Goal:** Speed up global sensitivity analysis (SA) of OPM Flow simulations using machine learning (ML)
- **Collaboration:** SINTEF Digital (Norway) & IT4Innovations (Czechia) (Praks, P., Rasmussen, A., Lye, K. O., Martinovič, J., Praksová, R., Watson, F., & Brkić, D.)
- **References:**
 - OPM Flow: Rasmussen et al., Computers & Mathematics with Applications, 2021, <https://doi.org/10.1016/j.camwa.2020.05.014>
 - SA & ML for OPM Flow: Praks et al., Heliyon, 2024. <https://doi.org/10.1016/j.heliyon.2024.e40044>



Development of fast interpretable ML approximations of OPM Flow results

(a) 1D model, (b) 2D model, ..., (f) 6D model

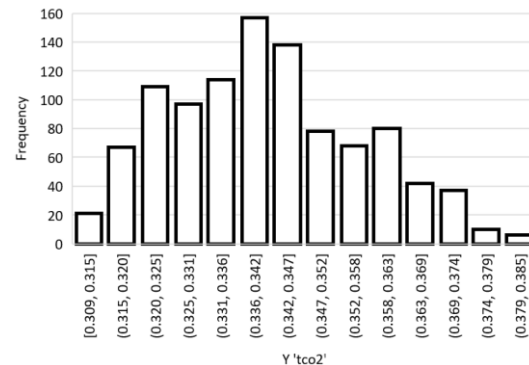
WORKFLOW FOR ML-ACCELERATED SENSITIVITY ANALYSIS IN OPM FLOW CARBON SEQUESTRATION

Parameter	Uncertainty type	Minimum	Maximum
temperature gradient (tegrad, x1)	Parametric/model	30 degrees C	40 degrees C
permeability of sand layers (pesand, x2)	Parametric/model	1100 mD	5000 mD
permeability of shale between sand layers (peshale, x3)	Parametric/model	0.00075 mD	0.0015 mD
permeability of feeder chimneys connecting sand layers (pefeeder, x4)	Parametric/model	1100 mD	5000 mD
porosities of sand, shale, and feeders (posand, x5)	Parametric/model	0.27	0.4
topography of top surface (totopsur, x6)	Parametric/model	-10 m	+10 m

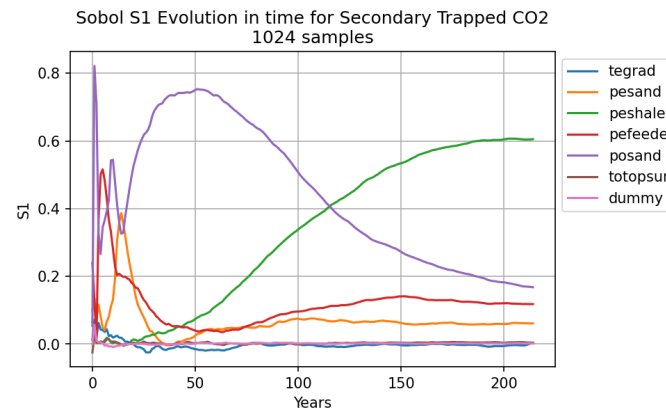
1. Define uncertain inputs

2. Generate quasi-random samples of model inputs

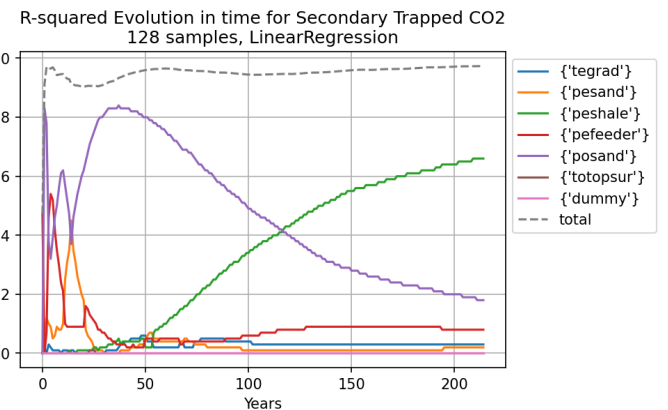
3. Run OPM Flow simulations on HPC cluster and extraction of outputs



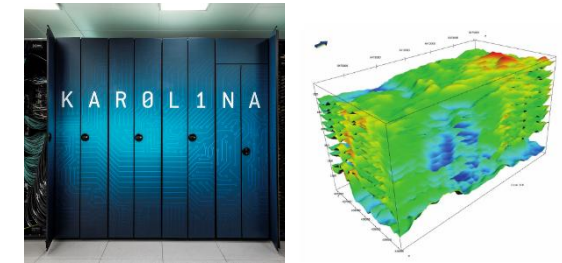
4. Uncertainty analysis of OPM Flow model output (secondary trapped CO₂)



5. Classical approach:
Time-dependent global sensitivity analysis
Requires many OPM Flow simulations



6. Novel accelerated approach:
Predict sensitivity indices using ML
Reduces computational cost



INPUTS AND OUTPUTS FOR SA & ML IN OPM FLOW CARBON SEQUESTRATION

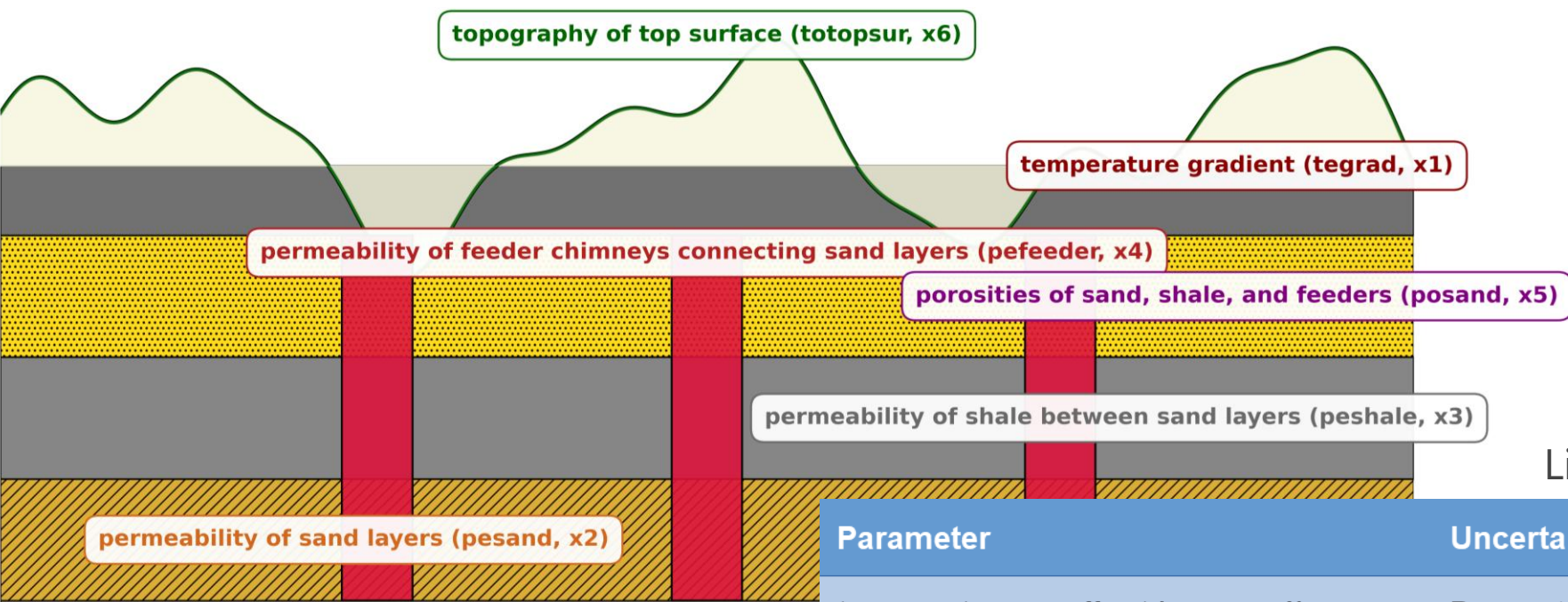


Diagram shows how these inputs relate to each other.

