MAX PLANCK INSTITUTE FOR DYNAMICS OF COMPLEX TECHNICAL SYSTEMS MAGDEBURG

COMPUTATIONAL METHODS IN SYSTEMS AND CONTROL THEORY

Reduced-order modeling for digital twins in the process industry: application to CO_2 methanation reactors

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November 11, 2025

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Workshop on Reduced Order and Surrogate Modeling for Digital Twins

Institute for Mathematical and Statistical Innovation, Chicago, USA, November 10 - 14, 2025

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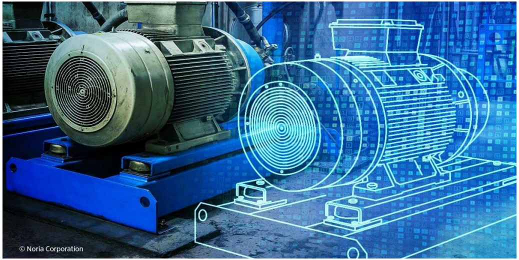
Digital Twins

Digital Twins provide a virtual model of a real-world object, device or process; they allow

- the simulation for analyzing behavior,
- optimizing design and control synthesis,
- surveillance and prediction,
- continuous improvement of the plant model and its controller.



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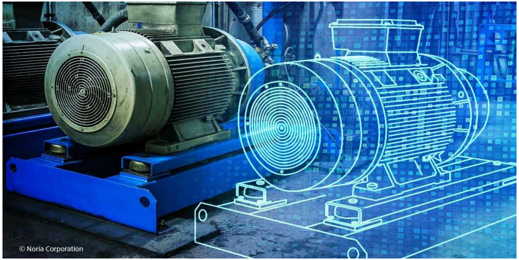
These require real-time response times!



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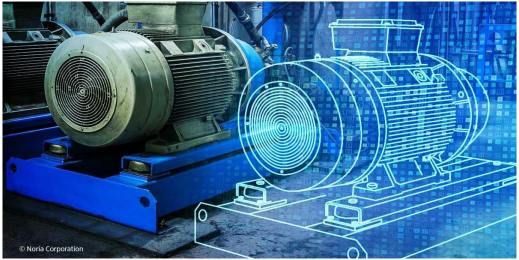

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Smart process engineering (SmartProSys) requires digital twins of, e.g., chemical reactors.

- This involves mathematical models (mass and energy balances, reaction kinetics,. . .).
- For high precision, this involves accurate discretizations of systems of nonlinear coupled partial differential equations.
- Real-time demands (but also, optimization and controller design) require fast-to-evaluate surrogate models.

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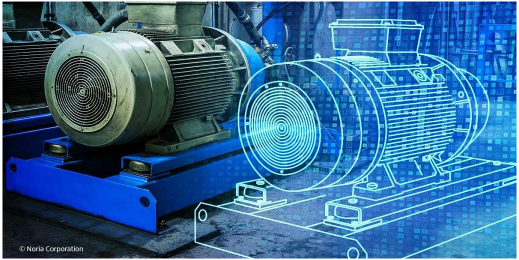

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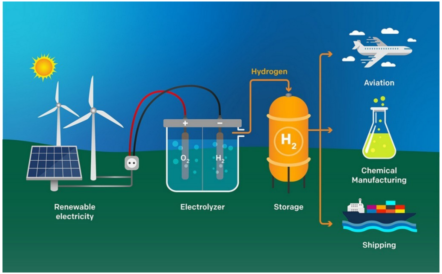
⇝ **MODEL REDUCTION is enabling technology!**

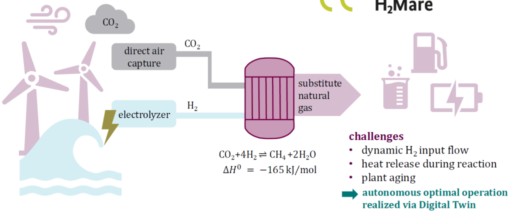
The application under study



CO_2 Methanation Case Study

Rentschler et al., *Chem. Ing. Tech.* (2024)

Leitprojekt H_2Mare



What is Green Hydrogen?

- It is made from water: it is produced by splitting water into hydrogen and oxygen, and this process is called electrolysis.
- Uses clean energy: the process of electrolysis is powered by renewable energy sources like solar and wind energy.

How does Green Hydrogen work?

- Electrolysis: electricity from renewable sources is used to power a device (an electrolyzer).
- Collecting: the gas is then collected and can be stored or transported to where it's needed.
- Using Hydrogen: it can then be used as a fuel (the only byproduct is water) or in reaction with carbon dioxide.

The long-term goal and some of our works

- The **goal** of our project is the development of a **Digital Twin** for a methanation reactor.
- Such a reactor is used to **convert renewable hydrogen** (coming from electrolysis) to more easily-distributable methane.

