Master’s Thesis Engineering Technology

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ENERGY MINIMIZATION OF DISTILLATION COLUMNS BY ARTIFICIAL NEURAL NETWORKS

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Master of chemical engineering technology

1 WHAT?

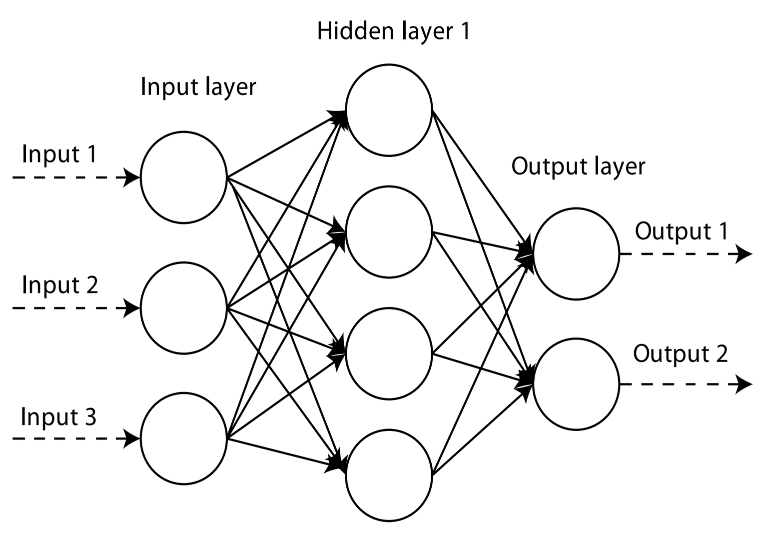

Figure 1: ANN structure

= Artificial Neural Network (ANN)

- Computing systems
- Allow for the detection of **non-linear relations** between features
- **Low simulation time** compared to chemical simulation software suites like Aspen Plus

2 PROBLEM DEFINITION

SUSTAINABILITY

- Design chemical installations with the goal of energy minimization
- **Energy minimization** → reduction of CO_2
- To design distillation columns in Aspen, a lot of simulations need to be performed
- ANN’s reduce this simulation time and can provide a good **prediction** of the actual optimal settings.

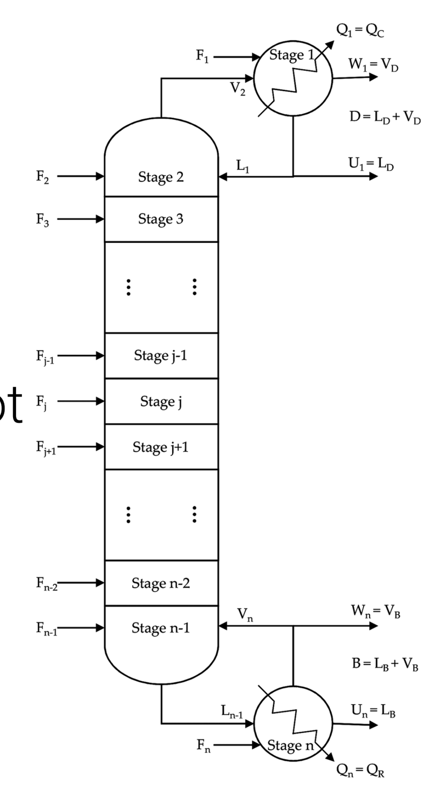

Figure 2: Distillation column [1,p.4]

4 TROUBLESHOOTING

IMBALANCED DATA PROBLEM

When performing simulations, data samples with a very pure distillate are overrepresented causing a bias during training.

Possible approaches:
- Redefining boundaries of input features
- Under-sampling
- Gathering more qualitative data

