DIGITAL TWIN

Department of Chemical Engineering

(CP-302 Project)

Presented by:

Arpita Singh - 2019CHB1042

Project Mentor:

Dr. Himanshu Paliwal

Digital Twin

- A digital twin is a virtual/digital copy of a device, system or process that accurately mimics actual performance, in real-time, that is executable and can be manipulated.
- Benefits include Operational Improvement, Predictive maintenance, cost reduction and effective-decision making.

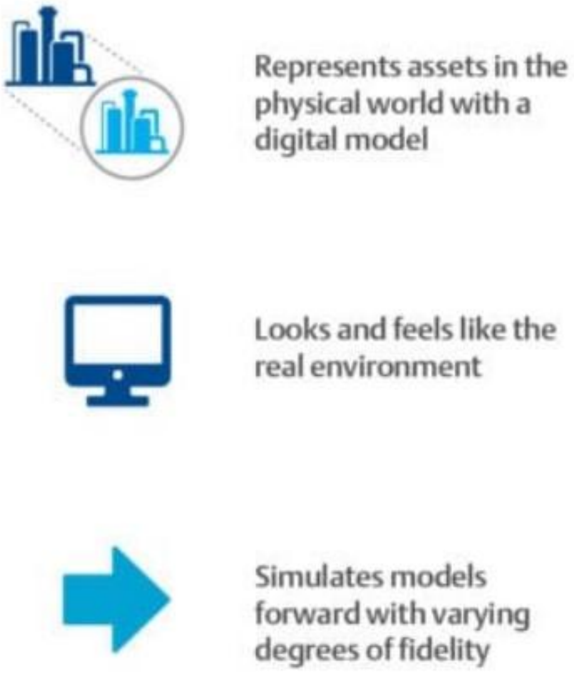


Fig 1: Digital twin technology[1]

[1] Berutti, M 2019, 'Understanding the digital twin', *IIOT Oil and Gas*. Understanding the Digital Twin - Chemical Engineering (chemengonline.com). (Accessed: 4 February 2022)

Why do we need Digital twin?

Fig 2: Steady, dynamic and real-time model[2]

[2] Berutti, M 2019, ‘Understanding the digital twin’, *IIOT Oil and Gas*. Understanding the Digital Twin - Chemical Engineering (chemengonline.com). (Accessed: 4 February 2022)

Problem Statement

Create a digital twin of Continuous Stirred Tank Reactor (CSTR).

- Model Assumptions:

    1. Irreversible and exothermic reaction: A —> B
    2. Constant volume, heat capacity and density
    3. Neglecting changes in Kinetic and Potential energy

- Balance on component A:

$$\frac{dCa}{dt} = f1(Ca,T) = \frac{F}{V}(C_{af} - C_a) - k_0\exp\left(\frac{-Ea}{RT}\right)Ca$$

- Reactor Energy Balance:

$$\frac{dT}{dt} = f2(Ca,T) = \frac{F}{V}(Tf - T) + \frac{(-\Delta H)}{\rho Cp} k_0\exp\left(\frac{-Ea}{RT}\right)Ca - \frac{UA}{V\rho Cp}(T - T_j)$$

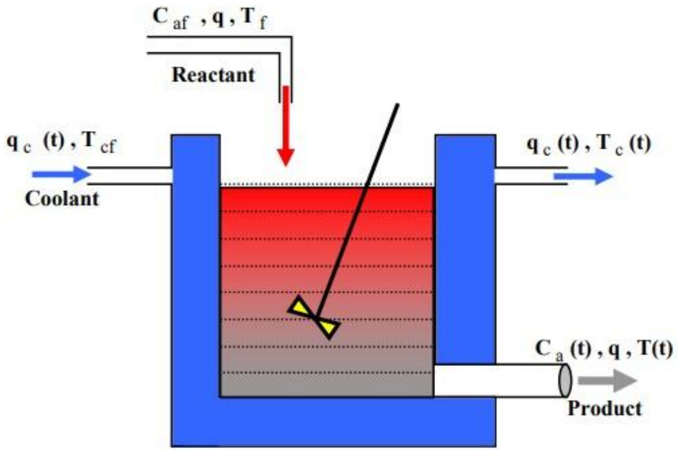


Fig 3: CSTR with cooling jacket[3]

