1. Given: ✓ Three reaction paths to the manufacture of monochlorodecane (MCD) are given below.

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Path 1: $C_{10}H_{22} + Cl_2 \xrightarrow{light} C_{10}H_{21}Cl + HCl$ (1)
(Decane, Da) (MCD)

with side reaction

$C_{10}H_{21}Cl + Cl_2 \longrightarrow C_{10}H_{20}Cl_2 + HCl$ (2)
(MCD) (dichlorodecane, DCD)

The ratio of DCD : MCD is 1 : 4 mol in the effluent.

Path 2: $C_{10}H_{20} + HCl \xrightarrow{Catalyst} C_{10}H_{21}Cl$ (3)
(decene, De)

Path 3: $C_{10}H_{21}OH + HCl \longrightarrow C_{10}H_{21}Cl + H_2O$ (4)
(decanol, DOH)

Compound	($/lbmol)
decane (Da)	4.80
decene (De)	12.00
decanol (DOH)	14.00
Cl_2	1.77
HCl	1.00
MCD	16.00
DCD	0.00

Want: ✓ Which process should be selected for further study?

Solution: ✓ Calculate EP's for each reaction path.

Rxn. (2) combines with rxn. (1) to yield

$C_{10}H_{22} + 2Cl_2 \longrightarrow C_{10}H_{20}Cl_2 + 2HCl$ (5)

Or, overall for path 1

$5C_{10}H_{22} + 6Cl_2 \longrightarrow 4C_{10}H_{21}Cl + 1C_{10}H_{20}Cl_2 + 6HCl$ (6)

EP_i = {value of products for path i} − {cost of raw materials}

$EP_1 = [(4\text{ lbmol MCD})(\$16.00/\text{lbmol}) + (1\text{ lbmol DCD})(\$0.00/\text{lbmol}) + (6\text{ lbmol HCl})(\$1.00/\text{lbmol})]$
$- [(5\text{ lbmol Da})(\$4.80/\text{lbmol}) + (6\text{ mol } Cl_2)(\$1.77/\text{lbmol})]$ (7)

$EP_1 = \$35.38$ for 4 lbmol MCD produced (7')

$EP_1 = \$8.845$ for 1 lbmol MCD produced ✓ (7'')

1 Solution: $EP_2 = [(1\ lbmol\ MCD)(\$16.00/lbmol)] - [(1\ lbmol\ De)(\$12.00/lbmol) + (1\ lbmol\ HCl)(\$1.00/lbmol)]$ (8)

$EP_2 = \$3.00$ for 1 lbmol MCD produced ✓ (8')

$EP_3 = [(1\ lbmol\ MCD)(\$16.00/lbmol) + (1\ lbmol\ H_2O)(\$0.00/lbmol)] - [(1\ lbmol\ DOH)(\$14.00/lbmol) + (1\ mol\ HCl)(\$1.00/lbmol)]$ (9)

$EP_3 = \$1.00$ for 1 lbmol MCD produced (9')

Answer: Reaction Path 1 shows the most promise ✓ based upon the economic potential ($EP_1 = \frac{\$8.845}{1\ lbmol\ MCD}$). ✓

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2. Given: Pilot plant studies on decane chlorination showed that the side reaction leading to DCD production can be reduced by feeding a larger excess of decane. ✓

When a mole ratio decane : chlorine is kept at 5:1, the effluent has 19 lbmol MCD : 1 lbmol DCD. All of the chlorine in the feed is consumed.

Want: How many moles of decane must be recycled per mole of MCD produced? Draw an input/output structure of the flowsheet showing (a) raw material requirements, (b) product and byproduct flowrates, and (c) the feed to the separations system. ✓

Solution: Use a basis of $100 \left(\frac{mol\ MCD\ produced}{hr}\right)$

Use the basis, the mole ratios, and equations (1) and (5) from problem 1 to calculate flows.

$100 \left(\frac{mol\ MCD}{hr}\right) \Rightarrow \left(\frac{1\ mol\ DCD}{19\ mol\ MCD}\right)\left(100\ \frac{mol\ MCD}{hr}\right) = \left(\frac{100}{19}\ \frac{mol\ DCD}{hr}\right)$ (10) ✓

Use these production values to determine how much Cl_2 is feed, and HCl produced.