The long-term goal and some of our works

- The **goal** of our project is the development of a **Digital Twin** for a methanation reactor.
- Such a reactor is used to **convert renewable hydrogen** (coming from electrolysis) to more easily-distributable methane.
- For this purpose, we study a *tubular catalytic wall reactor* and a **semi-discretized dynamic model constructed by mass and energy balances**; preliminary works are listed below ↓

Reactor for the catalytic CO_2 methanation

- I. V. G., L. Peterson, P. Goyal, J. Bremer, K. Sundmacher, and P. B.: *Learning reduced-order Quadratic-Linear models in Process Engineering using Operator Inference*, ENUMATH 2023 Proceedings.
- L. Peterson, A. Forootani, E. Sanchez Medina, I. V. G., K. Sundamcher, and P. Benner: *Towards Digital Twins for Power-to-X: Comparing Surrogate Models for a Catalytic CO_2 Methanation Reactor*, 2024.
- L. Peterson, L., M. Büttner, A. Forootani, I. V. G., P. Benner, and K. Sundmacher: *Greedy Sampling Neural Network SINDy with Control for a Catalytic CO2 Methanation Reactor, LSSC 2025 Proceedings.*

The complex model under study

- The synthetic data are generated from a first-principles reactor model adapted to a pilot plant setting.
- Specifically, we use a one-dimensional polytropic reactor model to generate synthetic data.

Mechanistic Reactor Model

Zimmermann et al., *Chem. Eng. J.* (2022)

reaction rate

$$\sigma_{\mathrm{eff}} = \eta\, \sigma_{\mathrm{int}}$$

$$\sigma_{\mathrm{int}} = k\, p_{\mathrm{CO_2}}^{n_{\mathrm{CO_2}}} p_{\mathrm{H_2}}^{n_{\mathrm{H_2}}} \left(1 - \frac{p_{\mathrm{CH_4}} p_{\mathrm{H_2O}}^2}{K_{\mathrm{eq}} p_{\mathrm{CO_2}} p_{\mathrm{H_2}}^4}\right)$$

$$k = k_{0,\mathrm{ref}} \exp\left(\frac{E_A}{R}\left(\frac{1}{T_{\mathrm{ref}}} - \frac{1}{T}\right)\right)$$

mass balance: $\varepsilon \frac{\partial c_i}{\partial t} = -\vec{u} \cdot \nabla c_i + \nabla(D_i^{\mathrm{eff}} \nabla c_i) + (1-\varepsilon)\nu_i\, \sigma_{\mathrm{eff}}$

energy balance: $(\rho c_p)_{\mathrm{eff}} \frac{\partial T}{\partial t} = -(\rho c_p)_{\mathrm{fluid}}\, \vec{u} \cdot \nabla T + \nabla \cdot (\Lambda_{\mathrm{eff}} \nabla T) + (1-\varepsilon)(-\Delta H_R)\, \sigma_{\mathrm{eff}}$

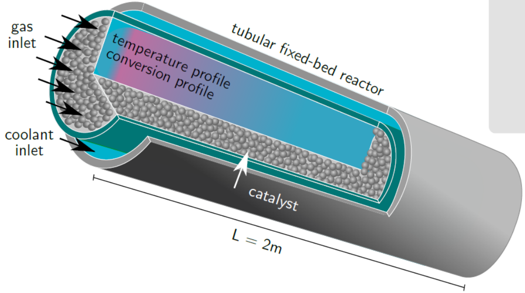
assumptions and details

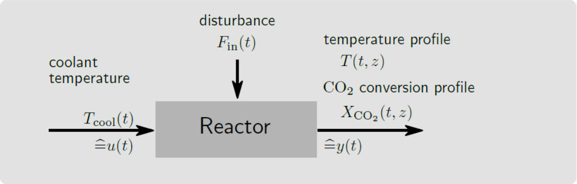
- one- & two-dimensional model
- parameters fitted to experimental data
- discretized via finite volume method
- integrated by use of Kvaerno5 solver (within the diffrax library)

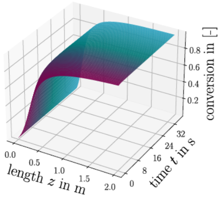
challenges

- nested parameter dependencies
- non-linearities → high disturbance sensitivity
- dynamics on different scales → stiff
- model solutions involve many states (after semi-discretization)

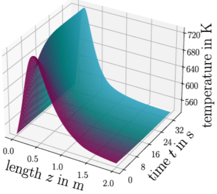
- Reaction kinetics and heat transfer parameters are calibrated against steady-state experimental data from a pilot plant.







