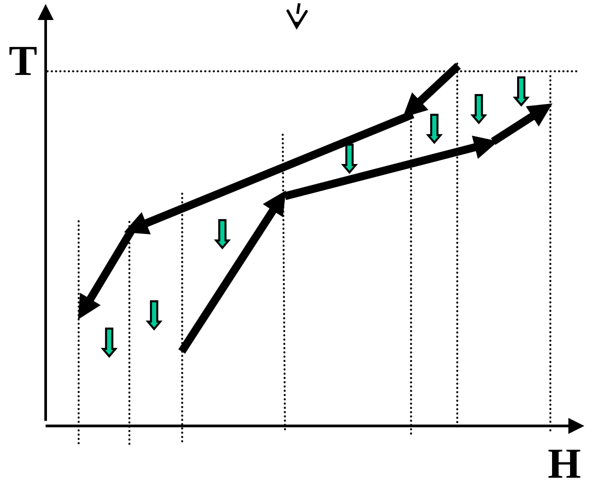
PART 6

HEAT INTEGRATION AND MATHEMATICAL PROGRAMMING

PINCH TECHNOLOGY SHORTCOMINGS

- It is a two-step procedure, where utility usage is determined first and the design is performed later.
- Trade-offs are optimized (through Super-targeting) using an approximation to the value of area (Vertical heat transfer) and using minimum number of exchangers.

$$\mathbf{N_{min} = (S\text{-}P)_{\text{above pinch}} + (S\text{-}P)_{\text{below pinch}}}$$

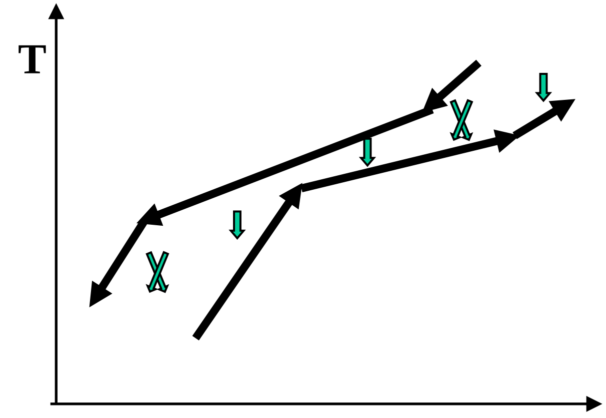


PINCH TECHNOLOGY SHORTCOMINGS

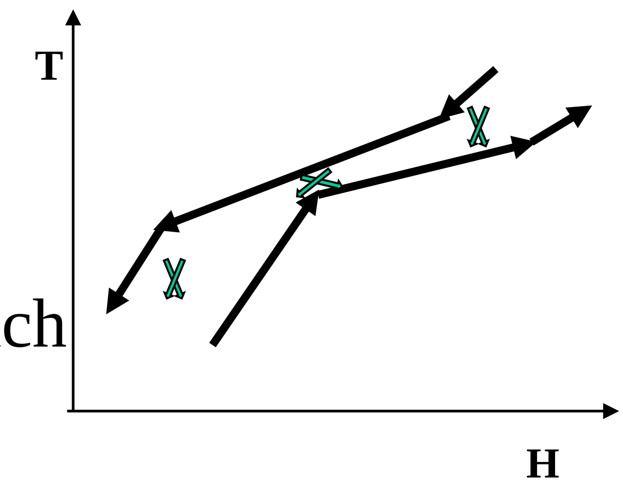
- Capital Investment trade-offs between area and number of units is resolved in favor of minimizing the number of units.
- All exchangers are subject to the same ΔT_{min}(HRAT).
- There is no shell counting
- No procedure is given for handling splitting away from the Pinch
- It is not systematic: After pinch matches are placed one is left using common sense built expertise
- Larger problems offer combinatorial challenges

PINCH TECHNOLOGY SHORTCOMINGS

- Vertical Transfer takes place in regions close to the pinch, while non-vertical transfer takes place away from it to minimize the number of units.



- Options allowing criss-cross at the pinch may offer some advantages .