$100(C_{10}H_{22} + Cl_2 \rightarrow C_{10}H_{21}Cl + HCl)$ (11)

$5.26(C_{10}H_{22} + 2Cl_2 \rightarrow C_{10}H_{20}Cl_2 + 2HCl)$ ✓ (12)

The net reaction is

$(105.26)C_{10}H_{22} + (110.52)Cl_2 \rightarrow 100\ C_{10}H_{21}Cl + 5.26\ C_{10}H_{20}Cl_2 + (110.52)HCl$ (13)

✓

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2. Solution: Since the reactor feed is 5 mol $C_{10}H_{22}$: 1 mol Cl_2, and since all Cl_2 fed reacts,

$$\dot{n}\left(\frac{mol}{hr}\right)_{C_{10}H_{22}\,fed} = 5\left(110.52\ \frac{mol\ Cl_2\ fed}{hr}\right) \quad (14)$$

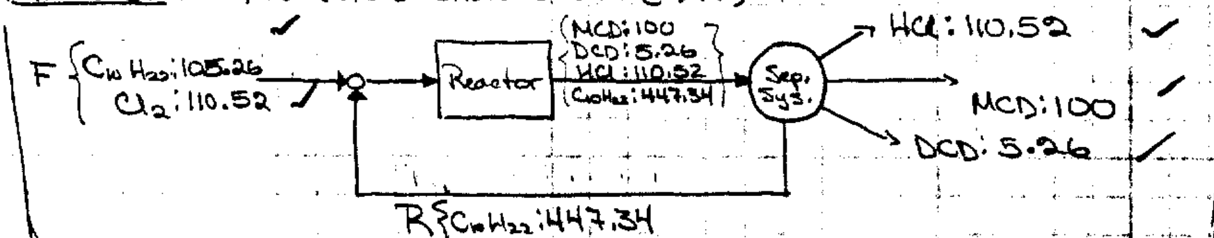
$$\dot{n} = 552.60\left(\frac{mol\ C_{10}H_{22}\ fed}{hr}\right) \checkmark \quad (14')$$

Of $C_{10}H_{22}$ fed, 105.26 (mol/hr) is consumed, ✓

thus there is 447.34 $\left(\frac{mol\ C_{10}H_{22}}{hr}\right)$ exiting the reactor. ✓

This excess $C_{10}H_{22}$ should be recycled.

Answer: All flows shown are in (mol/hr) ✓



The decane recycle is 4.4734 $\left(\frac{mol\ C_{10}H_{22}}{mol\ MCD\ made}\right)$. ✓

3. Given: The following physical properties are known:

Compound	Boiling point (°C)	Flow Rates
decane	174	
MCD	215	
DCD	241	
HCl	−85	
Cl_2	−34	

Want: Apply the sequential heuristics of Nadgir & Liu, and discuss the consequences of each. Synthesize a separation sequence and give the flow diagram.

Solution: Assume the feed to the separations sequence is that presented in problem 2.

M1: Ordinary distillation should be used for separations.

M2: Neither vacuum nor refrigerated distillation should be needed. cool product to condense all but HCl compress to avoid refrigeration.

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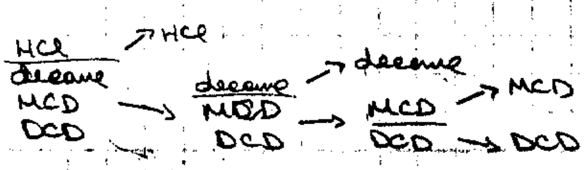
3. Solution: D1: None of the products, byproducts, or recycle components may be grouped.

S1: HCl is the only hazardous and corrosive material, and it should be removed first.

S2: The most difficult separation will probably be separating MCD and DCD, but none are particularly hard.

C1: The most plentiful component is decane. Remove it after the HCl (gv. S1).

C2: The separation sequence is set, and this heuristic need not be considered.



Answer: All flows shown are given in (mol/hr)