American Institute of Chemical Engineers

STUDENT CONTEST PROBLEM

1978

345 East 47 Street • New York, New York 10017

Refining of Isopropanol with Dehydration Agents Other than Benzene

A major chemical company is currently dehydrating isopropanol with benzene in a two-column distillation system. A process flow diagram for the existing system with a complete material balance is attached. It having recently been observed that benzene appears to promote leukemia in laboratory animals, human exposure to the system is to be avoided. Rather than assuming the cost of revisions to the facility and continuing an operation having the risk of exposure to benzene, the company has decided to convert its isopropanol refining system to a new dehydration agent. Several agents are being considered, such as isopropyl ether, *n*-hexane, and ethyl acetate. The agent yielding the best economic return (that is, the greatest total present value) will be recommended to company management for the change-over, which will be made in late 1978.

As a member of the Process Engineering Department, you are asked to evaluate isopropyl ether.

The manager of your department has specified that all evaluations will be made on a discounted-cash-flow basis, a 15 percent discount factor being used over a thirteen-year operating period beginning in 1979.* He has also stated that each dehydration agent is to be evaluated relative to benzene, that the existing system could be operated "as is" for the period of 1979 through 1991. Thus only the differences in total capital investment, income, manufacturing cost, etc., in the distillation system with isopropyl ether and with benzene are to be included in the evaluation.

* Economic terms are defined in Attachment F. In general, the economic terms are in accordance with those of Peters and Timmerhaus, *Plant Design and Economics for Chemical Engineers*, 2 ed. See pages 238-242 for a discussion of the terms *discounted cash flow*, *discount factor*, and *total present value*.

DESCRIPTION OF EXISTING PROCESS

The existing process using benzene is described in detail by the attached flow diagram. The diagram, which is somewhat simplified, does not necessarily represent modern practice. In summary, the feed consists of isopropanol-water azeotrope, which is fed to the upper side of a drying column. An adequate benzene concentration is maintained to produce an overhead vapor which, when condensed, forms two phases. The addition of condensate, Stream 5, to the decanter decreases the quantity of water which is returned in the reflux, Stream 7, to the drying column. (This operation can be confirmed by an examination of the attached phase diagram for benzene-isopropanol-water.) The use of condensate is not without penalty, however, as it increases utility usage in the downstream equipment. The upper, benzene-rich layer is refluxed to the drying column, and the lower, water-rich layer is fed to an organics removal still. Bottoms from this still are the water which is removed from the process. The organic recovery column has a small heads cut which contains acetone and is distilled in an available batch still periodically for the recovery of useful materials. An upper sidestream is recycled to the drying-column feed tank.

The final product is taken as a sidestream from the lower side of the drying column. It must meet specifications of 0.1 weight percent water maximum and 0.02 weight percent maximum of organic materials other than isopropanol. The drying agent may not exceed one part per million.

PROBLEM OBJECTIVES

1. Revise the attached flow diagram to show what you consider to be an optimized isopropyl ether system, giving particular attention to
   a. Material balance. (Assume zero loss from the system.)
   b. Utility usage. (Include a section in your report to detail any revisions you considered to improve energy conservation.) Because of corrosion and fouling problems, cooling-water return temperature is limited to 50°C.
   c. Any revisions to the instrumentation system.
   d. Equipment additions and revisions. (Detail these in a section of your report.)
2. Determine the total present value of your isopropyl ether system relative to the existing benzene system. This determination may be made on the cash-flow work sheet included in Attachment F.
3. Prepare an *outline* of procedures for assuring safe and efficient operation of the isopropyl ether system during start-ups; routine operation; "crash" shutdowns, such as may, for example, be caused by a utility failure; and planned shutdowns.

Note: All assumptions should be clearly stated in your problem solution.

Your manager has stressed two points.