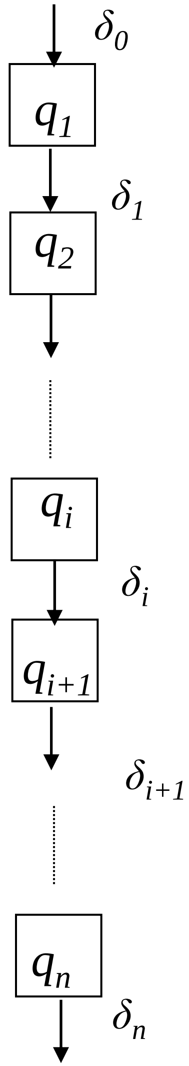
ALTERNATIVES

- Alternative models need to:
  - Treat all the trade-offs simultaneously through costs (energy, area, fixed costs for units/shells) and move away from two step procedures and relaxations. Let the true economics determine the design
  - Remove limitations on heat transfer (HRAT), and possibly introduce exchanger minimum approximation temperatures (EMAT) to specific pairs of streams when appropriate or desired.
  - Do not exhibit limitations like lack of control of splitting or isothermal mixing.
  - Be systematic and potentially automatic.

WE LOOK INTO MATHEMATICAL PROGRAMMING FOR THIS PURPOSE

MATHEMATICAL MODELS

Mathematical model to calculate the minimum utility.



$$S_{\min} = Min\ \delta_0$$

$$s.t$$

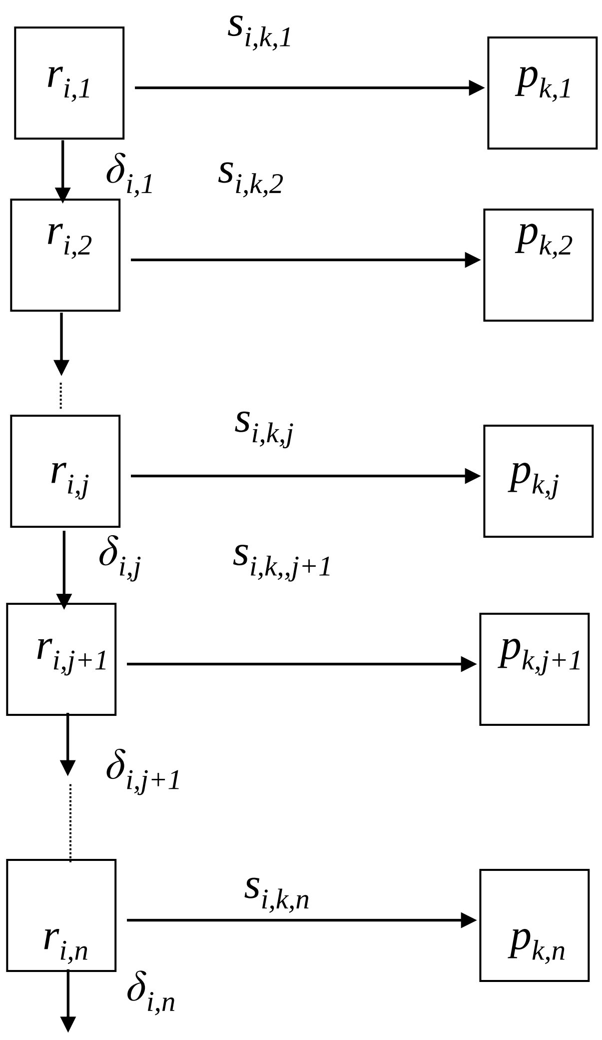
$$\delta_j = \delta_{j-1} + q_j \quad \forall j = 1,\ldots n$$

$$\delta_j \geq 0$$

Where

$$q_j = \sum_i F_i^H cp_i^H (T_{j-1} - T_j) - \sum_k F_k^C cp_k^C (T_{j-1} - T_j)$$

MATHEMATICAL MODEL



Assume now that we do the same cascade for each hot stream, while we do not cascade the cold streams at all. In addition we consider heat transfer from hot to cold streams in each interval.

