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Structured Data Management for Investigating an Optimum Reactive Distillation Design

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Abstract

Reaction and separation are the two most important processes in the chemical industry that significantly affect the overall energy and cost requirements. Therefore, the operation of integrated reactive separation in a single equipment, such as reactive distillation, potentially increases the chemical process efficiency remarkably. To achieve that advantage, it is vital to design an optimum reactive distillation configuration in the preliminary evaluation. This paper proposes structured data management that can be used to encounter an optimum reactive distillation design. The approach simplified and reduced the data necessity from thousands to dozens by applying a systematic data sorting for the simulation results obtained from the Aspen Plus simulator. Using a case study that is highly relevant to the real chemical processes, i.e., the metathesis of 2-pentene, this study showed that the rule of thumb for determining the optimum design of conventional distillation can be adapted for reactive distillation technology.

Keywords: Reactive Distillation, Data Management, Optimum Design, Aspen Plus.

1. Introduction

Reactive distillation (RD) technology attracts engineers in the chemical industry because of its superiority over conventional and sequential reaction-separation units[1]. The operation of RD potentially leads to many prominent benefits[2], [3]. For instance, it can boost reaction conversion and selectivity due to simultaneous reaction and separation that push the reaction preference to the products side, and therefore, it provides engineers with a compact, cheaper and energy-efficient process[4], [5].

Differently from conventional distillation that has been widely applied since more than two hundred years ago[6], reactive distillation technology was for the first time introduced commercially about three decades ago[7]. A conventional distillation column consists of trays or packed stages that enable the separation of mixed chemical compounds to two high-purity product streams because of the vapor-liquid interaction along the column. The exterior of RD looks almost identical to conventional distillation, but its interior is featured with stages that can hold solid catalysts and have a sufficient space for a larger liquid hold-up[8], [9].

As the RD technology is relatively new to conventional distillation, much more effective approaches to design its column configuration need to be further developed[10]. In conventional distillation processes, one can employ shortcut methods, such as the Fenske-Underwood-Gilliland method, to quickly estimate the optimum column design[11]. While, such approaches are not yet available for RD, therefore, designing an RD column are usually challenging[12].

To overcome that design constraint, this paper proposes structured data management to investigate an optimum RD configuration. With many combinations of number of theoretical stages (NTS), numbers of reactive and separation stages, and reflux ratio (RR), one can obtain thousands of RD configurations for a single chemical reaction. To handle that large data set, this work provides a systematic data sorting to select key dozens of data regarding the RD column design. Using a plot of RR vs. NTS, the present paper assessed the rule of thumb that can be used to design reactive distillation columns. By doing so, one can apply the proposed rule of thumb for many reaction systems in the chemical industry.

2. Research Method

The illustrative scheme of a reactive distillation column is displayed in Figure 1. A reactive distillation column contains reactive and separation stages, in which both reaction and separation take place at the same time along the reactive stages. The separation stages above and below reactive stages are called rectifying and stripping stages, respectively. The start and end of reactive stages are indexed by RS-1 and RS-2, respectively, in Figure 1. Reflux ratio is a term used to represent the ratio of the amount of chemicals being sent back to the column (reflux) and the amount of product B being released as the top product.

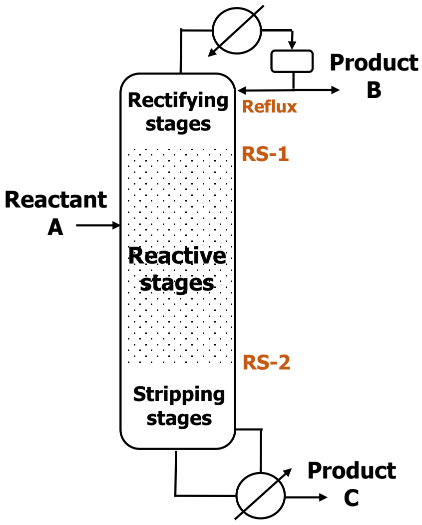


Figure 1. An illustrative scheme of reactive distillation

This work used the Aspen Plus v.11 process simulator to generate all technically feasible reactive distillation configurations for a chemical reaction. The procedures to run all simulations and to perform structured data management are shown in Figure 2. For a chemical reaction, thousands of data of feasible column configurations are usually achievable because of varied numbers of rectifying, reactive and stripping stages resulting in multiple solutions of reflux ratio. Therefore, as shown in Figure 2, only a single solution with the lowest RR is picked for each NTS. The plot of reflux ratio vs. number of theoretical stages plays an important role as both are proportional to the capital expenditure and operating costs[13]–[15].