List of uncertain input parameters:

Parameter	Uncertainty type	Minimum	Maximum
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INPUTS AND OUTPUTS FOR SA & ML IN OPM FLOW CARBON SEQUESTRATION

✓ **Inputs:**

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topography of top surface (totopsur, x6)	Parametric/model	-10 m	+10 m

✓ **Outputs:**

- OPM Flow simulations → trapped_co2.csv

trapped_co2
0.333245
0.336624
0.336523
0.343364
0.330078
0.342297
0.333459

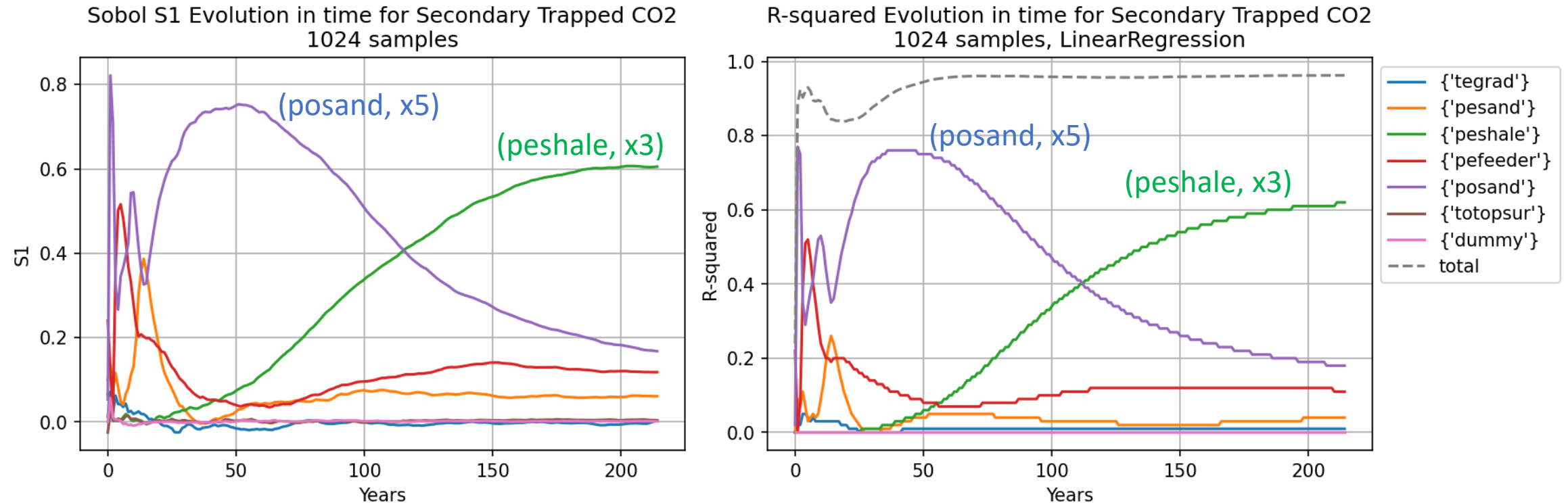
Quasi Monte-Carlo samples (input_params.csv)	Tegrad	pesand	peshale	pefeeder	posand	totopsur	dummy
• Includes dummy parameter for validation	30.01465	2568.213	0.001086	2998.584	0.342427	6.884766	0.241699
	35.87402	2568.213	0.001086	2998.584	0.342427	6.884766	0.241699
	30.01465	3817.432	0.001086	2998.584	0.342427	6.884766	0.241699
	30.01465	2568.213	0.001254	2998.584	0.342427	6.884766	0.241699
	30.01465	2568.213	0.001086	4304.932	0.342427	6.884766	0.241699
	30.01465	2568.213	0.001086	2998.584	0.38978	6.884766	0.241699
	30.01465	2568.213	0.001086	2998.584	0.342427	4.130859	0.241699

OPM Flow model and simulations:



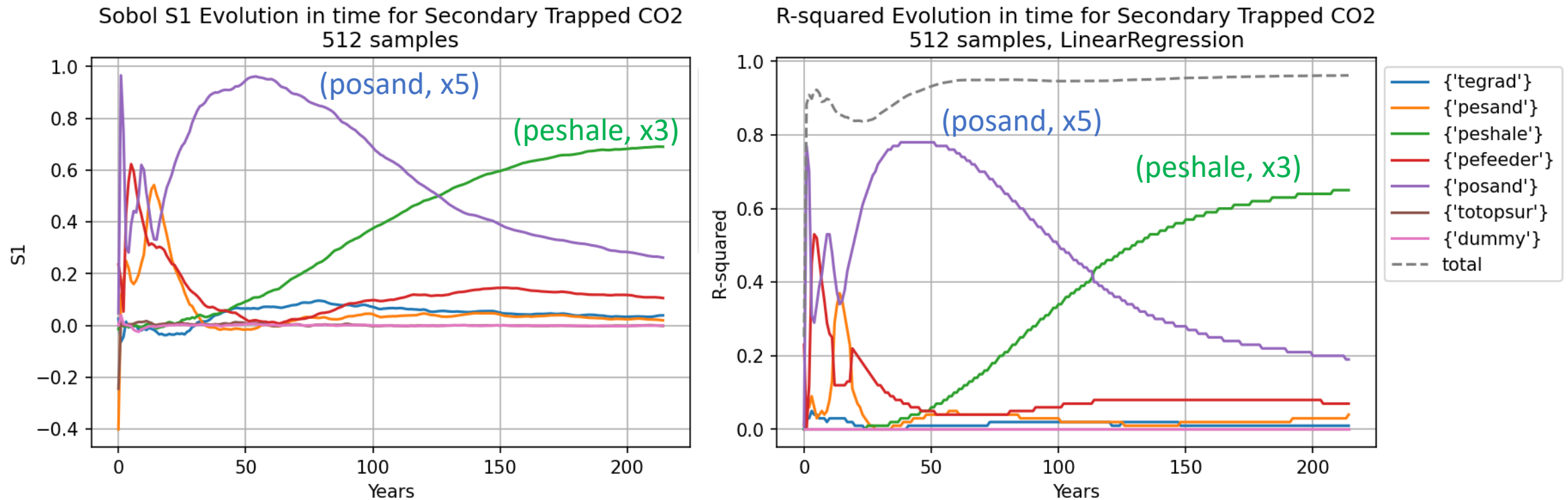
Sensitivity analysis & ML predictions:

SENSITIVITY ANALYSIS OF CARBON SEQUESTRATION: SOBOL VS NOVEL ML



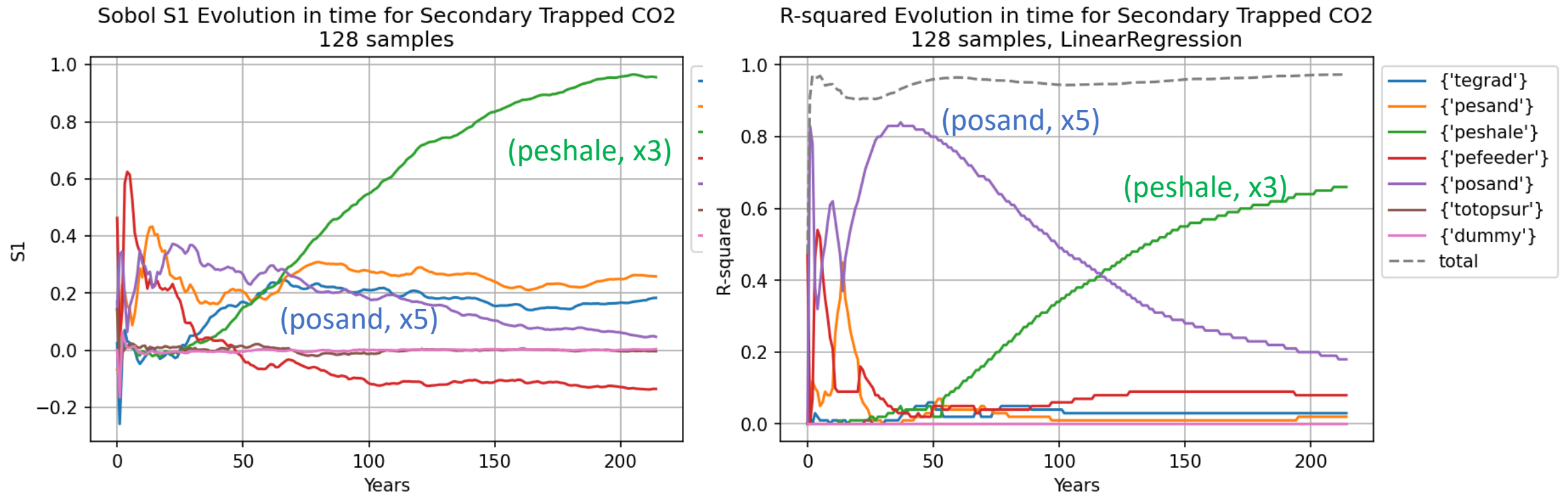
Sobol method and our novel machine learning approach discover the important properties of the time-dependent carbon sequestration process for 1 024 Quasi Monte Carlo (QMC) samples: Sand porosity (**posand, x5**) is more important than shale permeability (**peshale, x3**) for about the first 120 years.