The material balances for hot streams and utilities are:

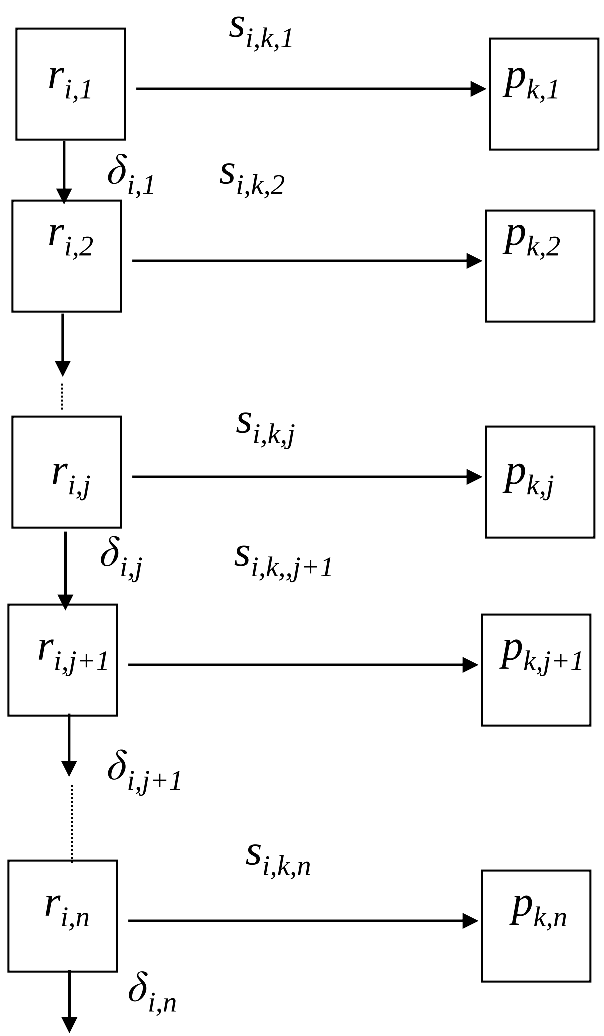
$$\begin{cases} \delta_{i,0} = 0 \qquad \delta_{U,0} \geq 0 \\ \delta_{i,j} = \delta_{i,j-1} + r_{i,j} - \sum_k s_{i,k,j} \quad \forall j = 1,\ldots n \end{cases}$$

The heat balances for cold streams are:

$$p_{k,j} = \sum_i s_{i,k,j} \quad \forall j = 1,\ldots n$$

where $r_{i,j}$ and $p_{k,j}$ are the heat content of hot stream *i* and cold stream *k* in interval *j*.

MATHEMATICAL MODEL



Although we have a simpler model to solve it, in this new framework, the minimum utility problem becomes:

$$Min \quad \delta_{U,0}$$

$$s.t$$

$$\delta_{i,0} = 0 \quad \forall i \neq U$$

$$\delta_{i,j} = \delta_{i,j-1} + r_{i,j} - \sum_k s_{i,k,j} \quad \forall i \cup U, \forall j = 1,\ldots n$$

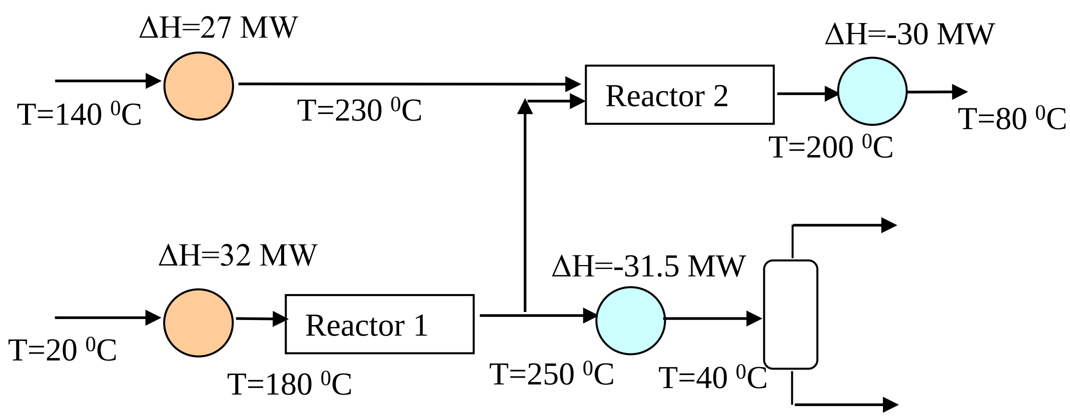
$$p_{k,j} = \sum_i s_{i,k,j} \quad \forall k, \forall j = 1,\ldots n$$

Note that the cascade equation for hot streams now includes the utility *U* as well. Cold streams include cooling water.