[3] Bequette, B 2002, Process Control Modeling. Process Control : Modeling, Design, and Simulation / B.W. Bequette. | Request PDF (researchgate.net). (Accessed: 10 February 2022)

Methodology

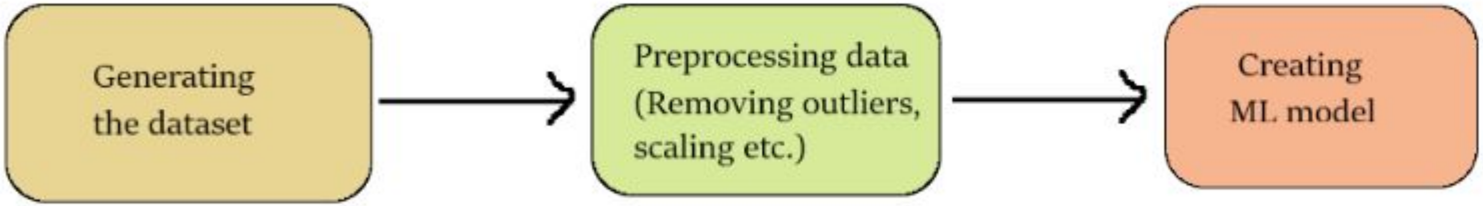


Fig 4: Flowchart for creating a digital twin

Tools used:

Data Generation

- For generating data, a dynamic model was created with the assumptions mentioned in slide(4).

```
# defining the reactor model
def simulation_model(t,x):
    Ca = x[0]
    T = x[1]
    k = k0*np.exp(-E_over_r/T)
    w = q*rho
    dcAdt = q*(cA_i - Ca)/V - k*Ca
    dTdt = 1/(V*rho*C)*(w*C*(Ti - T) - Hr*V*k*Ca + UA*(Tc - T))
    return dcAdt, dTdt
```

```
# simulation run time: 60 min (1 hr)

tspan = (0, 60)
t = np.linspace(*tspan, 1000)
```

```
Ca0 = 0.5     #mol/L
T0 = 350.0    #K
```

```
def simulate():
    res = solve_ivp(simulation_model, tspan, y0, t_eval=t)
    return res.y
```

```
# Generating a noise array
length = len(t)
noise = 0.001*np.random.randn(length)
```

Preprocessing Data

- Polynomial Regression

Gives better fit at very high

Degree (>5) of polynomial!