SENSITIVITY ANALYSIS OF CARBON SEQUESTRATION: SOBOL VS NOVEL ML



- Sobol method has incorrect negative sensitivity for Year 0 due to an insufficient number (512) of QMC samples.
- Our novel ML approach discovers the important properties of the time-dependent carbon sequestration process for 512 QMC samples: Sand porosity (posand, x5) is more important than shale permeability (peshale, x3) for about the first 120 years.

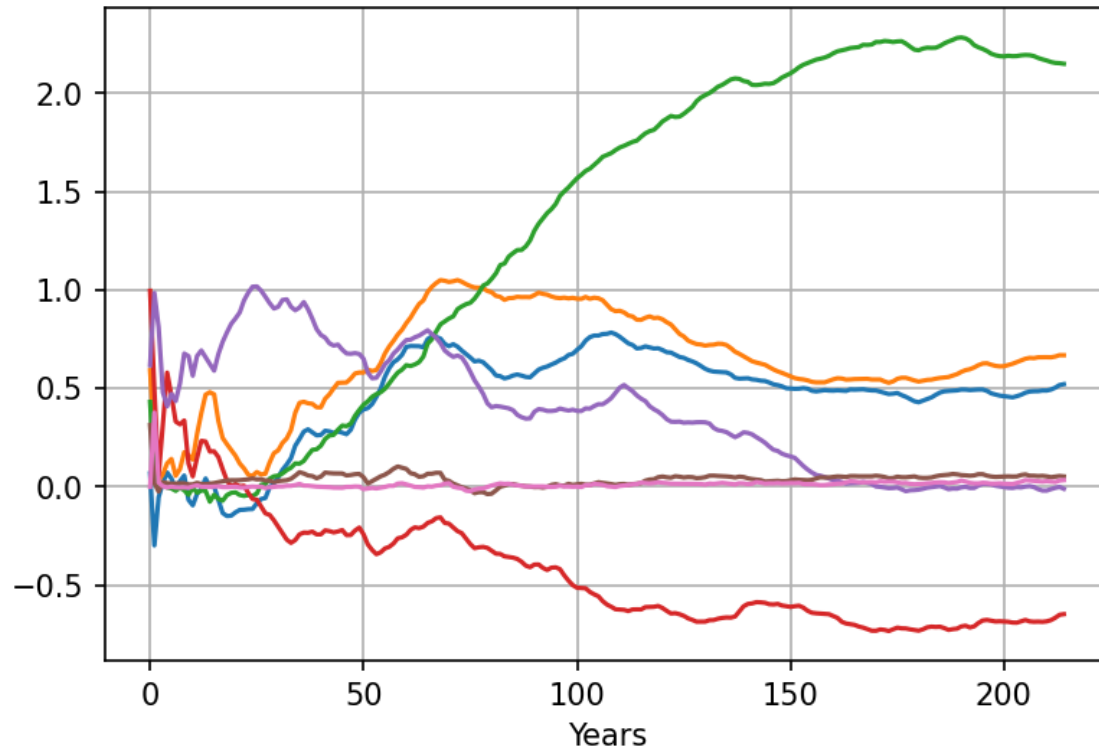
SENSITIVITY ANALYSIS OF CARBON SEQUESTRATION: SOBOL VS NOVEL ML



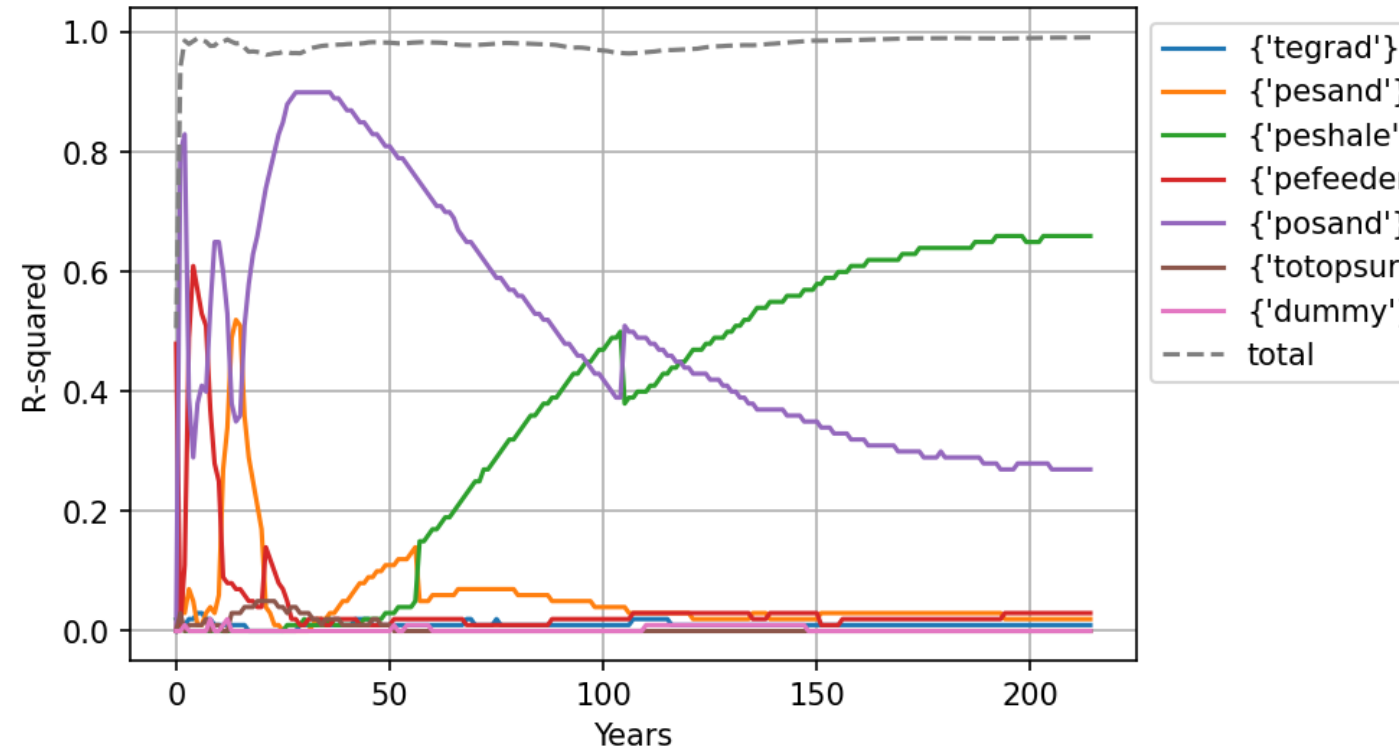
- Our novel ML approach discovers the important properties of the time-dependent carbon sequestration process for 128 QMC samples: Sand porosity (**posand, x5**) is more important than shale permeability (**peshale, x3**) for about the first 120 years.
- Sobol method does not detect the pattern and has incorrect negative sensitivity for Year 0 due to an insufficient number (128) of QMC samples.