More than one utility? Add it as another hot/cold stream

CAN THIS GIVE A NETWORK?

We use the following principle: Always satisfy cold stream requirements using hot process streams first. Consider the example given in Part I

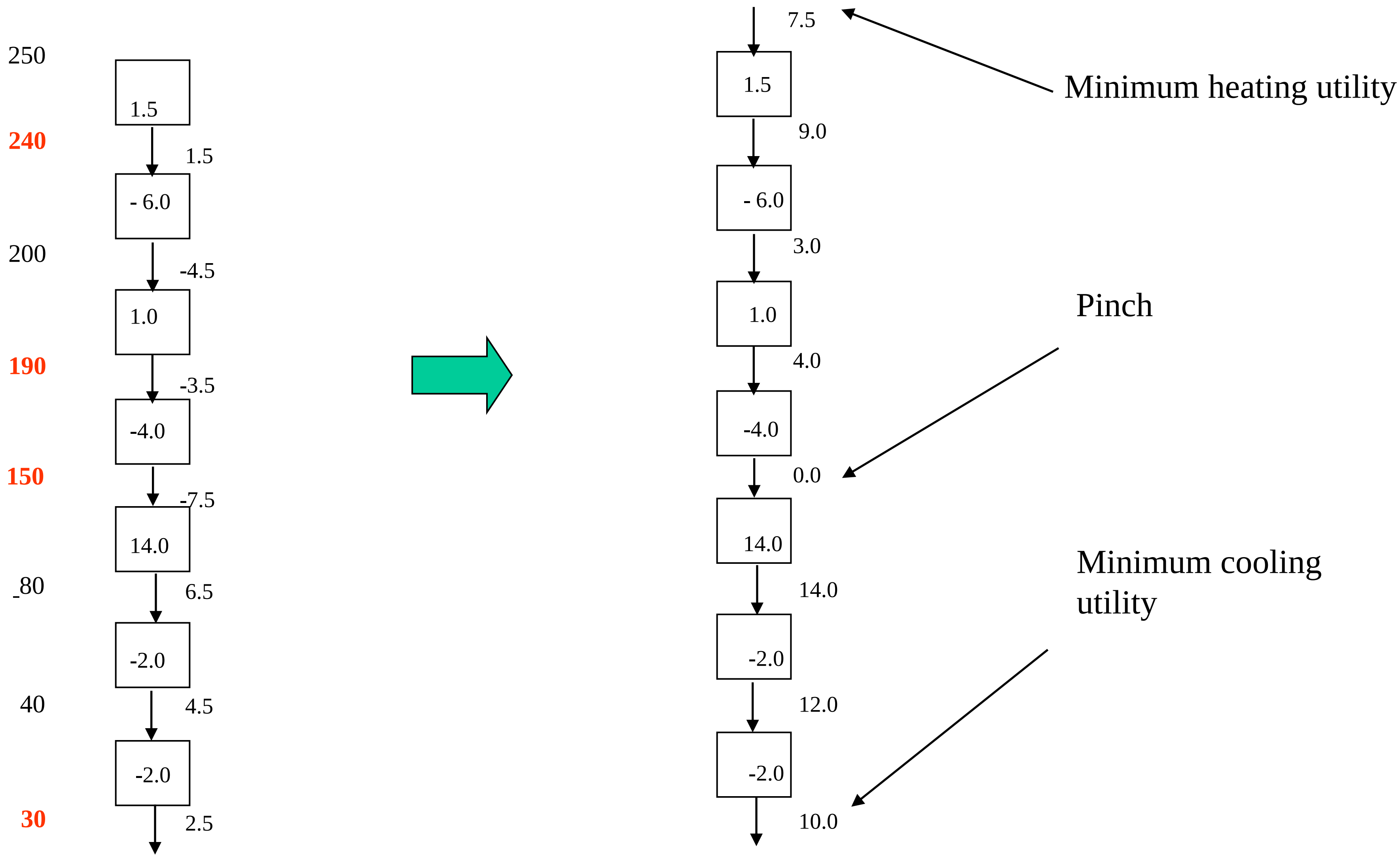


ΔT_{min}=10 ºC

Stream	Type	Supply T (ºC)	Target T (ºC)	ΔH (MW)	F*Cp (MW $^{o}C^{-1}$)
Reactor 1 feed	Cold	20	180	32.0	0.2
Reactor 1 product	Hot	250	40	-31.5	0.15
Reactor 2 feed	Cold	140	230	27.0	0.3
Reactor 2 product	Hot	200	80	-30.0	0.25