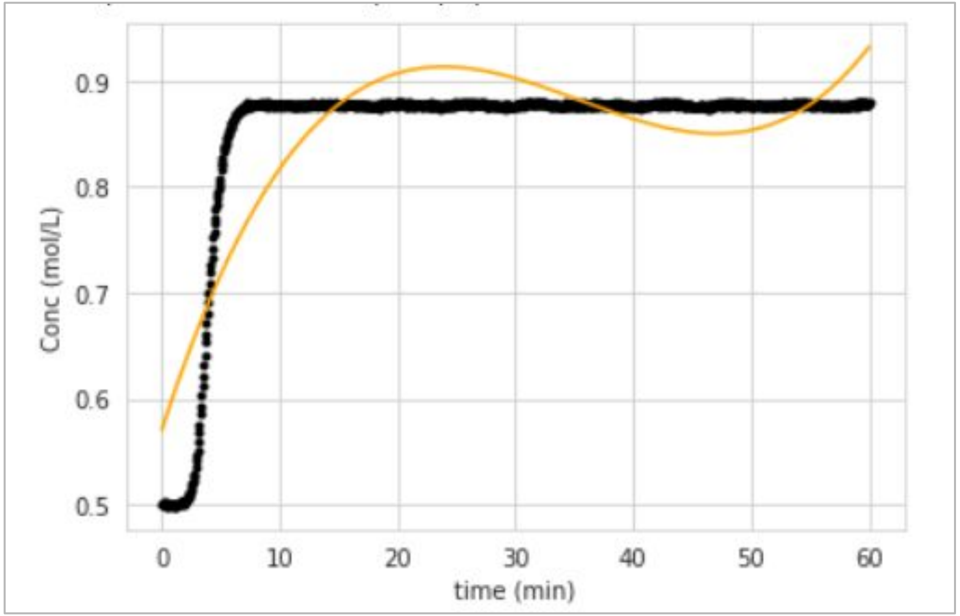


Fig 5: Concentration vs. time plot

```
#Fitting the Polynomial regression to the dataset
x_ = PolynomialFeatures(degree=3, include_bias=False).fit_transform(x2)
model = LinearRegression().fit(x_, y1)
intercept, coefficients = model.intercept_, model.coef_
y_pred = model.predict(x_)
```

Preprocessing Data

- Calculated Moving Average then used cubic spline to fit the data points

```
def moving_average(temp_avg, w):
    return np.convolve(temp_avg[:,0], np.ones(w), 'valid') / w

def moving_average(conc_avg, w):
    return np.convolve(conc_avg[:,0], np.ones(w), 'valid') / w

def moving_average(t_avg, w):
    return np.convolve(t_avg[:,0], np.ones(w), 'valid') / w
```

```
cs = CubicSpline(t, conc)
cs1 = CubicSpline(t, temp)
conc_new = cs(x2)
temp_new = cs1(x2)
```

```
xscaler = MinMaxScaler()
yscaler = MinMaxScaler()

X = xscaler.fit_transform(temp_avg.reshape(temp_avg.shape[0], 1))
Y = yscaler.fit_transform(conc_avg.reshape(conc_avg.shape[0], 1))
```