SENSITIVITY ANALYSIS OF CARBON SEQUESTRATION: SOBOL VS NOVEL ML

Sobol S1 Evolution in time for Secondary Trapped CO2
32 samples



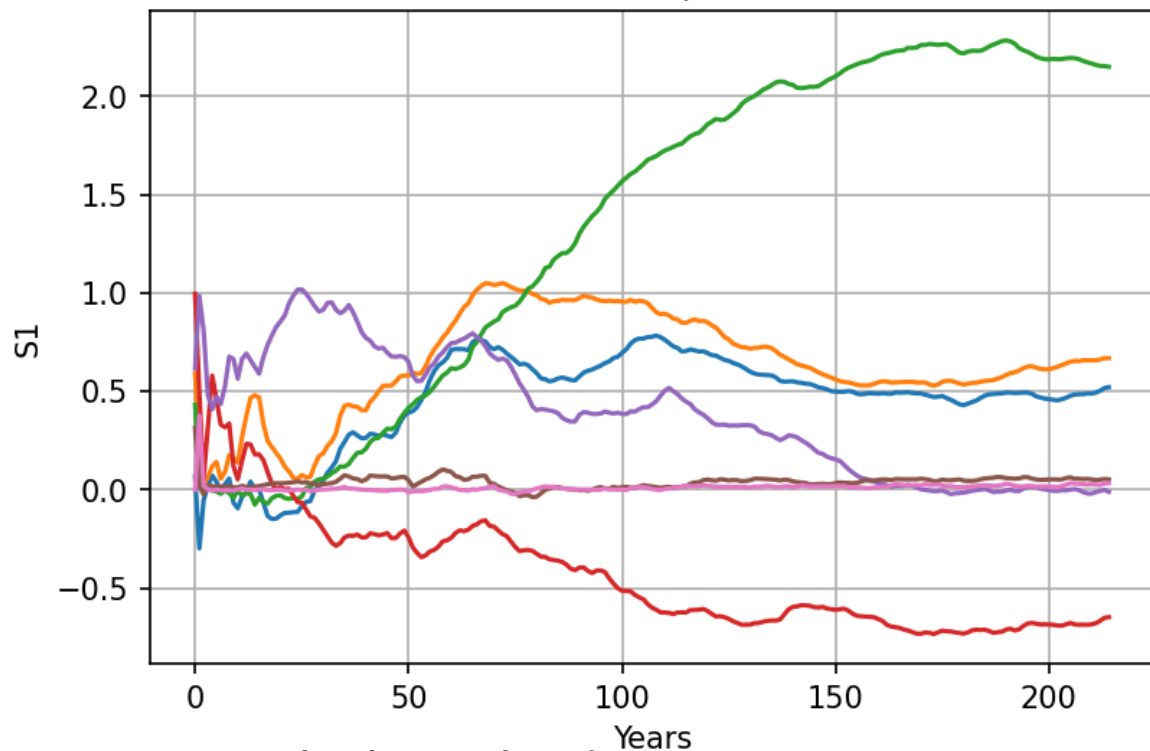
R-squared Evolution in time for Secondary Trapped CO2
32 samples, LinearRegression



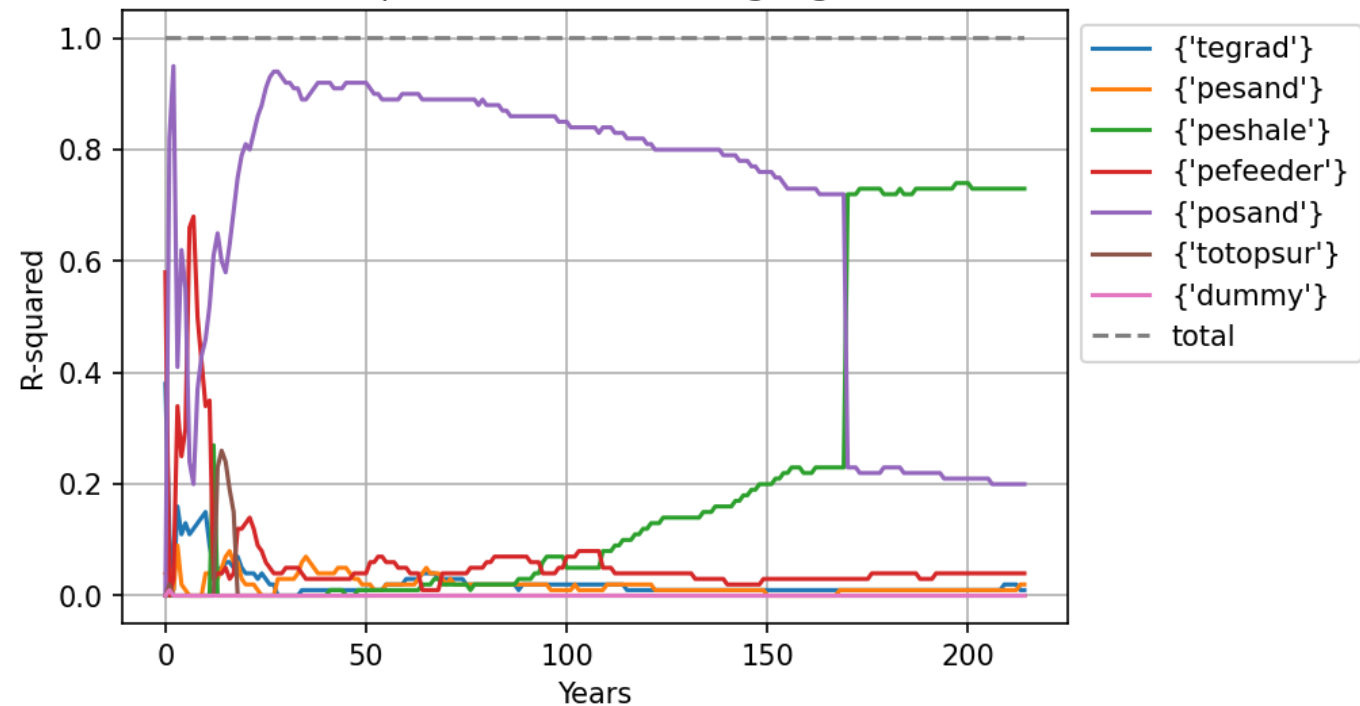
- Sobol method reports incorrect pattern of sensitivities (both negative and larger than one) due to an insufficient number (32) of QMC samples.
- Our novel ML approach discovers the important properties of the time-dependent carbon sequestration process even for 32 QMC samples: Sand porosity (**posand**, x5) is more important than shale permeability (**peshale**, x3) for about the first 95-120 years. (1 024 QMC samples estimate it for the first 120 years.)