CO_2 conversion profile



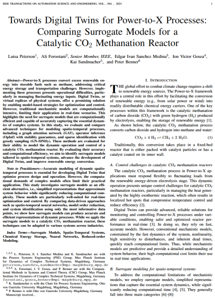
temperature profile

The proposed methods

SciML and surrogate modeling through stable Operator Inference (OpInf) ★ and GN-SINDy ⋆

- The results presented in what follows were published this year in the IEEE Transactions on Automation Science and Engineering (free copy available on TechRxiv):

  L. Peterson et al., *Towards Digital Twins for Power-to-X: Comparing Surrogate Models for a Catalytic CO_2 Methanation Reactor*, 2025



IEEE TRANSACTIONS ON AUTOMATION SCIENCE AND ENGINEERING, VOL. , NO. , 2024 1

Towards Digital Twins for Power-to-X Processes: Comparing Surrogate Models for a Catalytic CO_2 Methanation Reactor

Luisa Peterson[1], Ali Forootani[2], *Senior Member, IEEE*, Edgar Ivan Sanchez Medina[3], Ion Victor Gosea[4], Kai Sundmacher[5], and Peter Benner[6]

***Abstract*—Power-to-X processes convert excess renewable energy into storable fuels such as methane, addressing critical energy storage and transportation challenges. However, implementing these processes presents operational difficulties, particularly in managing fluctuating energy inputs. Digital Twins, or virtual replicas of physical systems, offer a promising solution by enabling model-based strategies for optimization and control. However, traditional mechanistic models are computationally intensive, limiting their application in real-time scenarios. This highlights the need for surrogate models that are computationally efficient and capable of accurately capturing the essential dynamics of complex systems. In this study, we evaluate and compare advanced techniques for modeling spatio-temporal processes, including a graph attention network (GAT), operator inference (OpInf) with stability guarantees, and sparse identification with greedy sampling (GN-SINDy). These methods are evaluated for their ability to model the dynamic operation and control of a catalytic CO_2 methanation reactor. By evaluating their accuracy and computational efficiency, we aim to identify surrogate models tailored to spatio-temporal systems, advance the development of Digital Twins, and improve renewable energy conversion.**

***Note to Practitioners*—Accurate modeling of dynamic spatio-temporal processes is essential for developing Digital Twins that optimize process design and operation. However, the computational demands of complex models often limit their practical application. This study investigates surrogate models as an efficient alternative, i.e., simplified representations that approximate system behavior while significantly reducing computational complexity. These models are particularly well-suited for real-time optimization and control. By comparing data-driven approaches such as spatio-temporal neural networks, model order reduction, and system identification using only the most informative data points, we show how surrogate models can produce accurate and efficient representations of dynamic processes. While we apply the surrogate models to a catalytic CO_2 methanation reactor, these techniques can be adapted to various systems across industries.**

***Index Terms*—Surrogate Models, Spatio-Temporal Systems, Chemical Energy Storage, Neural Networks, Reduced-order Modeling.**

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Manuscript received...

I. INTRODUCTION

THE global effort to combat climate change requires a shift to renewable energy sources. The Power-to-X framework plays a central role in this effort by facilitating the conversion of renewable energy (e.g., from solar power or wind) into readily distributable chemical energy carriers. One of the key processes within this framework is the catalytic methanation of carbon dioxide (CO_2) with green hydrogen (H_2) produced by electrolysis, enabling the storage of renewable energy [1].

As shown below, the catalytic CO_2 methanation process converts carbon dioxide and hydrogen into methane and water:

$$CO_2 + 4\,H_2 \rightleftharpoons CH_4 + 2\,H_2O. \qquad (1)$$

Traditionally, this conversion takes place in a fixed-bed reactor that is either packed with catalyst particles or has a catalyst coated on its inner wall.

A. Control challenges in catalytic CO_2 methanation reactors

The catalytic CO_2 methanation process in Power-to-X applications must respond flexibly to fluctuating loads from the renewable energy-driven electrolysis stage. This dynamic operation presents unique control challenges for catalytic CO_2 methanation reactors, particularly in managing the heat generated by the highly exothermic reaction, which often results in localized hot spots that compromise temperature control and reduce efficiency [2].

Digital Twins can provide advanced, reliable solutions for monitoring and controlling Power-to-X processes under variable conditions, enabling safer and optimized reactor performance in real-time [3]. In doing so, they rely on fast, accurate models. However, conventional mechanistic models, constrained by the fast dynamics of the system, nonlinearity, high sensitivity to disturbances, and inherent dead times, quickly reach computational limits. Thus, while mechanistic models are predictive and provide a detailed understanding of system behavior, their high computational cost limits their use in real-time applications.

B. Surrogate modeling for spatio-temporal systems

To address the computational limitations of mechanistic models, we employ surrogate models, simplified representations that capture the essential system dynamics, while significantly reducing computational time [4], [5]. They generally fall into three main categories [6]–[8]:

★ P. Goyal, I. Pontes Duff, P. Benner, *Guaranteed Stable Quadratic Models and their applications in SINDy and Operator Inference*, Physica D: Nonlinear Phenomena, Vol. 483, pp. 134893, 2025.

⋆ A. Forootani, P. Benner, *GN-SINDy: Greedy Sampling Neural Network in Sparse Identification of Nonlinear Partial Differential Equations*, arXiv:2405.08613, 2024.