Preprocessing Data

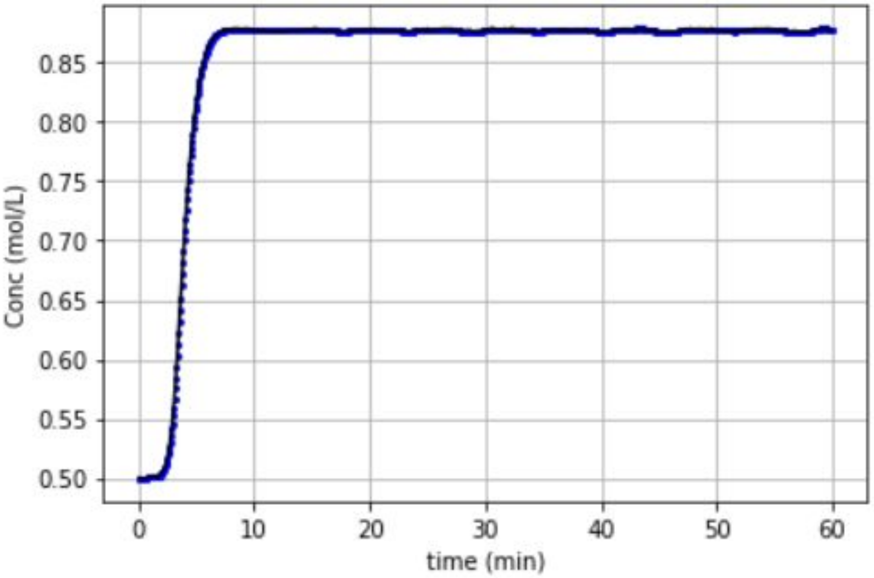


Fig 6: Concentration vs. time plot

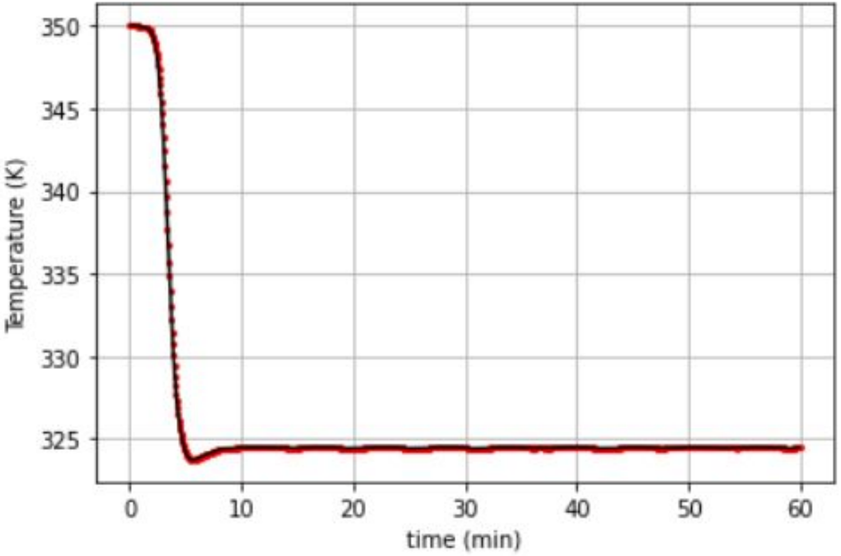
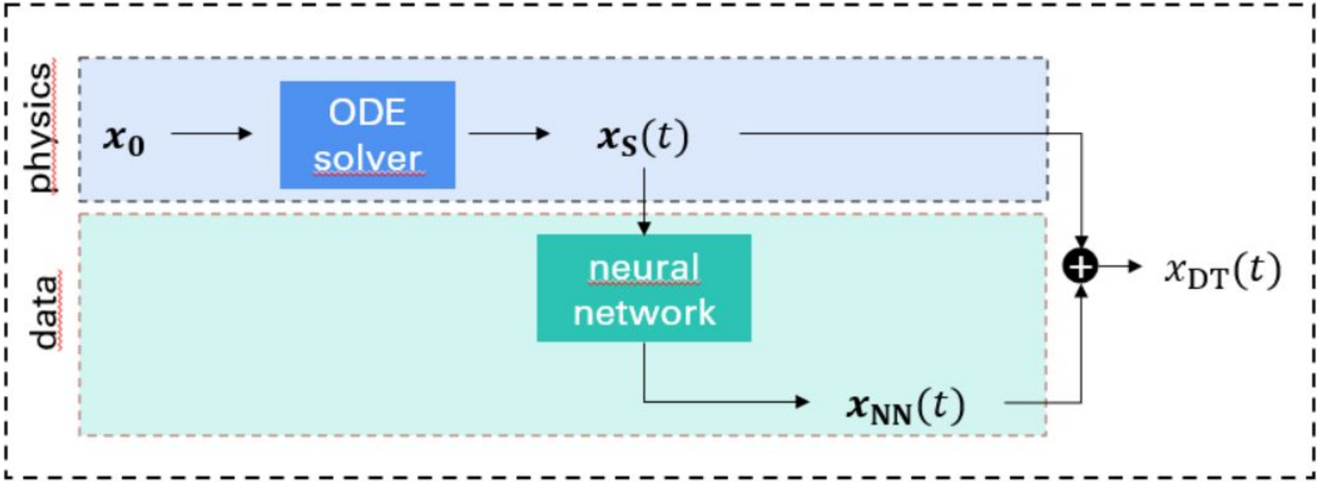