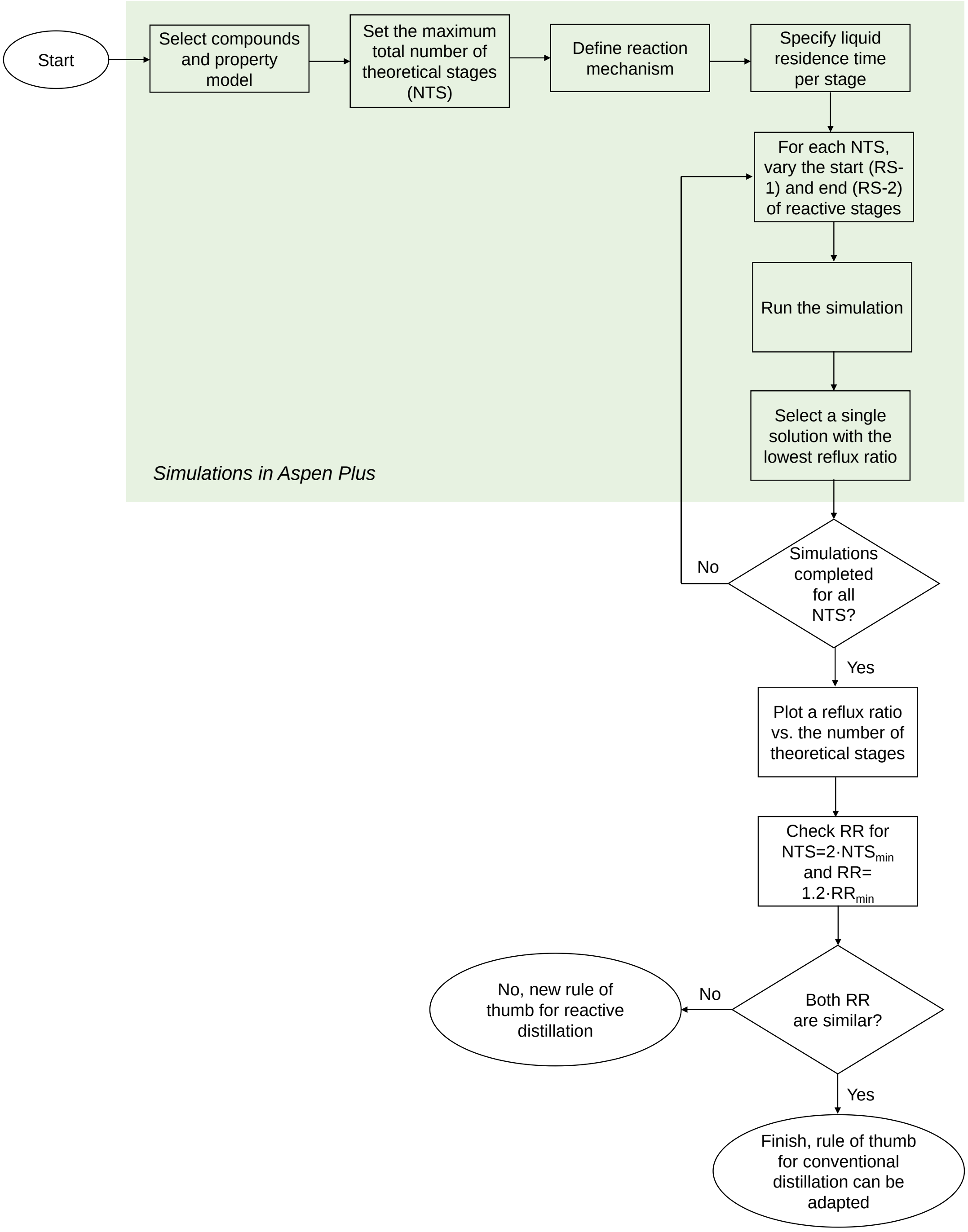


Figure 2. Simulations procedure and structured data management to obtain a rule of thumb for determining an optimum RD column configuration