Reduced-Order Model: Operator Inference

Peherstorfer & Willcox, *Comp. Meth. Appl. Mech. Eng.* (2016); Goyal et al., *Phys. D* (2025)

1 principal component analysis + projection

a) PCA via SVD

$$\underset{n \times d}{\boldsymbol{Q}} = \underset{n \times n}{\boldsymbol{U}} \; \underset{n \times d}{\boldsymbol{\Sigma}} \; \underset{d \times d}{\boldsymbol{V}^T}$$

$\boldsymbol{U}_\mathrm{r}$: $n \times r$, $\boldsymbol{\Sigma}_\mathrm{r}$: $r \times r$, $\boldsymbol{V}_\mathrm{r}^T$: $r \times d$

b) projection on low dimensional basis

$$\begin{matrix} \mathbf{Q} \\ \dot{\mathbf{Q}} \end{matrix} \xrightarrow{\cdot\, \boldsymbol{U}_\mathrm{r}^T} \begin{matrix} \hat{\mathbf{Q}} \\ \dot{\hat{\mathbf{Q}}} \end{matrix} \xrightarrow{\cdot\, \boldsymbol{U}_\mathrm{r}} \begin{matrix} \tilde{\mathbf{Q}} \\ \dot{\tilde{\mathbf{Q}}} \end{matrix}$$

compress decompress

2 low-dimensional regression

a) define reduced-order model structure

$$\dot{\hat{q}} = \hat{\mathbf{A}}\hat{q} + \hat{\mathbf{H}}(\hat{q} \otimes \hat{q}) + \hat{\mathbf{B}}u$$

b) get reduced operators

$$\min_{\hat{A},\hat{H}} \left\| \hat{Q}^T\hat{\mathbf{A}}^T + \left(\hat{Q} \odot \hat{Q}\right)^T \hat{\mathbf{H}}^T + \mathbf{U}^T\hat{\mathbf{B}}^T - \dot{\hat{Q}}^T \right\|_F^2$$

solve with **gradient-based optimization**

stable OpInf: choose a parameterization of $\hat{\mathbf{A}}$ and $\hat{\mathbf{H}}$, such that the inferred models are stable by design

Stable OpInf II: more details in [Goyal et al. '25], [Gkimisis et al. '25]

Asymptotic (exponential, Lyapunov) stability of linear systems

$$\dot{x}(t) = Ax(t), \qquad x(0) = x_0,$$

can be explicitly parameterized:

Theorem (Gillis/Sharma 2017)

A matrix $A \in \mathbb{R}^{n \times n}$ is asymptotically stable (Hurwitz, Lyapunov stable) if and only if it can be represented as

$$A = (J - R)Q,$$

where $J = -J^T$ and $R = R^T$, $Q = Q^T$ are both positive definite.

$\Longrightarrow$ **Stability-preserving OpInf for linear systems**:

$$(S_*, L_*, K_*) := \operatorname{argmin}_{\substack{L,K \text{ upper triangular} \\ \text{with positive diagonals}}} \left(\|\dot{X} - (S - S^T - L^T L) K^T K X\|_F^2 + \mathcal{R}(L, K, S) \right)$$

The matrix obtained from this nonlinear (regularized) least-squares problem,

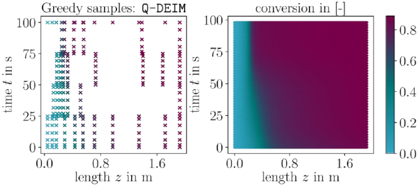
$$A_* = \left(S_* - S_*^T - L_*^T L_* \right) K_*^T K_*,$$

is guaranteed to be stable due to [Gillis/Sharma 2017]. Related work by *Schwerdtner, Voigt, ...*

Reduced-Order Model: Greedy Sparse Identification

Brunton et al., *Proc. Natl. Acad. Sci.* (2016), Forootani & Benner, *arXiv* (2024)

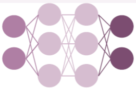
1 greedy sampling via Q-DEIM



a) **POD** to construct a reduced approximation of the snapshot matrix
b) **QR DECOMPOSITION** with column pivoting to select key time and space indices from reduced matrices

2 sparse regression on a library

$$\mathcal{L} = \mathrm{MSE}(u, \hat{u}) + \mathrm{MSE}\left(\hat{u}_t, \Theta\,\vec{\xi}\right) + \mathrm{L}_1(\vec{\xi})$$

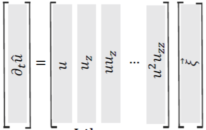


Auto. Diff. $\rightarrow$

$\leftarrow$ Include in $\mathcal{L}$

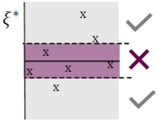
$(z, t) \longrightarrow \hat{u} \in \{\hat{X}, \hat{T}\}$

$$\hat{u}_t = \Theta\vec{\xi}$$



Normalize $\longrightarrow$

$$\xi^* = \xi \cdot \frac{\|\Theta\|}{\|u_t\|}$$



Steps (a) and (b)

The GN-SINDy approach introduces several **improvements to standard SINDy**:

- In step (a) of GN-SINDy, the Q-DEIM algorithm is used to sample the data set.
- Q-DEIM first applies the SVD to extract dominant features by retaining singular values above a precision threshold ϵ_{tresh} (linked to `DEIM_tolerance`), then uses QR decomposition with pivoting to select key spatio-temporal indices.
- This sensor placement strategy efficiently balances the trade-off between preserving essential dynamics and computational cost.