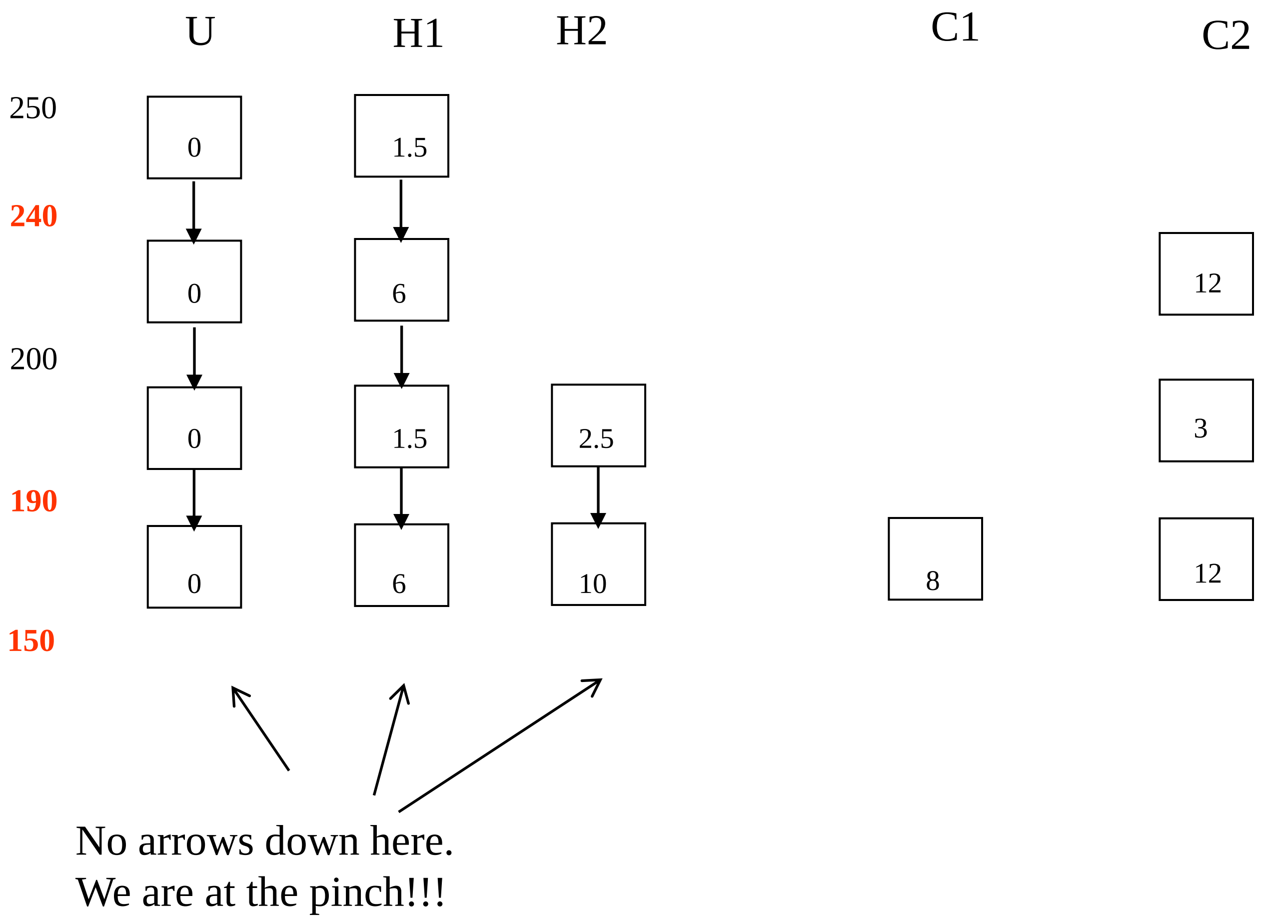
CASCADE

The problem had the following characteristics



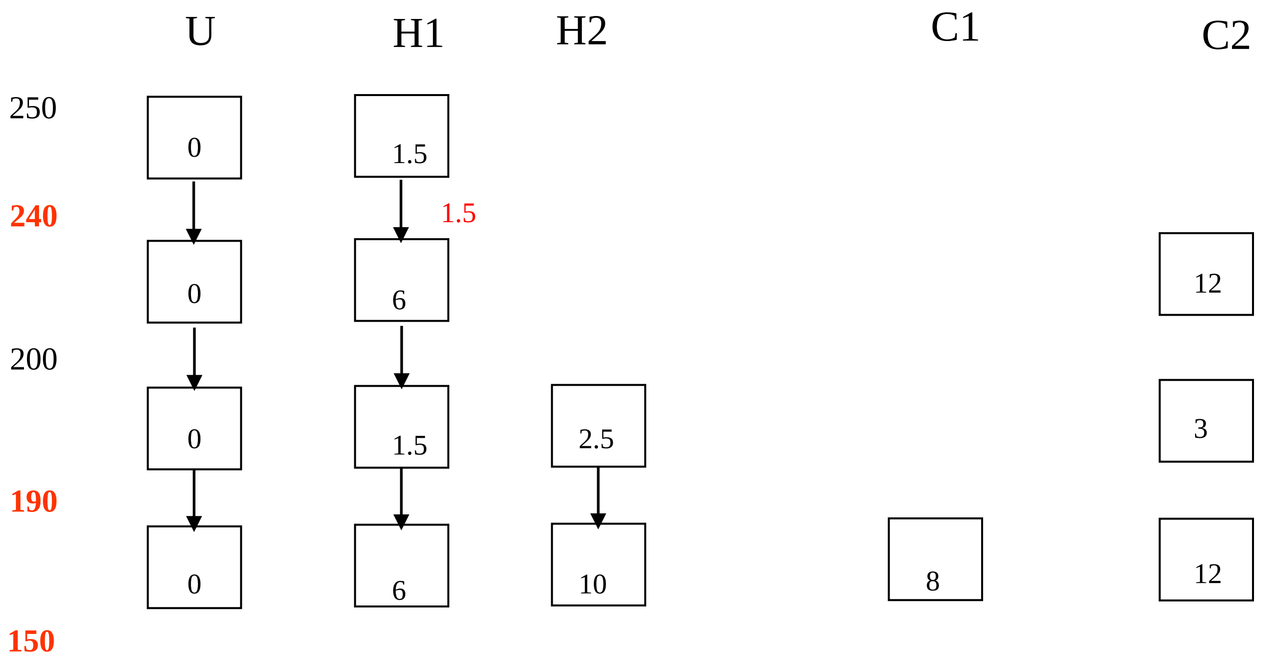
TRANSSHIPMENT

We will look at the intervals above the pinch only