SENSITIVITY ANALYSIS OF CARBON SEQUESTRATION: SOBOL VS NOVEL ML

Sobol S1 Evolution in time for Secondary Trapped CO2
32 samples



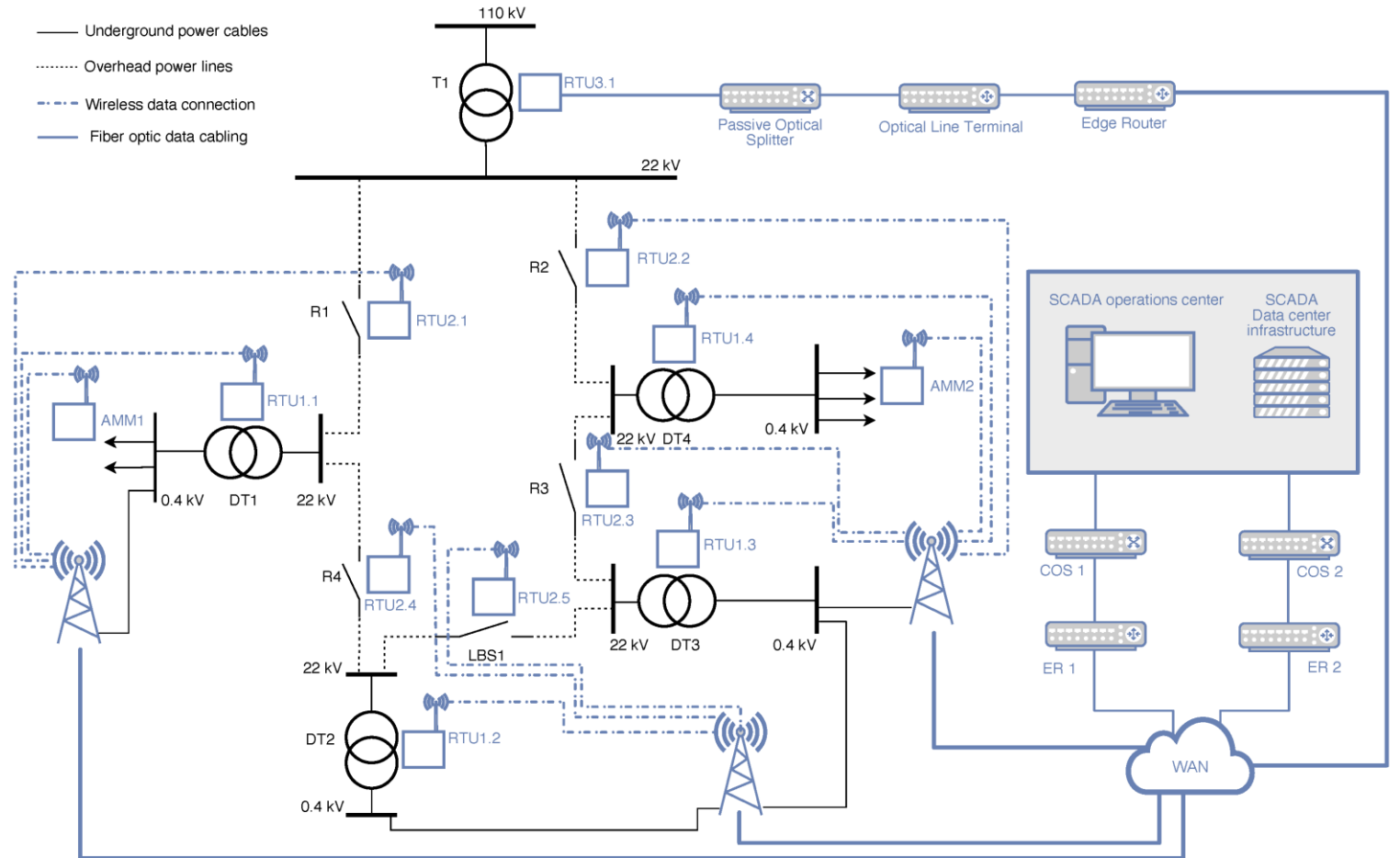
R-squared Evolution in time for Secondary Trapped CO2
10 samples, GradientBoostingRegressor



- Sobol method reports incorrect pattern of sensitivities (both negative and larger than one) due to an insufficient number (32) of QMC samples.
- Our novel ML approach discovers the important properties of the time-dependent carbon sequestration process even for 10 QMC samples: Sand porosity (**posand**, x5) is more important than shale permeability (**peshale**, x3) for about the first 170 years. (1 024 QMC samples estimate it for the first 120 years.)

INTERCONNECTED INFRASTRUCTURES

- Two interconnected networks:
 - Power distribution network
 - Communication network
- Power distribution network:
 - Based on Czech distribution grid
 - Ring topology structure



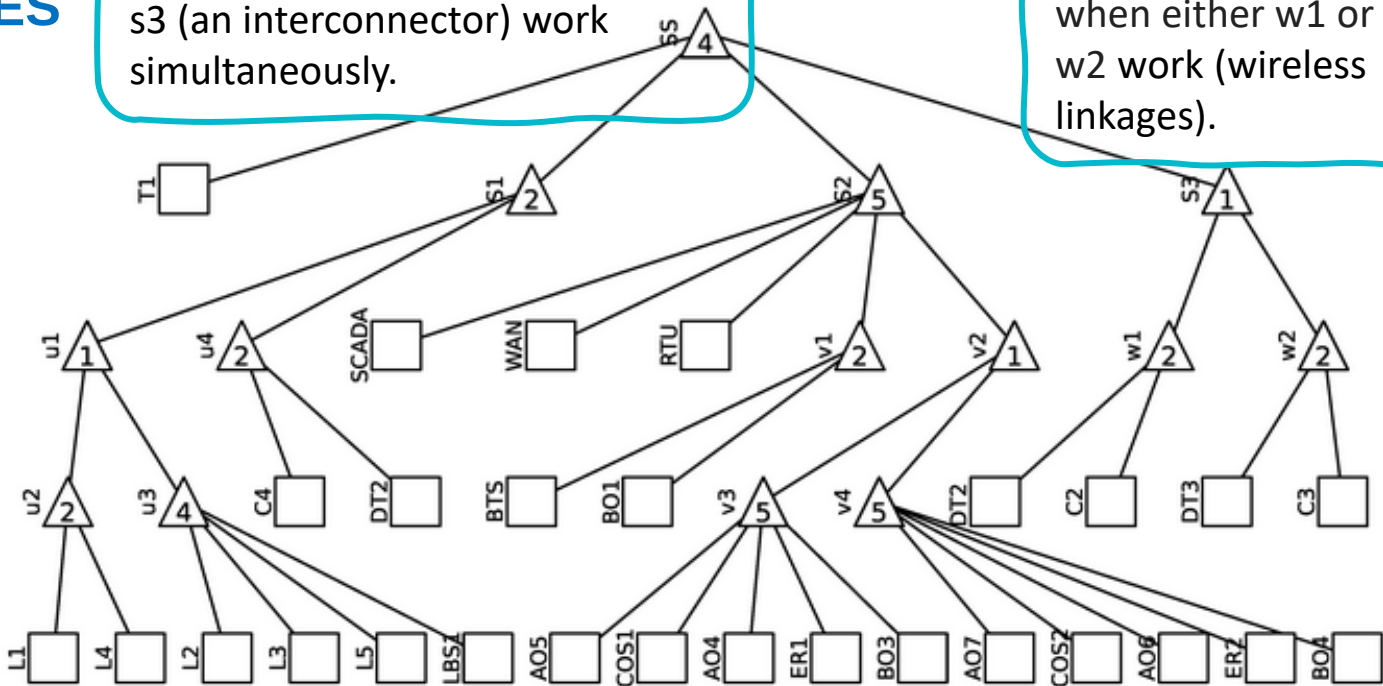
Parameters of the model and the reference solution is given by Běloch M., Praks P.; Praksová R.; Fujdiak R.; Vrtal M.; Briš R.; Brkić D. (2025). Evaluating the unavailability of interconnected power and communication networks with open-source tools on a petascale cluster. Energy Exploration & Exploitation. 2025;0(0). <https://doi.org/10.1177/01445987251377791>

INTERCONNECTED INFRASTRUCTURES

Components	MTBF (h)	MTTR (h)
Transformer T1	26,310.709	4.403
Overhead line L1	54,750.000	11.417
Overhead line L2	41,714.286	11.417
Overhead line L3	62,571.429	11.417
Overhead line L4	48,666.666	11.417
Overhead line L5	43,800.000	11.417
Load break switch LBS1	224,621.087	5.702
Underground cable C2	57,737.828	85.000
Underground cable C3	38,491.886	85.000
Underground cable C4	153,967.543	85.000
Transformer DT2	43,800.361	0.361
Transformer DT3	43,800.361	0.361
Buried optic fiber BO1	821,875.000	12.000
Buried optic fiber BO3	1,753,333.333	12.000
Buried optic fiber BO4	1,753,333.333	12.000
Edge router ER1	16,246.780	0.780
Edge router ER2	16,246.780	0.780
Aerial optic fiber AO4	500,000.000	6.000
Aerial optic fiber AO5	1,093,750.000	6.000
Aerial optic fiber AO6	500,000.000	6.000
Aerial optic fiber AO7	1,093,750.000	6.000

The system SS works when all T1, s1 (power grid), s2 (comm. grid), s3 (an interconnector) work simultaneously.

The node s3 works when either w1 or w2 work (wireless linkages).



The interconnected network represented by the success tree.

Components	MTBF (h)	MTTR (h)
Core optical switch COS1	5,000,014.000	14.000
Core optical switch COS2	5,000,014.000	14.000
SCADA operation and data center	175,200.000	184.600
Wide area network WAN	100,000.000	4.000
Remote terminal unit RTU	100,048.000	48.000
Base transceiver station BTS	100,000.000	4.000

Characteristic values of the power grid (and the communication network). In all cases, the shape parameter of Weibull $\beta=2$ is used. See Briš, R., Praks, P., Fujdiak, R., Vrtal, M., & Brkić, D. (2025). Maintenance optimization for unavailability enhancement of representative interconnected infrastructure based on minimum cost. Science Progress, 108(3) 1–23. <https://doi.org/10.1177/00368504251366357>

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Aerial optic fiber AO7	1,093,750.000	6.000

Reliability and maintainability metrics of components:

- **MTTR (Mean Time to Repair)**
Average time to repair or replace a component.
→ **Low MTTR** = quick recovery after failure → **high maintainability**
- **MTTF (Mean Time to Failure)**
Average operational time before a component fails.
→ **High MTTF** = long-lasting operation → **high reliability**
- **MTTR** measures *repair speed*, while **MTTF** measures *expected lifespan*.