One, it is desired to produce as much refined isopropanol from the available isopropanol-water constant boiling mixture as can be justified on a discounted-cash-flow basis. Note from the attached flow diagram that the contained isopropanol in the mixture is limited to 11,878 kilograms per hour. You are free to add equipment and to replace or to revise existing equipment, including either or both distillation columns, provided these additions and revisions result in an increase in total present value.

The manager's second point is that the revised system should be more utility efficient than the existing system. Therefore, you are to consider process modifications and equipment additions or revisions which would reduce the overall use of utilities provided such changes have no adverse effect on total present value. The manager has little confidence in the metered utilities reported for the existing system and has requested that utility consumption for both the existing and new systems be on a calculated basis.

The attachments to this memorandum include the basic information that you need for the evaluations:

A. Data for Determining Fixed-Capital Investment of New Equipment

O.D. × 16 BWG copper, 2.54 cm triangular pitch, 3.66 m long.

Product Cooler–Stream 2

Horizontal, four in series, fixed-tube sheet exchangers with product in tubes. Product and coolant piped countercurrent. 11.4 bar (abs.) working pressure, 33.66 cm I.D. shells.

Each body—136 tubes 1.9 cm O.D. × 14 BWG copper, 2.54 cm triangular pitch, 3.66 m long.

Waste Cooler–Stream 11

Horizontal, two in series, fixed-tube sheet exchangers with waste stream in tubes. Waste and coolant piped countercurrent. 11.4 bar (abs.) working pressure, 33.66 cm I.D. shells.

Each body— 136 Tubes 1.9 cm O.D. × 14 BWG copper, 2.54 cm triangular pitch, 3.66 m long.

Where incomplete information is presented for pressure-drop calculations for piping, orifices, control valves, and heat exchangers, assume that pressure drop through these items does not limit.

ATTACHMENT C

Operating Costs and Investments for Utilities

For decision-making purposes, use the following projected 1983 estimates of operating costs and investment for utilities. It is assumed that these estimates will be effective averages over the 13-year operating life of the project.

Utility	Unit	Operating Cost, ¢/unit	Investment, ¢/unit/year
Fuel	MJ	0.35	Ignore
Electricity	MJ	1.03	0.83
Steam, 43 bar abs.	kg	1.26	1.76
15 bar abs.	kg	1.11	1.54
5 bar abs.	kg	0.98	1.32
Cooling water	m^3	1.58	5.28
Condensate	m^3	105.6	264
Service gases (All gas flows are on the basis of one bar absolute and 0°C.)			
N_2 Purge gas	m^3	10.6	7.06
Instrument air	m^3	0.92	2.12

This project should be charged the excess operating cost and investment for extra utilities used by the converted system, and it may be credited with both operating cost and investment for reduced utility usage. For example, if revisions to the system required the use of an additional 10 m^3/h of cooling water, the incremental annual operating cost would be $1,343 (10 × 0.0158 × 8,500), and the incremental investment would be $4,488 (10 × 0.0528 × 8,500).

Nitrogen is assumed to be used at the rate of 3 m^3/h per vent header connection to each condenser; air for instruments, at 15 m^3/h. Entrainer-unaccounted-for losses from the system are estimated to be 2.5 kg/h. Entrainer costs for benzene and isopropyl ether are estimated to be 34¢/kg and 50¢/kg, respectively, in 1979 and to escalate at 7 percent every year thereafter.

Waste treatment costs for 1983 on a contained-organics basis are 86¢/kg operating cost plus an additional operating cost of 59¢/kg for capital-related charges.