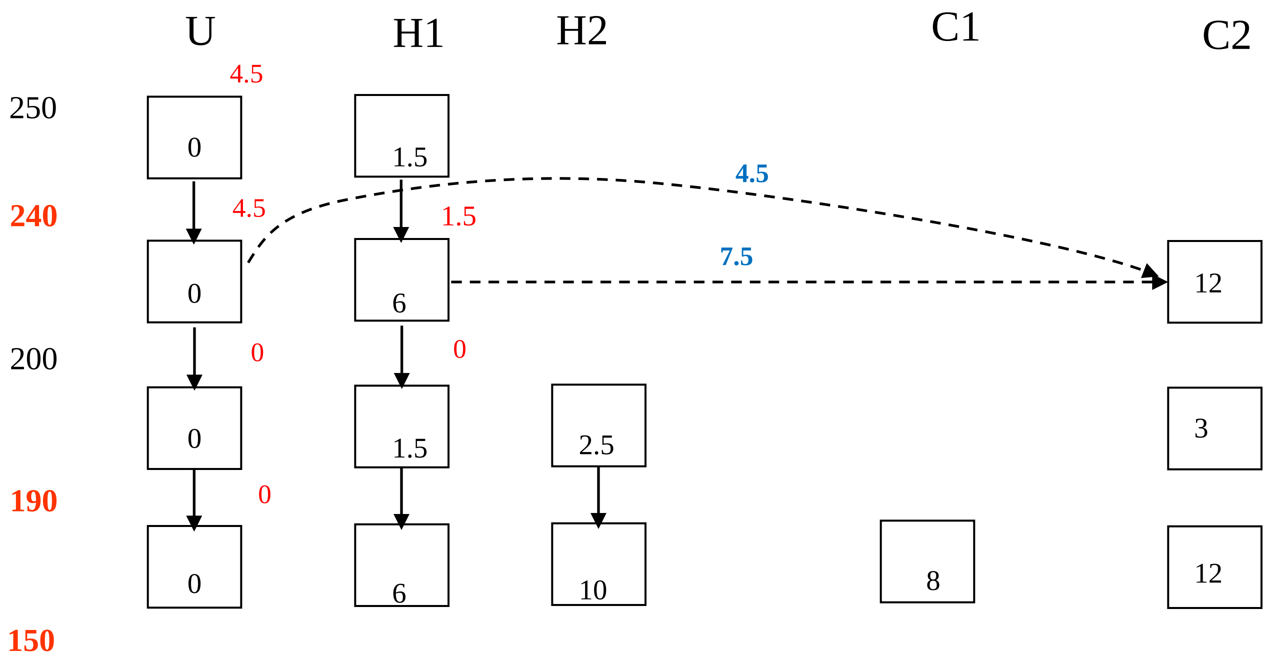
TRANSSHIPMENT

We start with the first hot stream (H1). There is no cold stream in the first interval. Then we cascade everything down