- In step (b), sample pairs (t_i, x_i) from Q-DEIM are entered into a DNN.
- The DNN learns the nonlinear mapping $(t, x) \mapsto u$ and the underlying physics via $\frac{\partial \boldsymbol{u}}{\partial t} = \boldsymbol{\theta}\boldsymbol{\xi}$.
- The output $\hat{\boldsymbol{u}}$ of the DNN serves as a function approximation used to construct the dictionary $\boldsymbol{\Theta}$ and compute $\frac{\partial \hat{\boldsymbol{u}}}{\partial t}$ by automatic differentiation.

Steps (c) and (d)

- Step (c) estimates $\boldsymbol{\xi}$ via stochastic gradient descent to minimize the loss function.
- The loss function for training the DNN comprises of a MSE component to capture the mapping $(t, x) \to \hat{\mathbf{u}}$, and an additional term to enforce constraints on the DNN solutions:

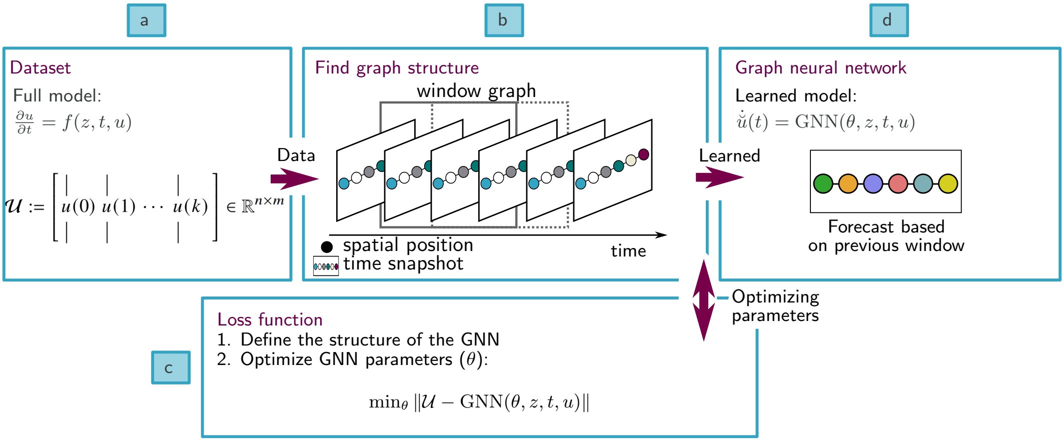
$$\mathcal{L} = \frac{1}{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} \Big(\mathbf{u}(t_i, x_i) - \hat{\mathbf{u}}(t_i, x_i) \Big)^2 + \frac{1}{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} \Big(\frac{\partial \hat{\mathbf{u}}(t_i, x_i)}{\partial t_i} - \boldsymbol{\Theta}\big(\hat{\mathbf{u}}(t_i, x_i)\big)(\boldsymbol{\xi} \odot \boldsymbol{g}) \Big)^2.$$

- (t_i, x_i) are the selected sample pairs in the domain, $\boldsymbol{u}(t_i, x_i)$ is calculated using the Q-DEIM algorithm applied to the snapshot matrix $\mathcal{U}$ and $\boldsymbol{g}$ is the sparsity mask.
- The DNN is constrained by the element-wise multiplication of $\boldsymbol{\xi}$ and $\boldsymbol{g}$, not by $\boldsymbol{\xi}$ alone.
- In step (d), the learned coefficient vector yields a model explaining the original data set.

$\rightsquigarrow$ see also the work in [Forootani et al. '24] (arXiv:2405.08613).

Comparison method: GNN (GAT)

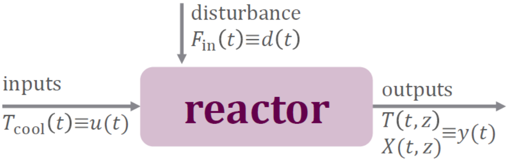
- GATs use attention mechanisms to assign adaptive weights to neighbors based on their relevance, making them effective for tasks where the importance of neighboring nodes varies significantly [Veličković et al. '18];



Numerics

Comparative Analysis – Study Design

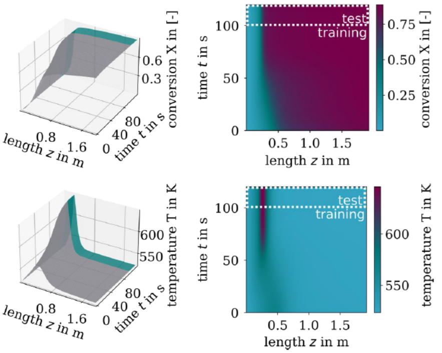
Peterson et al., *IEEE Trans. Autom. Sci. Eng.* (2025)



scenario (i):	$F_{in}(t)$ ↓
scenario (ii):	$F_{in}(t)$ ↑
scenario (iii):	$T_{cool}(t)$ ↓
scenario (iv):	$T_{cool}(t)$ ↑