ATTACHMENT D

Physical Property Data

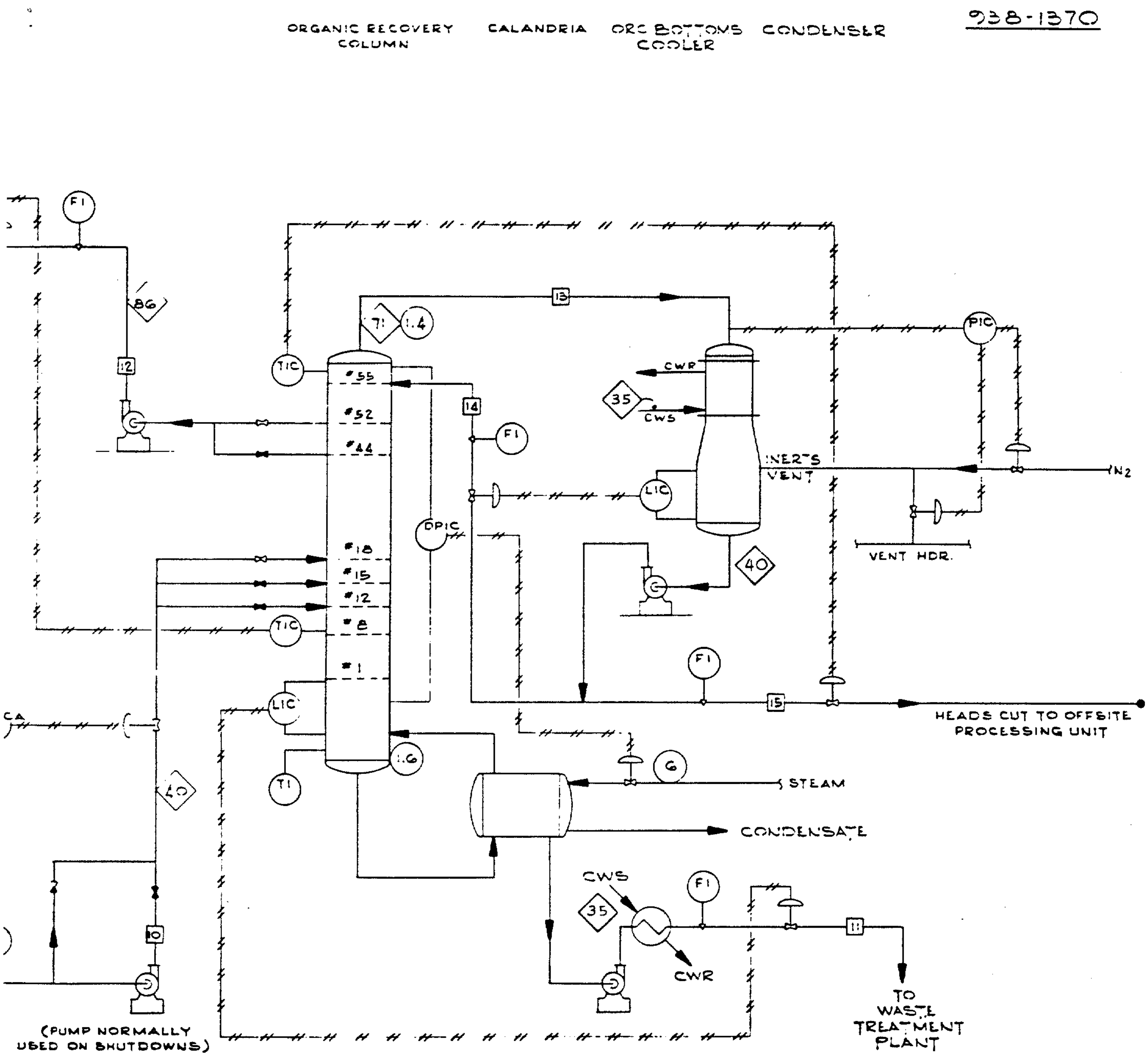
The following data are included in this attachment:

