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]