Simulation setup:

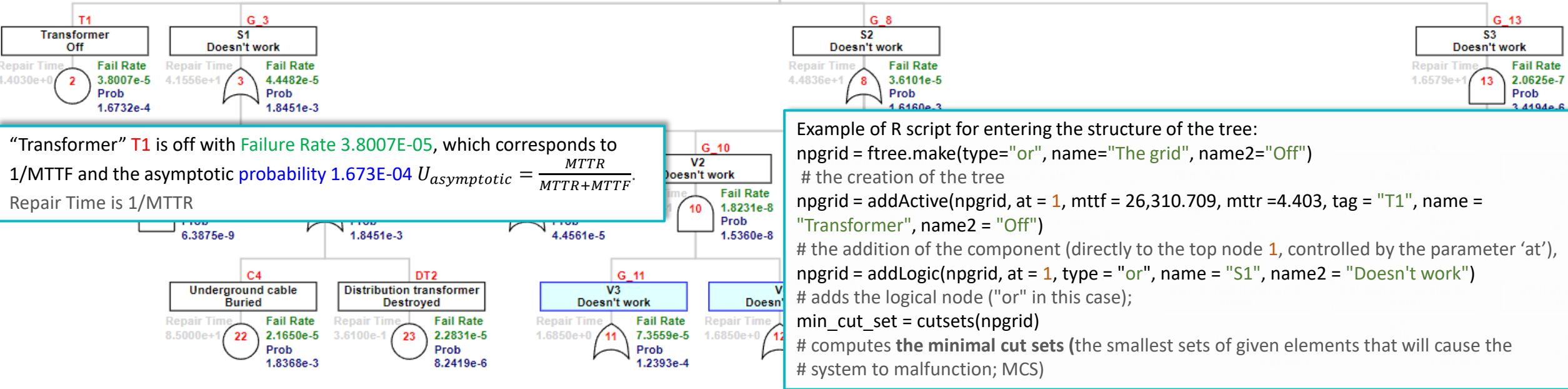
- We simulate component downtimes across a wide range:
0.1×MTTR to 10×MTTR
- How do these variations affect **system unavailability** at **t = 5 years**?

Characteristic values of the power grid and the communication network. In all cases, the shape parameter of Weibull $\beta=2$ is used. See Briš, R., Praks, P., Fujdiak, R., Vrtal, M., & Brkić, D. (2025). Maintenance optimization for unavailability enhancement of representative interconnected infrastructure based on minimum cost. Science Progress, 108(3) 1–23. <https://doi.org/10.1177/00368504251366357>

FaultTree¹

Number "1" represents node ID

The **top** node "The grid" is off, when **T1** transformer is off or **G_3** S1 power grid) doesn't work or **G_8** S2 (comm. grid) doesn't work, etc.



Example of R script for entering the structure of the tree:

```

npgrid = ftree.make(type="or", name="The grid", name2="Off")
# the creation of the tree
npgrid = addActive(npgrid, at = 1, mttf = 26,310.709, mttr = 4.403, tag = "T1", name = "Transformer", name2 = "Off")
# the addition of the component (directly to the top node 1, controlled by the parameter 'at'),
npgrid = addLogic(npgrid, at = 1, type = "or", name = "S1", name2 = "Doesn't work")
# adds the logical node ("or" in this case);
min_cut_set = cutsets(npgrid)
# computes the minimal cut sets (the smallest sets of given elements that will cause the
# system to malfunction; MCS)
    
```

Visualised fault tree

- Provides an interactive and easy-to-understand visualization of the fault tree structure.
- The tree structure is defined by addActive and addLogic commands.
- addActive individual elements (leaves) are described by Mean Time to Failure (MTTF) and Mean Time To Repair (MTTR)
- addLogic adds the logical node (“and”, “or”).
- For all logical nodes, FaultTree computes failure rates and asymptotic probabilities that the given node is not operating.
- The FaultTree uses the Binary Decision Diagrams (BDD) to efficiently compute the minimal cut sets of a fault tree.
- Given the asymptotic unavailability probabilities of the leaves (terminal events), BDD also computes the probability of the root event “The grid Off” by the Shannon's decomposition².



Used logic symbols (gates)

¹ Silkworth, D. (2023). FaultTree: Fault Trees for Risk and Reliability Analysis. R package version 1.0.1. URL: <https://CRAN.R-project.org/package=FaultTree>

² Rauzy, A. (1993). New algorithms for fault trees analysis. *Reliability Engineering & System Safety*, 40(3), 203–211. [https://doi.org/10.1016/0951-8320\(93\)90060-c](https://doi.org/10.1016/0951-8320(93)90060-c)

Ftapproxim³

Component	MTTF (h)	MTTR (h)
Transformer T1	26,310.709	4.403

```
T1 = list(  
  states=c("OK","F"),  
  G=rbind(c(NA,1), c(1,NA)), # G is a transition matrix describing the  
    probabilities of going from the state "OK" to "F" and vice versa.  
  dist=c("weibull", "unif"),  
  # definition of probability density function (pdf) of time to failure and  
    time to repair  
  # weibull represents pdf of the time to failure and uniform represents  
    the pdf of time to repair.  
  param=list(c(beta, T1_mttf/gamma(1+1/beta)), c(0, 2*T1_mttr)))  
# parameters of pdfs: (shape  $\beta$ , scale  $\theta$ ) for Weibull  
# and start and end of the interval for uniform pdf.
```

Definition of the component Transformer T1, which has 2 states.

- A deterministic iterative method for unavailability estimation for multistate systems
- Uses the minimal cut sets (MCSs) of the fault tree; individual elements (leaves) are described by density functions of time to failure and time to repair.
- MTTF of a given Weibull component is computed as $MTTF = \theta \cdot \Gamma(1 + 1/\beta)$, where θ is a scale, β is a known shape and Γ is a gamma function. As the θ parameter of the distribution is unknown, we have to factor it out.
- **Inputs:** list of the components and their **failures** and **repair** characteristics, MCS, mission time, time step, tolerance
- **The output:** the values of unavailabilities of each element in every time step (computed by the command FTUna)
- Very versatile tool, can work with all commonly used density functions (Weibull, exponential, uniform, normal)
- The time and space complexity of the algorithm is exponential in the number of discrete time steps⁴

³Niloofer, P., Haghbin, H., & Lazarova-Molnar, S. (2022). Ftapproxim - R Package for Proxel-Based Simulation of Fault Trees: A Case Study. In 2022 6th International Conference on System Reliability and Safety (ICSRS). 2022 6th International Conference on System Reliability and Safety (ICSRS). IEEE.

<https://doi.org/10.1109/icsrs56243.2022.10067562>

⁴G. Horton (2002), A new paradigm for the numerical simulation of stochastic petri nets with general firing times. Proceedings of the European Simulation Symposium (2002), pp. 129-136