Physical property	Water	Isopropanol	Benzene	Isopropyl ether	Acetone
Molecular formula	H_2O	C_3H_8O	C_6H_6	$C_6H_{14}O$	C_3H_6O
Molecular weight	18.015	60.096	78.114	102.176	58.079
Normal boiling point, °K	373.15	355.40	353.25	340.73	329.22
Normal freezing point, °K	273.15	184.65	278.68	187.65	178.45
Criticals:					
T_c, °K	647.3	508.29	562.09	500	508.2
P_c, N/m²	22,120,000.0	4,764,301.499	4,898,000	2,877,630	4,721,745.0
V_c, m³/kgmole	0.057108184	0.2200	0.2590	0.386	0.209
Z_c	0.23470993	0.248	0.2714	0.26718117	0.23354348
Pitzer's acentric factor v	0.344162	0.664946	0.21170	0.332881	0.308394

WATER

TEMPERATURE (DEGREES K)	DENSITY (KG/M3)	VAPOR PRESSURE (BARS)	LIQUID ENTHALPY (KJ/KGRAM)	VAPOR ENTHALPY (KJ/KGRAM)
298.15	996.142	0.032	-1877.70	552.39
300.15	995.521	0.036	-1869.33	556.13
302.15	994.880	0.040	-1860.97	559.86
304.15	994.218	0.045	-1852.60	563.60
306.15	993.535	0.050	-1844.24	567.34
308.15	992.832	0.056	-1835.87	571.08
310.15	992.108	0.063	-1827.51	574.82
312.15	991.364	0.070	-1819.15	578.57
314.15	990.598	0.078	-1810.79	582.31
316.15	989.812	0.086	-1802.43	586.06
318.15	989.006	0.096	-1794.07	589.80
320.15	988.178	0.106	-1785.71	593.55
322.15	987.330	0.117	-1777.36	597.30
324.15	986.462	0.130	-1769.00	601.05
326.15	985.572	0.143	-1760.64	604.80
328.15	984.662	0.157	-1752.28	608.56
330.15	983.731	0.173	-1743.91	612.31
332.15	982.780	0.190	-1735.55	616.07
334.15	981.808	0.208	-1727.19	619.82
336.15	980.815	0.228	-1718.82	623.58
338.15	979.802	0.250	-1710.46	627.34
340.15	978.768	0.273	-1702.09	631.10
342.15	977.713	0.298	-1693.72	634.87
344.15	976.638	0.325	-1685.34	638.63
346.15	975.542	0.354	-1676.97	642.40
348.15	974.425	0.385	-1668.59	646.16
350.15	973.288	0.418	-1660.20	649.93
352.15	972.129	0.454	-1651.82	653.70
354.15	970.951	0.493	-1643.43	657.47
356.15	969.751	0.534	-1635.04	661.24
358.15	968.531	0.577	-1626.64	665.02
360.15	967.290	0.624	-1618.24	668.79
362.15	966.029	0.674	-1609.84	672.57
364.15	964.747	0.728	-1601.43	676.35
366.15	963.444	0.784	-1593.01	680.13
368.15	962.120	0.845	-1584.59	683.91
370.15	960.776	0.909	-1576.17	687.70
372.15	959.411	0.977	-1567.74	691.48
374.15	958.025	1.050	-1559.30	695.27
376.15	956.619	1.127	-1550.86	699.06
378.15	955.192	1.208	-1542.42	702.85
380.15	953.745	1.295	-1533.97	706.64
382.15	952.276	1.386	-1525.50	710.43
384.15	950.788	1.483	-1517.04	714.23
386.15	949.278	1.585	-1508.57	718.02
388.15	947.748	1.693	-1500.09	721.82
390.15	946.197	1.807	-1491.60	725.62
392.15	944.625	1.927	-1483.10	729.42
394.15	943.033	2.054	-1474.60	733.22
396.15	941.420	2.187	-1466.09	737.03