The importance of data management and understanding the role of information technology for different fields has been assessed by many researchers. For instance, Atmadja and Gumilar[16] developed Fortran simulation program to improve the clinical management from predominant variables in order to reduce maternal mortality risks in the type C hospitals in East Java. Andriyan[17] assessed the role of technology in the learning process of college students at Universitas Raharja. Other findings are available in the literature[18]–[20].

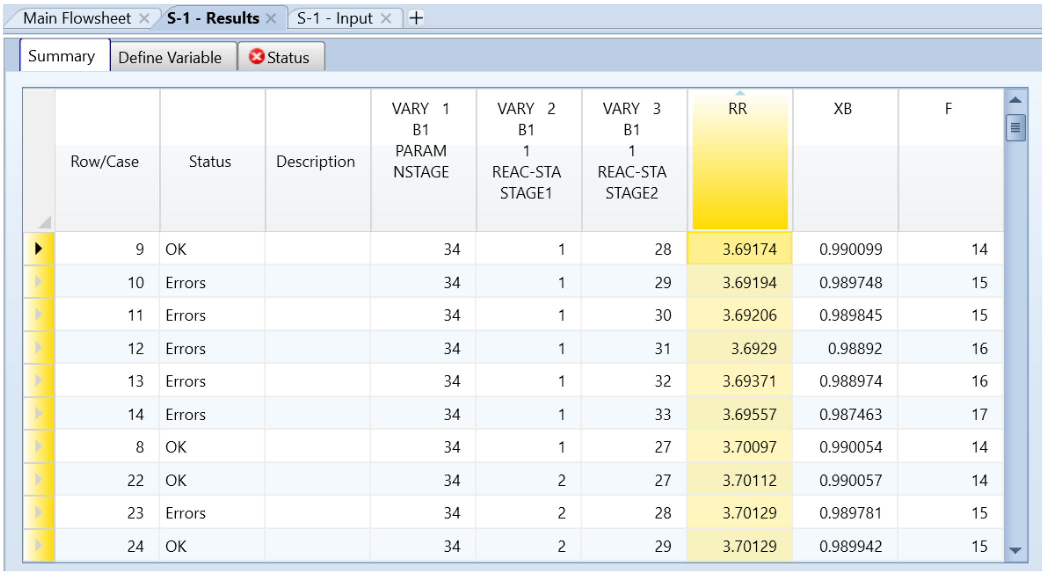
For the evaluation performed in this work, the case study of the metathesis of 2-pentene was considered. The case is highly relevant to the chemical industry[21], therefore, it represents the advantages of operating reactive distillation for real chemical processes. The metathesis reaction is usually performed to increase the values of olefins for wider purposes[22]. The reaction mechanism of the metathesis of 2-pentene is shown by Eq. 1,

	2 2-pentene **(A)** ⇌	2-butene **(B)** +	3-hexene **(C)**	
Boiling point (*T_b*) at 1 atm (°C)	6.3	0.9	67.1	(1)

Considering the boiling points of all chemicals in Eq. 1, one can expect to obtain 2-butene as the top product and 3-hexene as the bottom product in a reactive distillation column, which is illustrated in Figure 1. The Peng-Robinson property model was used to accounting for the system's thermodynamics behavior. The chemical equilibrium constant and the reaction rates refer to those suggested in the literature[23]. To enable the usage of cooling water in the condenser, the operating pressure of 5 atm is applied to the simulated columns[24]. The specified liquid residence time per stage was 30 s, which is inside the range of practical residence time that is commonly applied in the chemical industry[25].