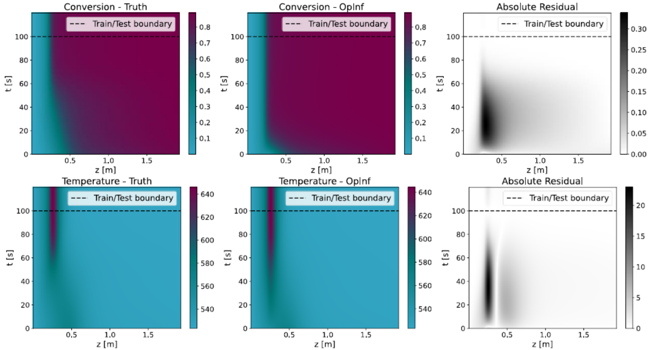
- get data based on the mechanistic model
- train on the first ~80 % of the time trajectory, **predict** the remaining ~20 %
- run each model **10×** for each scenario

trajectories for scenario (i)



Operator Inference - Results

Peterson et al., *IEEE Trans. Autom. Sci. Eng.* (2025)



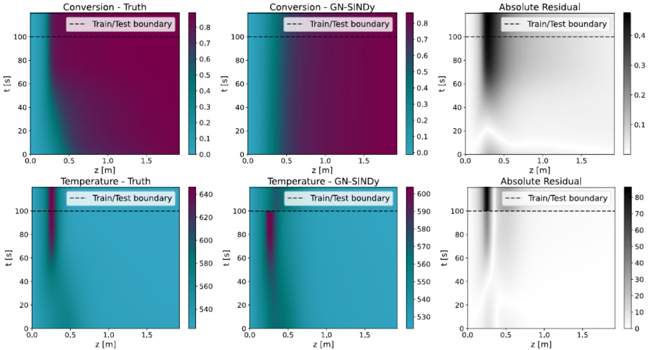
results for scenario (i)

forecasting speedup factor: 10.66

test (i)	test (ii)	test (iii)	test (iv)	training time	forecasting time	input parameter	model parameter
0.067 $\pm$ 0.046 %	0.075 $\pm$ 0.059 %	0.25 $\pm$ 0.010 %	0.30 $\pm$ 0.018 %	2816 $\pm$ 366 s	0.64 $\pm$ 0.15 s	6	42

Greedy Sparse Identification - Results

Peterson et al., *IEEE Trans. Autom. Sci. Eng.* (2025)



results for scenario (i)

forecasting speedup factor: 48.71

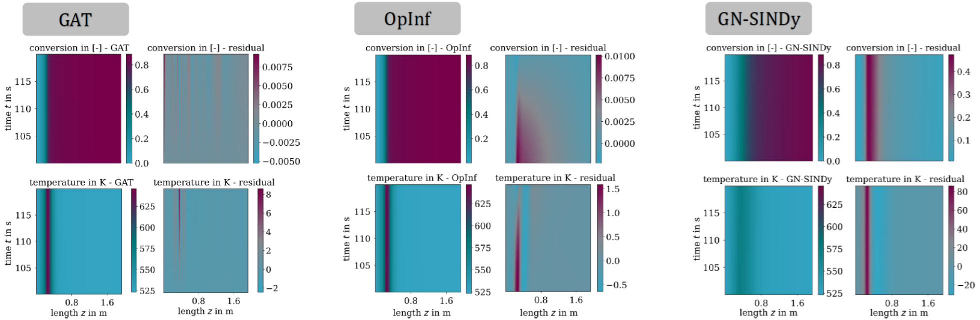
test (i)	test (ii)	test (iii)	test (iv)	training time	forecasting time	input parameter	model parameter
3.78 ± 0.018 %	1.09 ± 0.0080 %	6.47 ± 0.070 %	6.31 ± 0.069 %	96 ± 49 s	0.14 ± 0.012 s	792 – 1438	13186

Comparison: part I

Comparative Analysis – Prediction Error

Peterson et al., *TechRxiv* (2024)

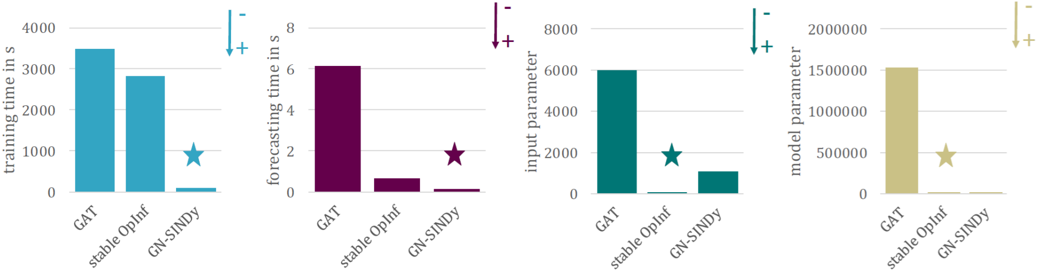
prediction results for scenario (i)



method	test (i)	test (ii)	test (iii)	test (iv)
GAT	0.17 ± 0.075 %	0.097 ± 0.059 %	0.29 ± 0.033 %	**0.21 ± 0.030** %
Stable OpInf	**0.067 ± 0.046** %	**0.075 ± 0.059** %	**0.25 ± 0.010** %	0.30 ± 0.018 %
GN-SINDy	3.78 ± 0.018 %	1.09 ± 0.0080 %	6.47 ± 0.070 %	6.31 ± 0.069 %