GRID SEARCH OF INPUT PARAMETERS IN FTAPROXIM

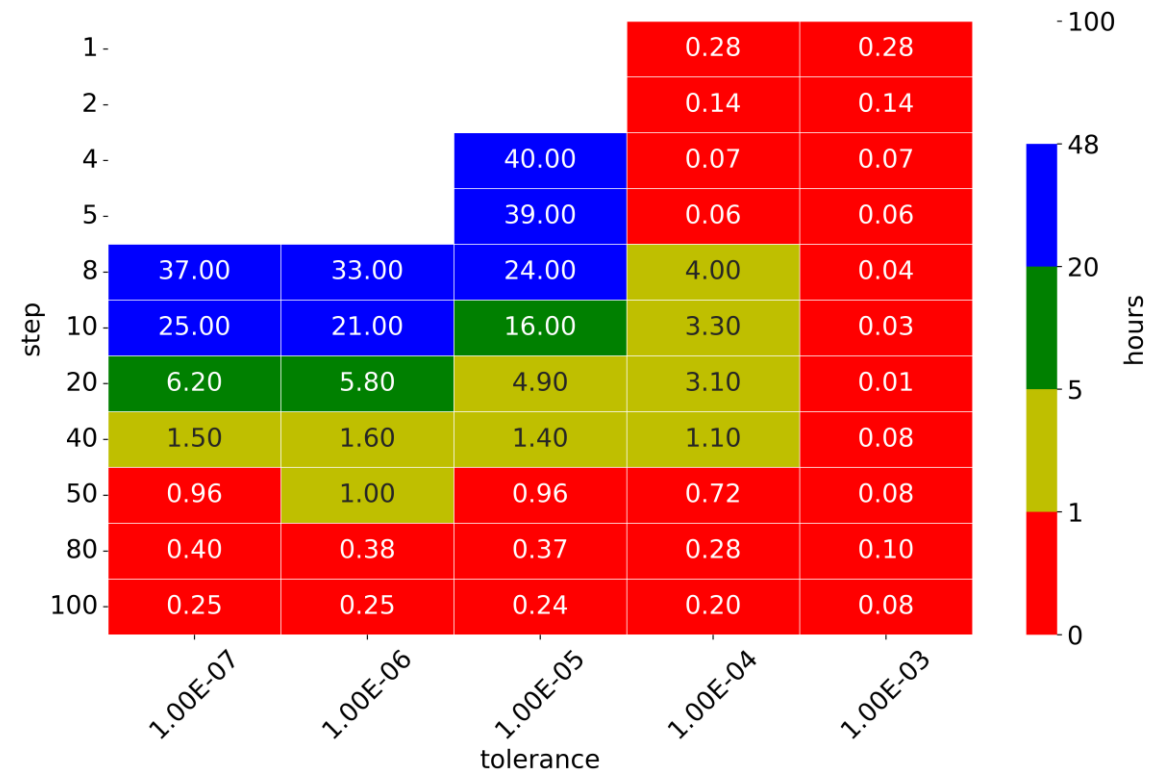
Objective: Analyze how **time step** and **tolerance** parameters influence the **computation time** and **result accuracy** of unavailability estimation in Ftaproxim's unavailability estimation.

Methodology:

- **Grid Search** on a distribution network model using Barbora cluster.
- **55 combinations:**
 - **Step sizes:** {1, 2, 4, 5, 8, 10, 20, 40, 50, 80, 100}
 - **Tolerances:** {1e-03, 1e-04, 1e-05, 1e-06, 1e-07}
- Executed as 55 **parallel processes**.
- **Max runtime per test:** 48 hours

Code availability: Python and R open-source implementations provided, see (Běloch, Praks et al., 2025):

- **Appendix A:** Python code
- **Appendix B:** R code



Heatmap shows impact of parameter choices on **computational time**. White cells: combinations exceeding 48h limit.

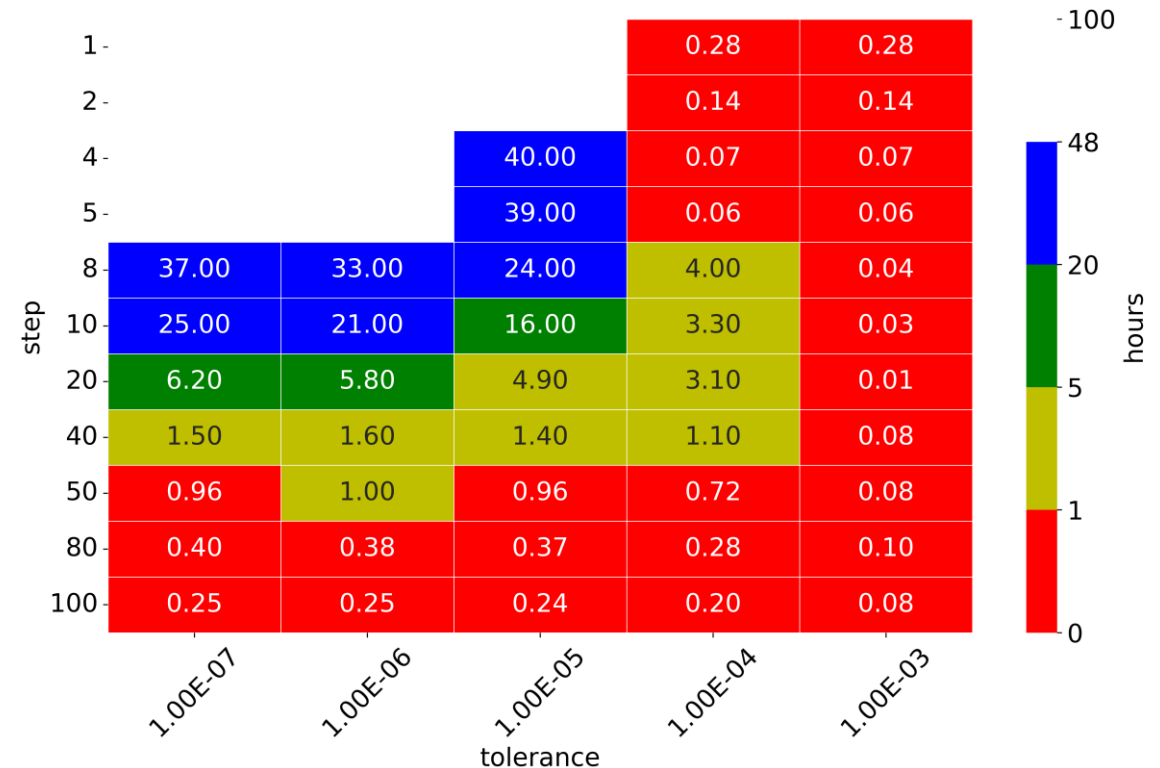
RESULTS OF GRID SEARCH ON BARBORA CLUSTER

Observations:

- Higher **tolerance** → faster computation.
- Larger **time steps** → reduced computation time.
- ⚠ **Trade-off**: Fastest runs often yield **invalid results**

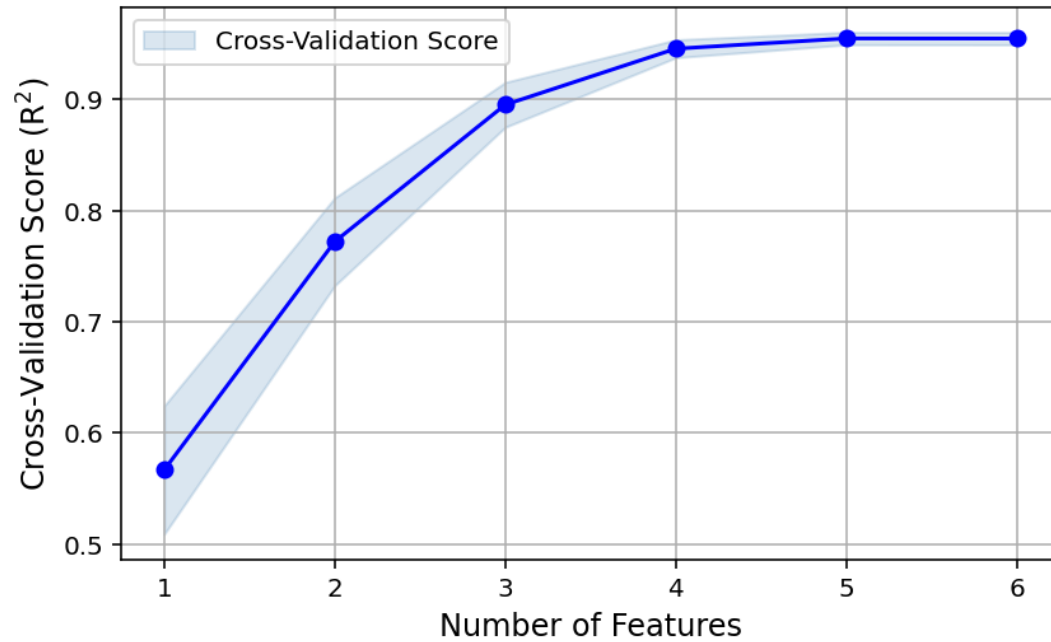
Key findings:

- **Tolerance** = 1×10^{-3} : Fastest, but **invalid results** (no transitions, unavailability = 0).
- **Optimal combinations**:
 - Tolerance = 1×10^{-4} , Step = 50 → **0.72 h**
 - Tolerance = 1×10^{-6} , Step = 8 → **33 h** ⚠
 - These combinations provide **plausible results**, balancing **accuracy** and **performance** (Běloch, Praks et al., 2025).