3. Findings

Figure 3 demonstrates the interface of the simulation results that were obtained in Aspen Plus v.11. The simulation results suggested that NTS = 16 is the smallest number of theoretical stages possible for feasible RD columns. Therefore, this number is called the minimum number of theoretical stages (NTS_{min}). As the NTS_{min} was obtained, the simulations were carried on for other larger numbers of theoretical stages. Assuming that the lowest reflux ratios for sufficiently high numbers of theoretical stages, i.e., NTS that is close to 60, are already similar, the investigation in this work limited the observation to NTS = 60. Therefore, the lowest reflux ratio for NTS = 60 is called the minimum reflux ratio (RR_{min}). Varying the numbers of rectifying, reactive and stripping stages from NTS = 16 to NTS = 60 already gave 37,820 possible solutions.



Row/Case	Status	Description	VARY 1 B1 PARAM NSTAGE	VARY 2 B1 1 REAC-STA STAGE1	VARY 3 B1 1 REAC-STA STAGE2	RR	XB	F
9	OK		34	1	28	3.69174	0.990099	14
10	Errors		34	1	29	3.69194	0.989748	15
11	Errors		34	1	30	3.69206	0.989845	15
12	Errors		34	1	31	3.6929	0.98892	16
13	Errors		34	1	32	3.69371	0.988974	16
14	Errors		34	1	33	3.69557	0.987463	17
8	OK		34	1	27	3.70097	0.990054	14
22	OK		34	2	27	3.70112	0.990057	14
23	Errors		34	2	28	3.70129	0.989781	15
24	OK		34	2	29	3.70129	0.989942	15

Figure 3. The interface of the simulation results in Aspen Plus

Table 1 provides all feasible configurations for NTS= 20. RS-1 and RS-2 are the start and end of reactive stages, respectively. While, RR and XB stand for reflux ratio (mol/mol) and the bottom product purity (mol%), respectively. Following the suggested procedure in Figure 1, only the configuration with the lowest reflux ratio (as highlighted in blue in Table 1) was picked for generating a plot of reflux ratio vs. number of theoretical stages. The same procedures were done for all numbers of theoretical stages.

Table 1. Simulation results for NTS = 20

Row/Case	Status	NTS	RS-1	RS-2	RR	XB
18	OK	20	1	18	7.40	0.99
37	OK	20	2	17	7.42	0.99
17	OK	20	1	17	7.42	0.99
56	OK	20	3	16	7.44	0.99
36	OK	20	2	16	7.44	0.99
55	OK	20	3	15	7.49	0.99
75	OK	20	4	15	7.49	0.99
16	OK	20	1	16	7.54	0.99
74	OK	20	4	14	7.57	0.99
15	OK	20	1	15	7.58	0.99
35	OK	20	2	15	7.59	0.99
94	OK	20	5	14	7.59	0.99
34	OK	20	2	14	7.65	0.99
54	OK	20	3	14	7.67	0.99
93	OK	20	5	13	7.74	0.99
115	OK	20	6	15	7.77	0.99
53	OK	20	3	13	7.81	0.99
113	OK	20	6	13	7.81	0.99
73	OK	20	4	13	7.82	0.99
134	OK	20	7	14	8.02	0.99
72	OK	20	4	12	8.10	0.99
92	OK	20	5	12	8.12	0.99
112	OK	20	6	12	8.13	0.99
14	OK	20	1	14	8.18	0.99
133	OK	20	7	13	8.22	0.99
13	OK	20	1	13	8.32	0.99
33	OK	20	2	13	8.32	0.99
132	OK	20	7	12	8.33	0.99
32	OK	20	2	12	8.60	0.99
52	OK	20	3	12	8.61	0.99
153	OK	20	8	13	8.62	0.99
91	OK	20	5	11	8.67	0.99
111	OK	20	6	11	8.77	0.99
131	OK	20	7	11	8.99	0.99
152	OK	20	8	12	9.07	0.99
51	OK	20	3	11	9.14	0.99