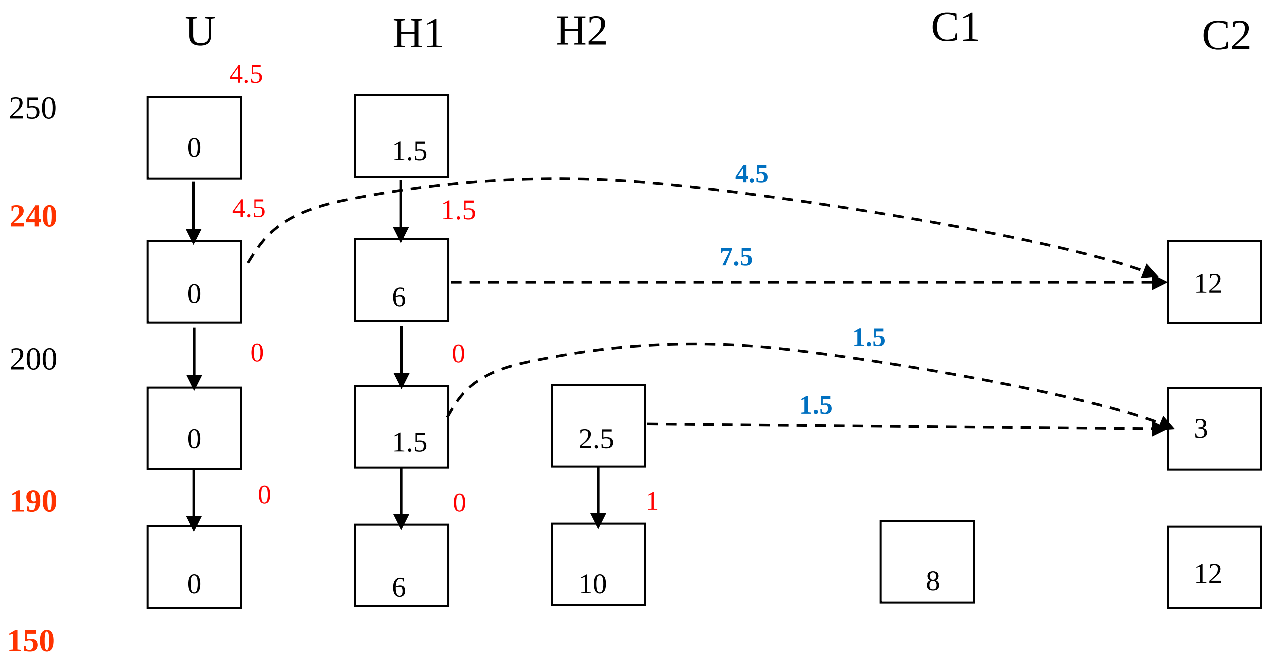
TRANSSHIPMENT

We now send 7.5 to the cold stream and use utility cascaded to fulfill the 12 units the cold stream C2 requires