Heatmap shows impact of parameter choices on **computational time**. White cells: combinations exceeding 48h limit.

MACHINE LEARNING FOR IDENTIFYING KEY PARAMETERS IN RELIABILITY MODELING



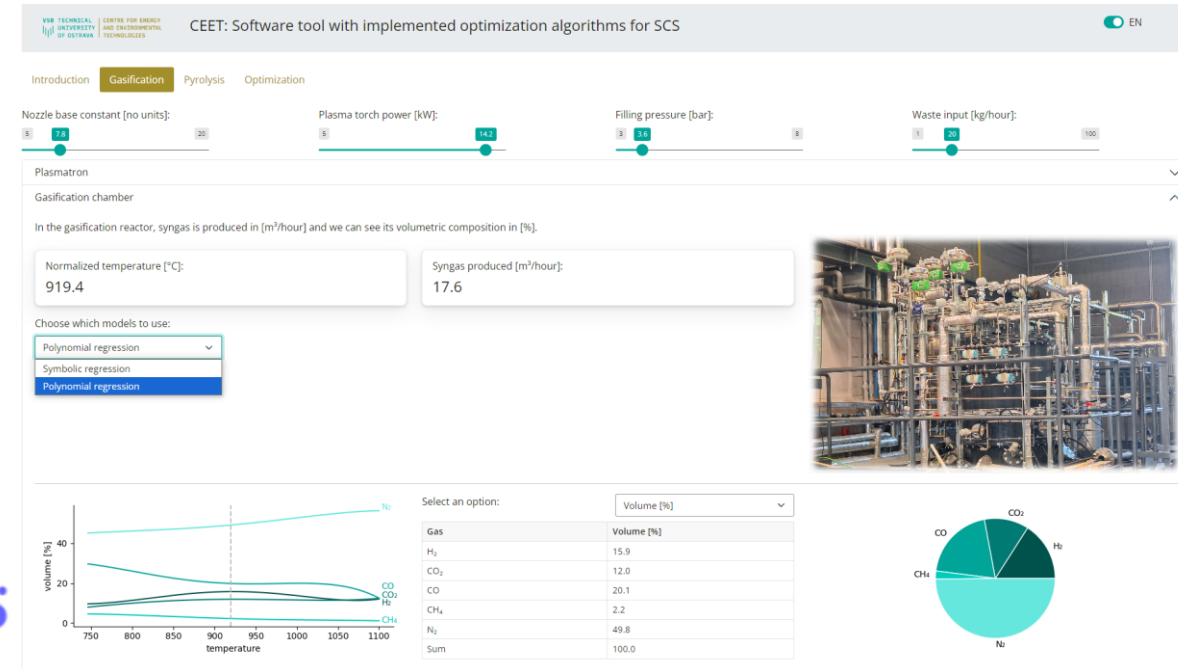
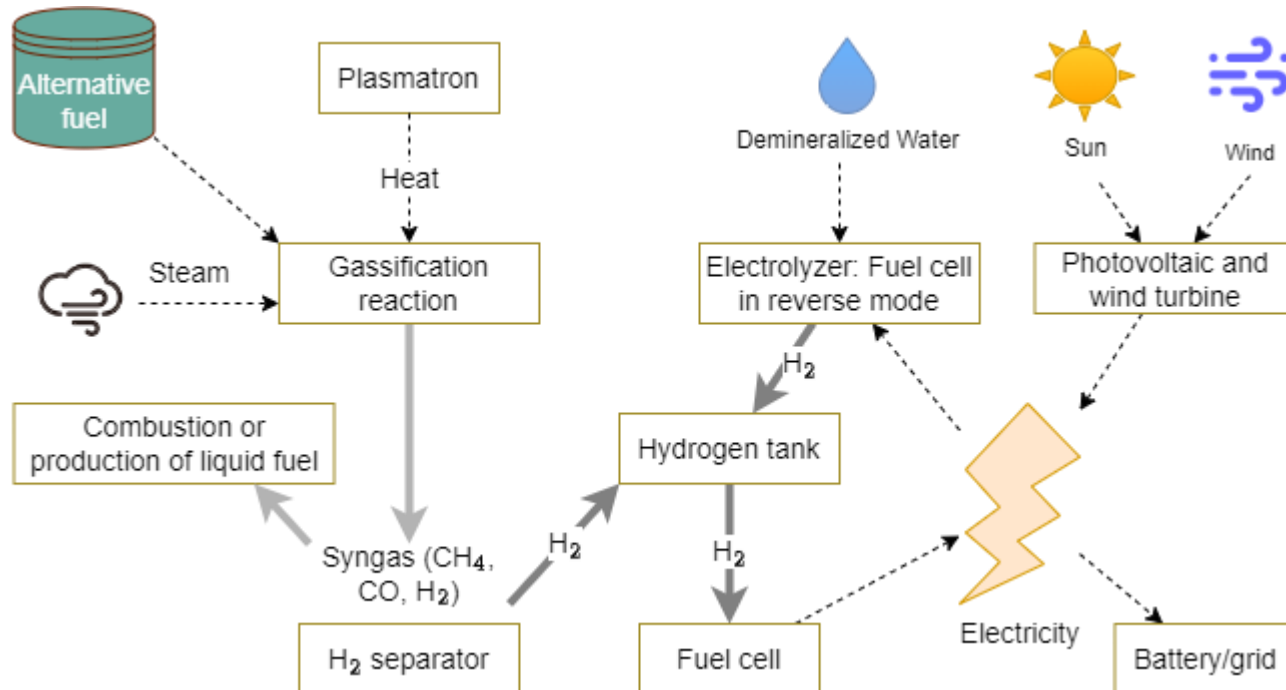
- **Objective:**
Use machine learning to identify parameters that most influence system availability in interconnected **power and communication networks**.
- **Method:**
An optimization algorithm selects input parameters that maximize the **R² (coefficient of determination)**.
- **Key result:**
Out of **27 parameters**, using only **four** – SCADA, RTU, C4, T1 – achieves an **R² = 0.9938**, explaining **99.38%** of the variability in system availability over a time horizon **t = 5 years**.

ML performance and parameter impact

Number of Features	Selected Features	Selected Features Names	R-squared	Std. Error
1	(24)	('SCADA')	0.4394	0.0149
2	(23, 24)	('SCADA', 'RTU')	0.7971	0.0082
3	(11, 23, 24)	('SCADA', 'RTU', 'C4')	0.9057	0.0041
4	(0, 11, 23, 24)	('SCADA', 'RTU', 'C4', 'T1')	0.9938	0.0003
5	(0, 11, 23, 24, 25)	('BTS', 'SCADA', 'RTU', 'C4', 'T1')	0.9968	0.0002
6	(0, 11, 23, 24, 25, 26)	('WAN', 'BTS', 'SCADA', 'RTU', 'C4', 'T1')	0.9981	0.0001

Developed Tool: Shinyenet

- **Developed Tool: *Shinyenet*** — an online software tool implementing **optimization algorithms** for selected **waste-to-energy processes**.
- **Application Context:** Designed for the innovation polygon **CEETe** at **VSB – Technical University of Ostrava**.
- Software is running on the **IT4Innovations** infrastructure.



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The software will be **open-source** and is available for testing:
<https://shinyenet.vsb.cz/>

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Thank You for Your attention!

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MINISTRY OF EDUCATION,
YOUTH AND SPORTS

Increasing the resilience of power grids in the context of decarbonisation, decentralisation, and sustainable socioeconomic development

- Acronym: ZEUS
- 2025 – 2028
- Project ID: CZ.02.01.01/00/23_021/0008759
- Provider: Programme Johannes Amos Comenius (MEYS)
- The project focuses on research and development of software tools for analysing installation efficiency and resilience of new energy sources and storage capacities for use within energy communities and research in the field of hydrogen production, transport and storage. This includes social science research to promote acceptance of these specialised technologies by the general public, development of cooperation with the application sector, project preparation, infrastructure upgrade, and compliance with RIS3.

<https://www.it4i.cz/en/research/research-projects>