938-1370



13	14	15
937	924	13
153	151	2
347	342	5
861	850	11
2,298	2,267	31

LEGEND

(6) - PRESSURE IN BARS ABSOLUTE

⟨30⟩ - TEMPERATURE IN °C

PROCESS FLOW DIAGRAM

ANHYDROUS ISOPROPANOL REFINING

BY: CHECKED: WW/RCJ DATE: 8-26-77

BENZENE

TEMPERATURE (DEGREES K)	DENSITY (KG/M3)	VAPOR PRESSURE (BARS)	LIQUID ENTHALPY (KJ/KGRAM)	VAPOR ENTHALPY (KJ/KGRAM)
298.15	873.667	0.127	-337.13	90.87
300.15	871.495	0.139	-333.84	92.97
302.15	869.322	0.152	-330.52	95.09
304.15	867.150	0.166	-327.19	97.22
306.15	864.977	0.181	-323.83	99.37
308.15	862.804	0.198	-320.46	101.53
310.15	860.632	0.215	-317.07	103.72
312.15	858.459	0.234	-313.66	105.92
314.15	856.286	0.254	-310.23	108.13
316.15	854.114	0.275	-306.78	110.36
318.15	851.941	0.298	-303.32	112.61
320.15	849.769	0.322	-299.83	114.87
322.15	847.596	0.348	-296.32	117.15
324.15	845.423	0.376	-292.80	119.45
326.15	843.251	0.405	-289.26	121.76
328.15	841.078	0.436	-285.69	124.09
330.15	838.906	0.469	-282.11	126.43
332.15	836.733	0.504	-278.51	128.79
334.15	834.560	0.541	-274.90	131.17
336.15	832.388	0.580	-271.26	133.56
338.15	830.215	0.621	-267.60	135.97
340.15	828.042	0.665	-263.93	138.39
342.15	825.870	0.710	-260.24	140.83
344.15	823.697	0.759	-256.53	143.29
346.15	821.525	0.810	-252.80	145.75
348.15	819.352	0.864	-249.05	148.24
350.15	817.179	0.920	-245.28	150.74
352.15	815.007	0.979	-241.50	153.26
354.15	812.834	1.042	-237.70	155.79
356.15	810.662	1.107	-233.87	158.33
358.15	808.489	1.175	-230.03	160.89
360.15	806.316	1.247	-226.18	163.47
362.15	804.144	1.322	-222.30	166.06
364.15	801.971	1.401	-218.41	168.67
366.15	799.798	1.483	-214.49	171.29
368.15	797.626	1.569	-210.56	173.93
370.15	795.453	1.659	-206.61	176.58
372.15	793.281	1.752	-202.65	179.24
374.15	791.108	1.850	-198.66	181.92
376.15	788.935	1.951	-194.66	184.62
378.15	786.763	2.057	-190.64	187.33
380.15	784.590	2.168	-186.60	190.05
382.15	782.417	2.283	-182.54	192.79
384.15	780.245	2.402	-178.46	195.55
386.15	778.072	2.526	-174.37	198.31
388.15	775.900	2.655	-170.26	201.10
390.15	773.727	2.789	-166.13	203.89
392.15	771.554	2.927	-161.99	206.70
394.15	769.382	3.071	-157.82	209.53
396.15	767.209	3.221	-153.64	212.37

Isopropanol—Water
Vapor-Liquid Equilibria, P = 1 atm
[Reference: Yorizane, Kagaku. Kogaku, 31(5), 451 (1967)]

x, mole fraction isopropanol in liquid phase	y, mole fraction isopropanol in vapor phase
0.000	0.000
0.005	0.060
0.008	0.160
0.016	0.285
0.025	0.325
0.032	0.365
0.065	0.435
0.110	0.490
0.235	0.546
0.340	0.570
0.420	0.590
0.550	0.625
0.560	0.635
0.590	0.650
0.720	0.700
0.750	0.730
0.780	0.750
0.830	0.790
0.870	0.820
0.900	0.850
0.945	0.900
0.960	0.920
0.990	0.965
1.000	1.000

