SUPPLEMENTARY INFORMATION

Model Predictive Control using Physics Informed Neural Networks for Process Systems.

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Table S1. Model Parameters of CSTR System

Parameter	**Units**	**Nominal Operating Points**
Coolant flow rate ($U_1 = F_C$)	*m^3/min*	15
Inlet flow rate of A ($U_2 = F$)	*m^3/min*	1
Reactor concentration of A ($X_1 = C_A$)	*$kmol/m^3$*	0.265
Reactor temperature ($X_2 = T$)	*K*	393.954
Inlet concentration of A ($D = C_{AO}$)	*$kmol/m^3$*	2.0
Parameter	**Units**	**Values**
Reaction rate constant (k_0)	*min^{-1}*	10^{10}
Density of the reagent A (ρ)	*g/m^3*	10^6
Specific heat capacity of A (C_p)	*cal/g°C*	1.0
Heat of reaction (ΔH_r)	*cal/kmol*	$-130*10^6$
Density of the coolant (ρ_c)	*g/m^3*	10^6
Specific heat capacity of coolant (C_{pc})	*cal/g°C*	1.0
Volume of the CSTR (V)	*m^3*	1.0
Inlet temperature of the coolant (T_{cin})	*K*	365
Inlet temperature of A (T_o)	*K*	323
a	(cal/min)/K	$1.678*10^6$
Reaction Rate Parameter (E/R)	*K^{-1}*	8330
b		0.5

Table S2. Model Parameters of Electrochemical System

Parameter	**Values**
F	96487
R	8.314
$\varphi_{eq,1}$	0.420
$\varphi_{eq,2}$	0.303
ρ	3.4
W	92.7
V	1×10^{-5}
i_{app}	1×10^{-5}
i_{01}	1×10^{-04}
i_{02}	1×10^{-08}

Table S3. Bounds of variables for PINN training and MPC

For a CSTR ODE System:			
Inputs	**Lower Bound**	**Upper Bound**	**Max Move**
U_1	12	18	1.2
U_2	0.5	1.5	0.2
X_1	0.01	0.9	-
X_2	330	450	-
Timestep (t)	0	0.8	-
For an Electrochemical DAE System:			
Inputs	**Lower Bound**	**Upper Bound**	**Max Move**
U_1	273	343	10
X_1	0.01	1	-
X_2	0.3	0.54	-
Timestep (t)	0	500	-

Table S4. MPC Parameters

For a CSTR ODE System:	
Parameter	**Value**
Prediction Horizon (P)	20
Control Horizon (M)	6
No of simulation steps	130
α	[10000, 0]
β	[1, 1]
For an Electrochemical DAE System:	
Inputs	**Lower Bound**
Prediction Horizon (P)	7
Control Horizon (M)	3
No of simulation steps	50
α	[10000, 0]
β	[0.05]

PINN Data Generation

The PINN models for both the ODE system and DAE system are trained on a dataset consisting of the inputs $[t, U, X_k]$. X_k are the initial values at the k^{th} step. This input dataset is generated by obtaining collocation points for each U and X in a range given in Table S3. The internal collocation points incorporating the varying timesteps t are additionally appended with zeros to evaluate residuals at the

ICs. The predictions X_{K+1} are obtained from PINN which has been trained by minimizing the residuals of the loss function incorporating the physics, as described in Fig. 1. While the ODE and DAE systems are trained using the unlabeled dataset, their initial conditions are enforced using labeled samples.