Comparative Analysis – Complexity

Peterson et al., *TechRxiv* (2024)



method	training time	forecasting time	input parameter	model parameter
GAT	3475 ± 213 s	6.11 ± 0.039 s	6000	1528130
Stable OpInf	2816 ± 366 s	0.64 ± 0.15 s	**6**	**42**
GN-SINDy	**96 ± 49 s**	**0.14 ± 0.012 s**	792 – 1438	13186

Summary & Outlook

why Digital Twin?

- concept that **bi-directionally links** a physical entity to a model
- goal: enable **optimal control** for PtX
- **real-time** model execution needed

key findings

	ST-NN	GN-SINDy	OpInf
accuracy	✓		✓
speed		✓	✓

what we did

- compared three surrogate models:
  - Spatio-Temporal Neural Networks (**ST-NN**),
  - Greedy Sparse Identification (**GN-SINDy**),
  - Operator Inference (**OpInf**)
- focus: speed, accuracy, and generalizability

next steps

- **closed-loop control** integration
- Analysis of other **ROM methods**
- Full **Digital Twin** implementation

Special thanks also to Pawan Goyal (appliedAI Initiative GmbH), Jens Bremer (TU Clausthal), Ronny Zimmermann & Alexander Geschke (MPI, PSE), Miriam Büttner (TU Berlin) . . .

Extensive survey published

Our recent survey paper (one of the first **Digital Twin** survey in **Process Engineering**), addresses the following relevant topics*:

- **Guidance for practitioners:** Providing guidance to researchers and practitioners in **Process Engineering** and chemical engineering fields.
- **Real-time representation:** Addressing real-time representation challenges in **Digital Twin** development and offering practical solutions.
- **Numerical methods review:** Comprehensive review of state-of-the-art numerical methods and tools for constructing **Digital Twin**s, with a focus on applications in **Process Engineering**.
- **Unlocking potential:** Highlighting the transformative potential of **Digital Twin**s in **Process Engineering** and offering insights into essential mathematical tools to be harnessed.

* L. Peterson, I. V. G., P. Benner and K. Sundmacher: *Digital twins in process engineering: An overview on computational and numerical methods*, Computers & Chemical Engineering, Vol. 193, pp. 108917, February, 2025.

The team behind it

GEFÖRDERT VOM
Bundesministerium für Bildung und Forschung

Leitprojekt H_2Mare

SmartProSys

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Peterson et al., Comput. Chem. Eng. (2025)

Thank you for your attention!

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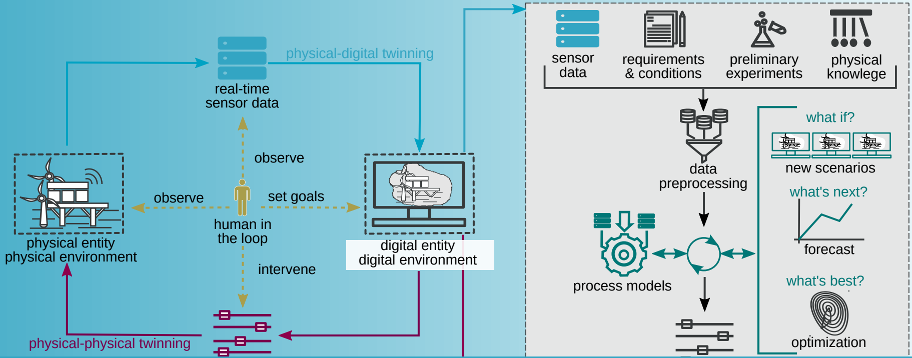
Thank you!