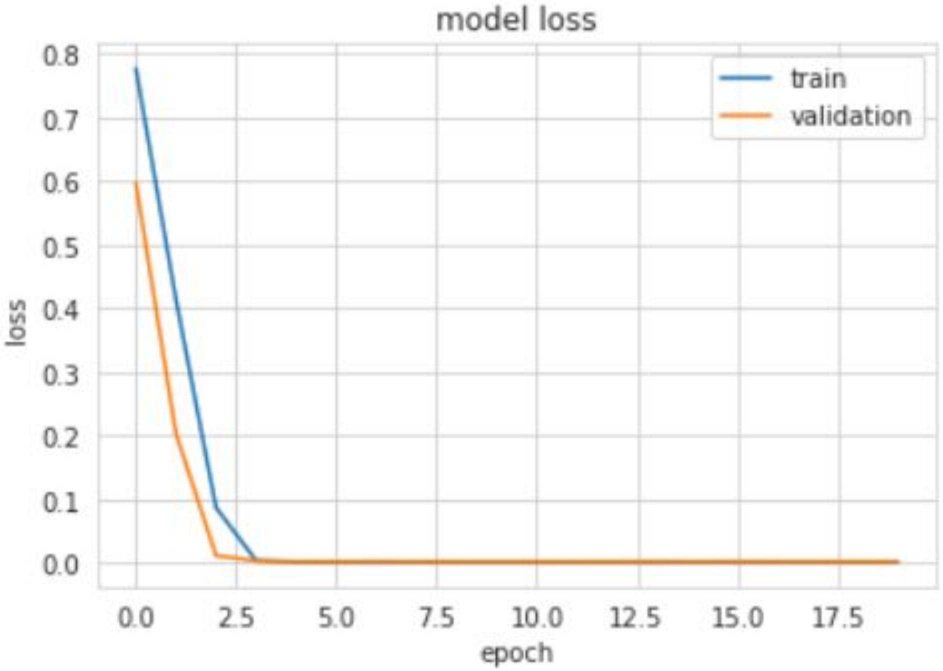
Fig 7: Temperature vs. time plot

Creating Digital Twin




```python
# making a simple neural network model
model = Sequential()
model.add(Dense(64, activation='relu'))
model.add(Dense(64, activation='relu'))
model.add(Dense(1))
```

Results: Digital Twin



count	329.000000
mean	0.003485
std	0.008385
min	0.000034
25%	0.000938
50%	0.001740
75%	0.002443
max	0.073614

Fig 8: (a) Model losses **(b) errors**

Results: Digital Twin

```
model.evaluate(x_test,  y_test, verbose=2)
```

```
11/11 - 0s - loss: 0.0026 - mae: 0.0150 - 27ms/epoch - 2ms/step
[0.0025860609021037817, 0.014950723387300968]
```

```
mean_absolute_error(y_test_unscaled, result_unscaled)
```

```
0.005671175529108492
```

```
# RMSE
mean_squared_error(y_test_unscaled, result_unscaled)
np.sqrt(mean_squared_error(y_test_unscaled, result_unscaled))
```

```
0.019289935740105374
```

```
# R-squared
r2_score(y_test_unscaled, result_unscaled)
```

```
0.9515097652431731
```

R-squared value = 0.9515. Therefore, model is **95.15%** accurate !!