Row/Case	Status	NTS	RS-1	RS-2	RR	XB
71	OK	20	4	11	9.16	0.99
151	OK	20	8	11	9.63	0.99
174	OK	20	9	14	9.67	0.99
110	OK	20	6	10	9.87	0.99
12	OK	20	1	12	9.88	0.99
173	OK	20	9	13	10.02	0.99
172	OK	20	9	12	10.09	0.99
70	OK	20	4	10	10.19	0.99
90	OK	20	5	10	10.23	0.99
130	OK	20	7	10	10.26	0.99
31	OK	20	2	11	10.44	0.99
11	OK	20	1	11	10.44	0.99
150	OK	20	8	10	11.27	0.99
171	OK	20	9	11	11.35	0.99
30	OK	20	2	10	11.53	0.99
50	OK	20	3	10	11.54	0.99
193	OK	20	10	13	11.65	0.99
195	OK	20	10	15	11.81	0.99
178	OK	20	9	18	11.82	0.99
89	OK	20	5	9	12.30	0.99
109	OK	20	6	9	12.55	0.99
192	OK	20	10	12	12.74	0.99
129	OK	20	7	9	12.77	0.99
197	OK	20	10	17	13.19	0.99
49	OK	20	3	9	13.68	0.99
69	OK	20	4	9	13.70	0.99
191	OK	20	10	11	14.44	0.99
10	OK	20	1	10	14.80	0.99
149	OK	20	8	9	14.81	0.99
214	OK	20	11	14	14.91	0.99
216	OK	20	11	16	15.84	0.99
213	OK	20	11	13	15.93	0.99
9	OK	20	1	9	17.16	0.99
29	OK	20	2	9	17.17	0.99
212	OK	20	11	12	17.19	0.99
108	OK	20	6	8	17.35	0.99
68	OK	20	4	8	18.28	0.99
88	OK	20	5	8	18.44	0.99
218	OK	20	11	18	18.60	0.99
128	OK	20	7	8	19.22	0.99
200	OK	20	10	20	21.23	0.99
235	OK	20	12	15	21.49	0.99
190	OK	20	10	10	22.04	0.99

Row/Case	Status	NTS	RS-1	RS-2	RR	XB
28	OK	20	2	8	22.18	0.99
48	OK	20	3	8	22.19	0.99
169	OK	20	9	9	22.20	0.99
234	OK	20	12	14	22.55	0.99
233	OK	20	12	13	23.33	0.99
237	OK	20	12	17	23.90	0.99
219	OK	20	11	19	23.99	0.99
220	OK	20	11	20	23.99	0.99
236	OK	20	12	16	24.11	0.99
211	OK	20	11	11	24.99	0.99
148	OK	20	8	8	26.39	0.99
239	OK	20	12	19	29.52	0.99

Figure 4 displays the plot of RR vs NTS for the selected case study. The solid line in Figure 4 indicates the lowest reflux ratios obtainable for different numbers of theoretical stages from NTS = 16 to NTS = 60. Note that above the solid line, there are multiple configurations of RD that are technically feasible, including those listed in Table 1. The square marker in Figure 4 points out the RR for NTS = $2 \cdot NTS_{min}$ (RR = 3.18), while the triangle marker indicates the RR for RR = $1.2 \cdot RR_{min}$ (RR = 3.01). According to these markers, the difference of the two RRs is only 5%, which can be claimed as very similar between each other. Therefore, following the procedure proposed in Figure 1, the determination of an optimum reactive distillation configuration can be done using the rule of thumb for conventional distillation. Note that, in conventional distillation process, both approaches of estimating NTS = $2 \cdot NTS_{min}$ and RR = $1.2 \cdot RR_{min}$ also provide similar results in terms of an optimum conventional distillation design.

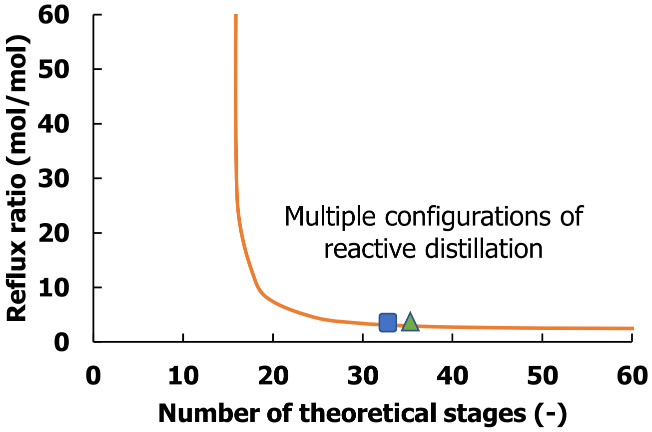


Figure 4. The plot of reflux ratio vs. number of theoretical stages for the metathesis of 2-pentene