ATTACHMENT E

Data for Determining Stream Compositions and Capacities when Operating with Isopropyl Ether

Your Research and Development Department has simulated the drying-column operating condition, shown on the flow diagram, in a pilot plant distillation unit. With this same distillation unit, the following overhead composition was obtained when isopropyl ether was used as the dehydration agent:

Component	Weight percent
Isopropanol	4.575
Water	4.00
Acetone	0.025
Isopropyl ether	91.400
	100.00

It was noted that operating pressures up to two bars absolute had little effect on this composition. Temperatures were noted at several operating pressures as follows:

Temperature, °C	Pressure, bars absolute
62	1.00
71	1.40
81	2.05
95	3.08

The isopropanol specifications were met when the bottoms withdrawal rate was controlled at 2 percent of the CBM feed rate.

A column in the same pilot plant was used to confirm the operation of the organic recovery column. (This column basically "strips" organics from the water before the water is routed to the waste treatment plant.) Conclusions from the pilot plant test are

1. The distillation below the feed point may be considered as a water-isopropanol binary. The column in the production unit has adequate trays above the feed point provided that reflux ratios similar to those for the benzene system are maintained.
2. The upper sidestream, which is recycled to the drying-column feed tank, has a water composition of 14.5 weight percent, which is the same as for the benzene system. The stream temperature was found to be 86°C at a column pressure of 1.4 bars absolute.
3. The flow-rate ratio of the heads-cut stream, which is processed in an off-sites batch still, to the isopropanol constant-boiling-mixture stream is the same for both the benzene and isopropyl ether streams.

The capacities of either column when benzene or isopropyl ether is used may be approximated from the following equations:

$$W_v = 275\ A_B \rho V \sqrt{\frac{\rho L - \rho V}{\rho V}} \tag{1}$$

$$Q_L = 175\ A_D \tag{2}$$

$$A_C = A_B + 2\ A_D \tag{3}$$

where

W_V = vapor rate, Kg/h
ρV = vapor density, Kg/m^3
ρL = liquid density, Kg/m^3
Q_L = liquid rate, m^3/h
A_B = tray bubbling area, m^2
A_D = downcomer area, m^2
A_C = column cross-sectional area, m^2

Constant molal overflow may be assumed for all column conditions.

DISCOUNTED-CASH-FLOW WORK SHEET

PROJECT: Refining of Isopropanol with Dehydration Agents Other Than Benzene
CASE: Isopropyl Ether System Relative to Continued Operation of Existing Benzene System
NOTES: 1. All monies are in thousands of dollars and rounded to the nearest $1,000.
2. Cost elements which are anticipated to be the same for both systems, such as operating labor, administration, etc., are not included in the analysis.

Line	Item	YEAR 1978	1979	1980	1981	1982	1983	1984	1985	1986	1987	1988	1989	1990	1991	1992
1.	Fixed-Capital Investment															
2.	Working Capital															
3.	Total Capital Investment															
4.	Annual Income (Sales)															
5.	Annual Manufacturing Cost															
a.	Isopropanol CBM															
b.	Utilities															
c.	Maintenance and Repairs															
d.	Local Taxes and Insurance															
	Total of Line 5															
6.	Annual General Expense															
a.	Distribution and Selling															
b.	Interest															
	Total of Line 6															
7.	Total Product Cost															
8.	Annual Operating Income (4 − 7)															
9.	Depreciation															
10.	Income Before Tax (8 − 9)															
11.	Income After Tax (0.52 × 10)															
12.	Annual Cash Income (9 + 11)															
13.	Investment Tax Credit															
14.	Annual Cash Flow (3 + 12 + 13)															
15.	15% Discount Factors	1.000	0.870	0.756	0.658	0.572	0.497	0.432	0.376	0.327	0.284	0.247	0.215	0.187	0.163	0.141
16.	Annual Present Value (14 × 15)															
17.	Total Present Value (sum of Line 16)															