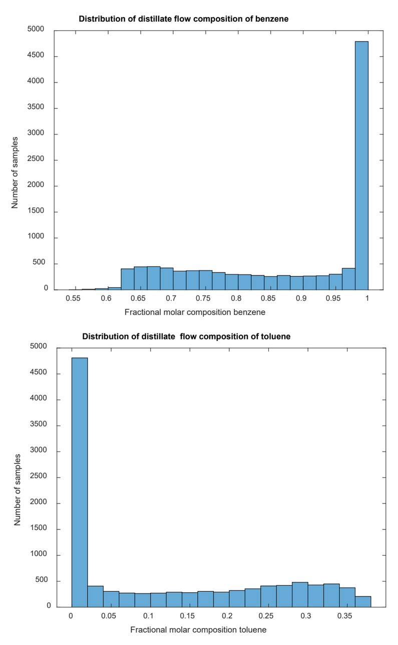

Figure 4: Distributions Of distillate flow rates

3 METHOD

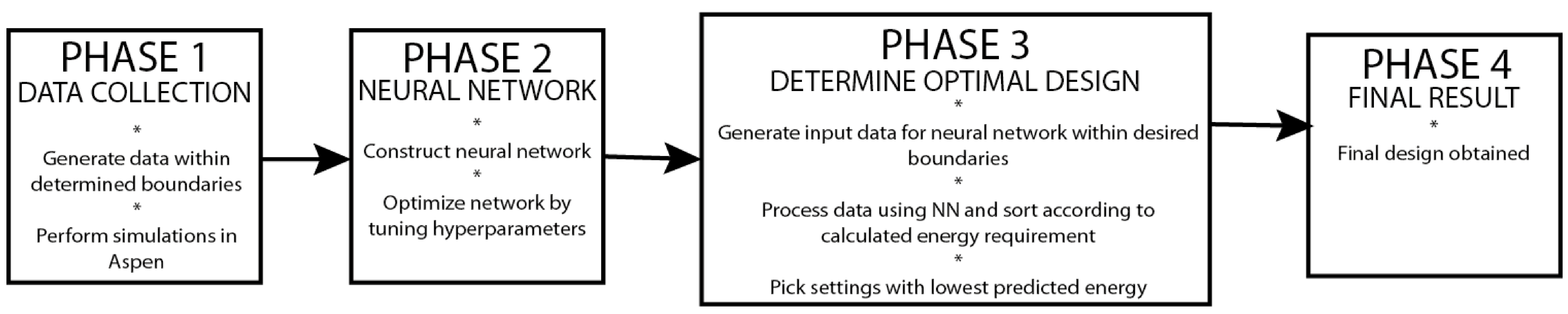

Figure 3: Methodology

5 RESULTS

CASE STUDY 1

Creating a model to find optimal design (reflux ratio, feed stage) and compare the result to the use of Driving Force Method given specific feed conditions [2]

		Neural network	Accuracy check(1)	DFM
No. of stages, Ns		21		21
No. of feed location, NF		15		13
Reflux ratio		1.3722		1.41
Composition at top	Benzene	0.9900	0.9718	0.9900
	Toluene	0.0100	0.0282	0.0100
	p-xylene	0.0000	0.0000	0.0000
Composition at bottom	Benzene	0.0415	0.0585	0.0415
	Toluene	0.5714	0.5543	0.5714
	p-xylene	0.3871	0.3871	0.3871
Energy condenser (kW)		933.6	937.3	953.9
Energy reboiler (kW)		1181.3	1182.9	1201.6
Total energy (kW)		2114.9	2120.2	2155.5

CASE STUDY 2

Expand model of first case study with number of stages, feed composition and feed temperature

		IMPURE FEED		PURE FEED	
		Neural network	Accuracy check	Neural network	Accuracy check
No. of stages, Ns		26		17	
No. of feed location, NF		15		9	
Reflux ratio		0.4184		0.4007	
Feed temperature (°C)		78.9628		77.5054	
Composition at top	Benzene	0.9900	0.7964	0.9900	0.9593
	Toluene	0.0100	0.1832	0.0100	0.0400
	p-xylene	0.0000	0.0204	0.0000	0.0007
Composition at bottom	Benzene	0.0286	0.1618	0.2540	0.3424
	Toluene	0.5640	0.4503	0.5523	0.4661
	p-xylene	0.4074	0.3880	0.1937	0.1916
Energy condenser (kW)		423.2	452.8	836.4	851.8
Energy reboiler (kW)		682.1	694.0	983.3	996.3
Total energy (kW)		1105.3	1146.8	1819.7	1848.1

6 CONCLUSION & FUTURE WORK

- Model performs well in predicting the required energy for the separation
- Imbalanced data set needs to be taken into account when gathering data
- The model needs to have the reflux ratio at the output, together with the reboiler and condenser duty.
- Further optimization of the model needs to be performed by varying other hyperparameters

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[1] V. Steffen and E. A. da Silva, “Steady-State Modeling of Equilibrium Distillation,” in *Distillation - Innovative Applications and Modeling*, InTech, 2017.

[2] M. Faris, A. Noor, F. Mohd, A. Asri, I. Norazana, and K. Mohd, “Design of Energy Efficient Distillation Columns Systems,” in International symposium on green manufacturing and applications, 2014, no. June, pp. 66–69.

(1) The accuracy check is performed to see if the calculated values of the ANN correspond to the values that are found in Aspen.

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