4. Conclusion

This work successfully demonstrates the implementation of structured data management to handle 37,820 data and sort it to obtain dozens of key data (44 data of column configurations with the lowest reflux ratios for NTS = 16 – 60). The proposed systematic approach provides a clear understanding in determining the optimum RD column configuration for the metathesis of 2-pentene. Based on the findings, it can be observed that the rule of thumb for conventional distillation, in terms of determining the optimum column configuration, can be used for reactive distillation in the conceptual design level.

References

[1] A. A. Kiss, “Reactive Distillation,” in *Process Intensification: by Reactive and Membrane-Assisted Separations*, M. Skiborowski and A. Górak, Eds. Germany: Walter de Gruyter GmbH & CoKG, 2022, pp. 265–322.

[2] S. P. Pushkala and R. C. Panda, “Design and analysis of reactive distillation for the production of isopropyl myristate,” *Cleaner Chemical Engineering*, vol. 5, p. 100090, 2023, doi: https://doi.org/10.1016/j.clce.2022.100090.

[3] C. Li, C. Duan, J. Fang, and H. Li, “Process intensification and energy saving of reactive distillation for production of ester compounds,” *Chin J Chem Eng*, vol. 27, no. 6, pp. 1307–1323, 2019, doi: https://doi.org/10.1016/j.cjche.2018.10.007.

[4] A. A. Kiss, M. Jobson, and X. Gao, “Reactive Distillation: Stepping Up to the Next Level of Process Intensification,” *Ind Eng Chem Res*, vol. 58, no. 15, pp. 5909–5918, Apr. 2019, doi: 10.1021/acs.iecr.8b05450.

[5] A. A. Kiss, “Novel Catalytic Reactive Distillation Processes for a Sustainable Chemical Industry,” *Top Catal*, vol. 62, no. 17, pp. 1132–1148, 2019, doi: 10.1007/s11244-018-1052-9.

[6] U. Kim, J. Kim, T.-W. Kim, and J. Choi, “Analysis of distillation characteristics via CFD (computational fluid dynamics) of Korean traditional ‘Sojutgori’ and study on structure for distillation efficiency enhancement,” *Food Sci Nutr*, vol. 11, no. 1, pp. 590–598, Jan. 2023, doi: https://doi.org/10.1002/fsn3.3099.

[7] C. Shu, X. Li, H. Li, and X. Gao, “Design and optimization of reactive distillation: a review,” *Front Chem Sci Eng*, vol. 16, no. 6, pp. 799–818, 2022, doi: 10.1007/s11705-021-2128-9.

[8] M. Wierschem and A. Górak, “Reactive Distillation,” *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*, pp. 1–10, 2018.

[9] Z. Wang, Y. Zhang, Z. Zhang, D. Zhou, Z. Cao, and Y. Sha, “Investigation on catalytic distillation for ethyl acetate production with different catalytic packing structures,” *Chin J Chem Eng*, vol. 53, pp. 63–72, 2023, doi: https://doi.org/10.1016/j.cjche.2022.02.012.

[10] M. Skiborowski, “Process synthesis and design methods for process intensification,” *Curr Opin Chem Eng*, vol. 22, pp. 216–225, 2018, doi: https://doi.org/10.1016/j.coche.2018.11.004.

[11] C. Yin and G. Liu, “Synthesis of optimal reaction-separation system with sufficient operational flexibility,” *Chem Eng Sci*, vol. 249, p. 117316, 2022, doi: https://doi.org/10.1016/j.ces.2021.117316.

[12] A. Iftakher *et al.*, “RD-toolbox: A computer aided toolbox for integrated design and control of reactive distillation processes,” *Comput Chem Eng*, vol. 164, p. 107869, 2022, doi: https://doi.org/10.1016/j.compchemeng.2022.107869.