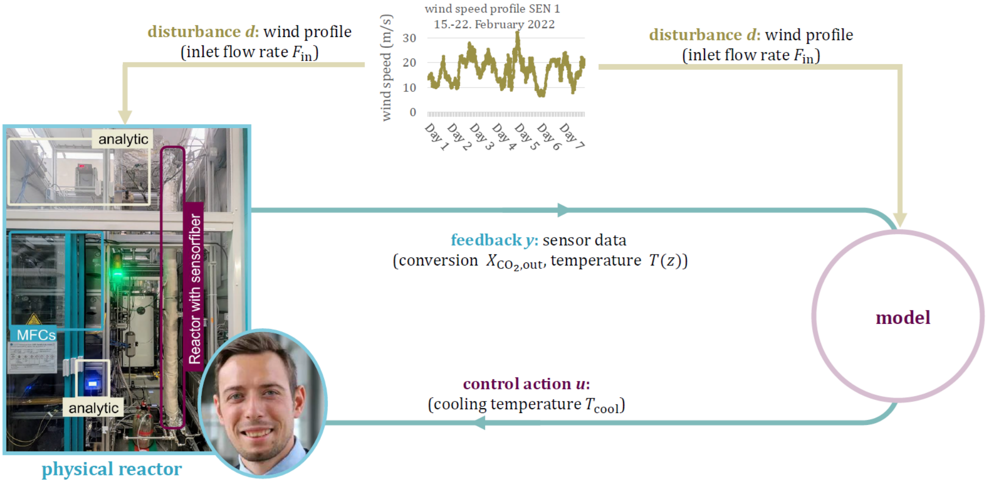
Any questions?

The twinning scenario

- Real-time sensor data and physical models of an existing chemical plant (the physical entity), are used to represent its current state as a virtual entity.
- This virtual entity can provide several benefits, e.g., scenario exploration, prediction, and optimization.
- The virtual and physical entities are thus connected in real time through bi-directional data exchange.



Digital Twin Data Flow



- The energy balance equation describes the energy distribution in the reactor, taking into account heat conduction, convective heat transport, heat exchange with the environment.

$$(\rho c_p)_{\text{eff}} \frac{\partial T}{\partial t} = -u_{\text{in}}\, \rho_{\text{in}} c_p \frac{\partial T}{\partial z} + \frac{\partial}{\partial z}\left[\Lambda_{\text{z}} \frac{\partial T}{\partial z}\right] - \frac{4\,U}{D}\,(T - T_{\text{cool}}) - \Delta H_{\text{r}}\,(1 - \varepsilon_R)\,\zeta\,\sigma_{\text{eff}}$$

- Each term represents a specific aspect of heat transport and heat reaction in the reactor:
  1. $(\rho c_p)_{\text{eff}} \frac{\partial T}{\partial t}$: indicates how quickly the temperature in the reactor changes over time. It depends on the reactor's effective heat capacity, which is determined by the reactor's material.
  2. $-u_{\text{in}}\, \rho_{\text{in}} c_p \frac{\partial T}{\partial z}$: reflects the influence of convective heat transport along the reactor axis.
  3. $\frac{4\,U}{D}\,(T - T_{\text{cool}})$: represents the heat loss due to heat transfer at the wall of the reactor.
  4. $-H_{\text{r}}\,(1 - \varepsilon_R)\,\zeta\,\sigma_{\text{eff}}$: takes into account the heat released/absorbed due to the chemical reaction.

- The resulting mass balance equation for the conversion of CO_2 is:

$$\varepsilon_R \frac{\partial X}{\partial t} = -u \frac{\partial X}{\partial z} + \frac{M_{\mathrm{CO_2}}}{\rho \, y_{\mathrm{CO_2,in}}} (1 - \varepsilon_R) \, \zeta \, \sigma_{\mathrm{eff}} \tag{1}$$

with the following terms:

1. $\varepsilon_R \frac{\partial X}{\partial t}$: reflects how quickly the conversion of CO_2 in the reactor changes over time.
2. $-u \frac{\partial X}{\partial z}$: describes the influence of the flow velocity on the spatial distribution of the CO_2 conversion in the reactor (convective transport in the z-direction).
3. $\frac{M_{\mathrm{CO_2}}}{\rho \, y_{\mathrm{CO_2,in}}} (1 - \varepsilon_R) \, \zeta \, \sigma_{\mathrm{eff}}$: encompasses the chemical reaction itself, where σ_{eff} represents the effective reaction rate.

- **Taking into account the conversion law for mass and energy, for any control volume of different shape and size within the reactor, the following basic set of equilibrium equations (Euler specification) applies:**

$$\textbf{Totale Masse}\ \frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \vec{u}) \tag{2}$$

$$\textbf{Komponenten Masse}\ \rho \frac{\partial \omega_\alpha}{\partial t} = -\rho \vec{u} \nabla \cdot \omega_\alpha - \nabla \cdot \vec{j}_\alpha + M_\alpha \sum_\beta \nu_{\alpha,\beta} \tilde{r}_\beta \tag{3}$$

$$\textbf{Energie}\ \rho c_p \frac{\partial T}{\partial t} = -\rho c_p \vec{u} \nabla T - \nabla \cdot \vec{\dot{q}} - \sum_\beta \nu_{\alpha,\beta} \left(\Delta_R \tilde{H}_\beta \right) \tilde{r}_\beta \tag{4}$$

- **When considering a single reaction, the mass balance equation of the components CO_2, H_2, CH_4, H_2O and N_2 can be summarized in a single equation by using the carbon dioxide conversion X_{CO_2}:**

$$\dot{n}_i = \dot{n}_{i,\mathrm{in}} + \nu_i X_{CO_2} \dot{n}_{CO_2,\mathrm{in}} \tag{5}$$