Results: Digital Twin

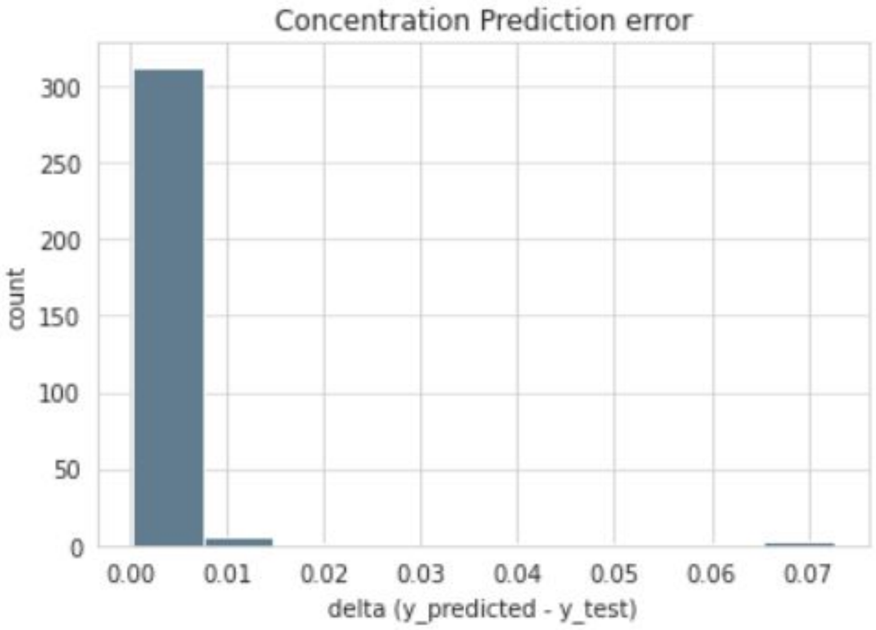


Fig 9: delta (y_predicted - test) plot

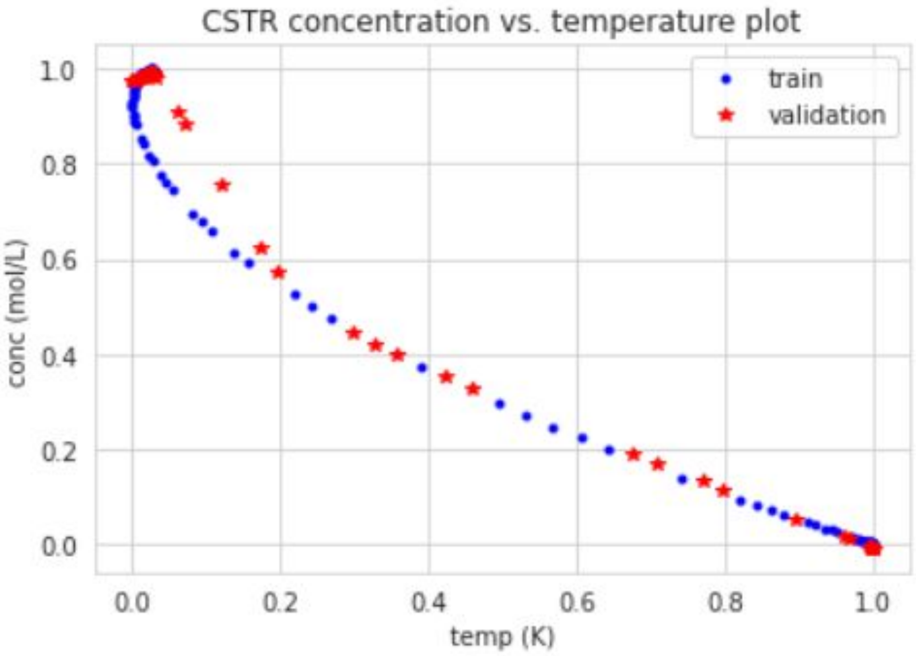


Fig 10: Concentration vs. temperature_plot

Conclusion

- Digital twin can be used to study a process model's performance and predict possible improvements.
- Deep learning has immense potential in the field of Chemical engineering.
- The Neural network model is able to predict the concentration of reactant at a given temperature with **95.15%** accuracy.

Future Scope

- The model used in this project is trained on a very small set of data. More data extraction can be done by increasing the simulation runtime.
- The amount of cold utility required to cool the reactor can be calculated.
- Effect of change in ambient temperature can be incorporated.
- It can also be used to model non-jacketed CSTR and other reactors in the chemical industry.

References

1. Digital twin: The key to effective decision making, *Yokogawa*. Digital Twin White Paper X09.pdf (yokogawa.com). (Accessed: 1 February 2022)
2. Berutti, M 2019, ‘Understanding the digital twin’, *IIOT Oil and Gas*. Understanding the Digital Twin - Chemical Engineering (chemengonline.com). (Accessed: 4 February 2022)
3. Digital twin technology, *TWI*. What is Digital Twin Technology and How Does it Work? - TWI (twi-global.com). (Accessed: 5 February 2022)
4. Jones, D, Snider, C, Nassehi, A & Yon, J 2020, ‘Characterizing the digital twin: A systematic literature review’, *CIRP Journal of Manufacturing Science and Technology,* doi: https://doi.org/10.1016/j.cirpj.2020.02.002. (Accessed: 7 February 2022)
5. Bequette, B 2002, Process Control Modeling. Process Control : Modeling, Design, and Simulation / B.W. Bequette. | Request PDF (researchgate.net). (Accessed: 10 February 2022)
6. The Sequential model | TensorFlow Core https://www.tensorflow.org/guide/keras/sequential_model (Accessed: 15 April 2022).

THANK YOU!