[13] P. Kale, S. Pujari, J. G. Gujar, R. Sontakke, E. I. Haddadi, and S. S. Sonawane, “Batch distillation for separating the acetone and n-heptane binary azeotrope mixture: Optimization and simulation,” *Journal of the Indian Chemical Society*, vol. 100, no. 1, p. 100795, 2023, doi: https://doi.org/10.1016/j.jics.2022.100795.

[14] B. Mondal and A. K. Jana, “Techno-economic Feasibility of Reactive Distillation for Biodiesel Production from Algal Oil: Comparing with a Conventional Multiunit System,” *Ind Eng Chem Res*, vol. 58, no. 27, pp. 12028–12040, Jul. 2019, doi: 10.1021/acs.iecr.9b00347.

[15] M. A. Khan and Y. G. Adewuyi, “Techno-economic modeling and optimization of catalytic reactive distillation for the esterification reactions in bio-oil upgradation,” *Chemical Engineering Research and Design*, vol. 148, pp. 86–101, 2019, doi: https://doi.org/10.1016/j.cherd.2019.05.037.

[16] S. Atmadja and G. Gumilar, “Fortran Program Forecasting on Maternal Mortality in Type C Hospitals in East Java based on Predominant Variables,” *ADI Journal on Recent Innovation*, vol. 1, no. 1, pp. 7–13, 2019.

[17] W. Andriyan and V. Anesti, “Visual Audio Communication Design on the Role of Information Technology on Student Life Style of Universitas Raharja,” *ADI Journal on Recent Innovation*, vol. 2, no. 1, pp. 16–25, 2020.

[18] R. Rosdiana, P. Padeli, R. S. S. Handayni, and R. Alfian, “Design And Development of Population Service Administration System With Pieces Method In Kemiri Village Head Office Banten,” *ADI Journal on Recent Innovation*, vol. 1, no. 1, pp. 33–45, 2019.

[19] F. W. Ramadhan, H. T. Sukmana, L. K. Oh, and L. K. Wardhani, “Analysis Of Warganet Comments On It Services In Mandiri Bank Using K-Nearest Neighbor (K-Nn) Algorithm Based On Itsm Criteria,” *ADI Journal on Recent Innovation*, vol. 1, no. 1, pp. 14–19, 2019.

[20] M. Maimunah, H. Haris, and N. Priliasari, “The Design of Web-Based Training Management Information Systems at PT. Sintech Berkah Abadi,” *ADI Journal on Recent Innovation*, vol. 2, no. 2, pp. 216–222, 2021.

[21] W. Yan, Z. You, K. Meng, F. Du, S. Zhang, and X. Jin, “Cross-metathesis of biomass to olefins: Molecular catalysis bridging the gap between fossil and bio-energy,” *Chin J Chem Eng*, vol. 48, pp. 44–60, 2022, doi: https://doi.org/10.1016/j.cjche.2021.10.008.

[22] B. Zhang, M. E. Ford, E. Ream, and I. E. Wachs, “Olefin metathesis over supported MoOx catalysts: influence of the oxide support,” *Catal Sci Technol*, vol. 13, no. 1, pp. 217–225, 2023, doi: 10.1039/D2CY01612E.

[23] Y. Tian and E. N. Pistikopoulos, “Toward an Envelope of Design Solutions for Combined/Intensified Reaction/Separation Systems,” *Ind Eng Chem Res*, vol. 59, no. 24, pp. 11350–11354, Jun. 2020, doi: 10.1021/acs.iecr.0c01196.

[24] H.-Y. Lee, Y.-Y. Chen, P. Eiamsuttitam, and J. R. Alcántara-Avila, “Comparison of optimization methods for the design and control of reactive distillation with inter condensers,” *Comput Chem Eng*, vol. 164, p. 107871, 2022, doi: https://doi.org/10.1016/j.compchemeng.2022.107871.

[25] R. Muthia *et al.*, “Novel method for mapping the applicability of reactive distillation,” *Chemical Engineering and Processing - Process Intensification*, vol. 128, pp. 263–275, 2018, doi: https://doi.org/10.1016/j.cep.2018.04.001.