

Figure 1: The setup of a common Continuous Stirred-Tank Reactor (CSTR)

( 1)

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|  | 1.287 |
|  | 1.287 |
|  | 9.043 |
|  | 8.31432 |
|  | 9758.3 |
|  | 9758.3 |
|  | 8560.0 |
|  | 04.20 |
|  | -11.00 |
|  | -41.85 |
|  | 0.9342 |
| *Specific Heat capacity* | 3.01 |
| *Coolant heat capacity* | 2.00 |
|  | 0.215 |
|  | 10.01 |
|  | 5.0 |
|  | 130.0 |
|  | 4032.0 |
|  | 5.10 |

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| **S.No** | **HYPERPARAMETERS** | **HYPERPARAMETERS’ RANGE** | **BEST HYPERPARAMETERS** |
| 1 | NARX Delay Size |  |  |
| 2 | Activation Function on the Hidden Layers |  |  |
| 3 | Number of Nodes on Hidden Layers |  |  |
| 4 | Number of Hidden Layers |  |  |
| 5 | Optimizer’s Learning Rate |  |  |
| 6 | Batch Size |  |  |
| 7 | Optimizer’s Momentum Rate |  |  |
| 8 | Tuner Class in KerasTuner |  |  |
| 9 | Loss Objective Function |  |  |
| 10 | Epochs |  |  |
| 11 | Shuffle of the Data |  |  |

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| **S.No** | **NEURAL NETWORK’S PARAMETERS** | **DESCRIPTION** | **PROPERTIES** |
| 1 | Input Data for Training (NARX) |  |  |
| 2 | Input Data for Testing (NARX) |  |  |
| 3 | Target Data for Training |  |  |
| 4 | Target Data for Testing |  |  |
| 5 | Keras Optimizer Used |  |  |
| 6 | Callbacks |  |  |
| 7 | Epochs |  |  |
| 8 | Loss Objective Function |  |  |
| 9 | Loss Metrics |  |  |
| 10 | Train and Test Split |  |  |

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| **S.No** | **PGNN Constraints** | **DESCRIPTION** |  |
| 1 | Concentration of reactant A () greater than 0 |  |  |
| 2 | Concentration of reactant B () greater than 0 |  |  |
| 3 | Product of Rate of Change of Heat Flow and Rate of Change of Temperature of Jacket |  |  |