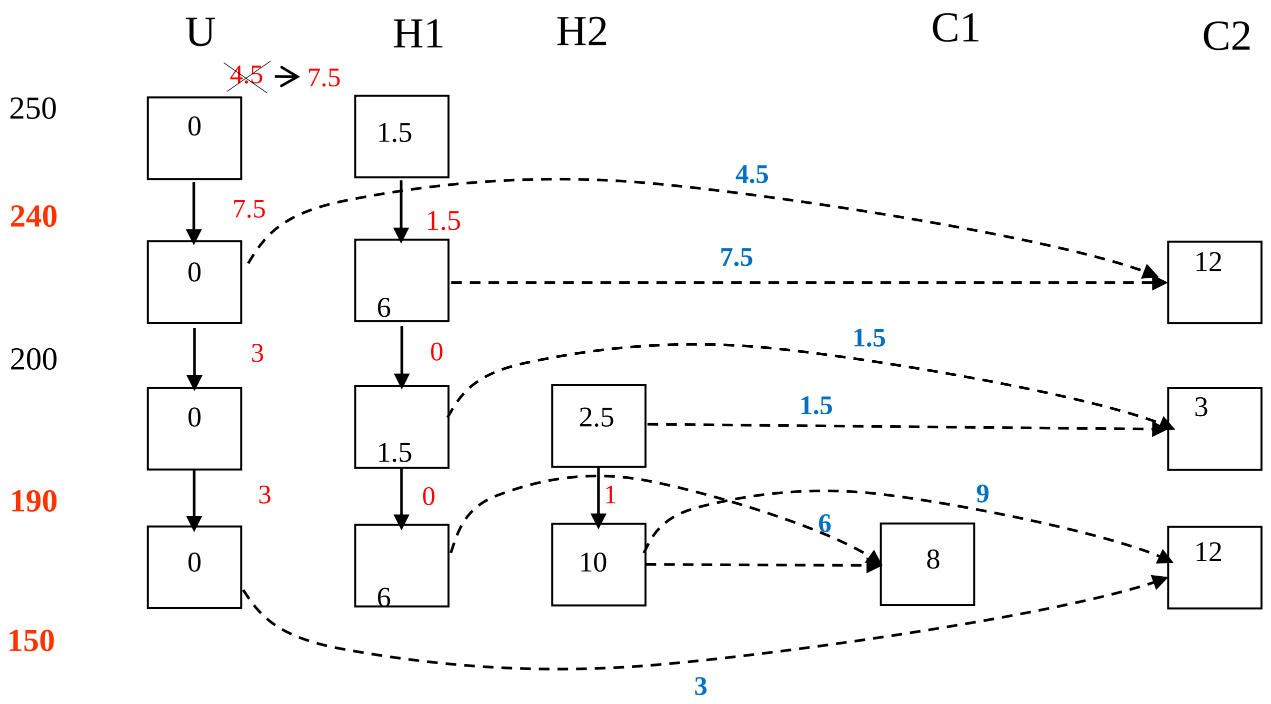
TRANSSHIPMENT

In interval 3 there are two streams. We use H1 first and then H2 if needed



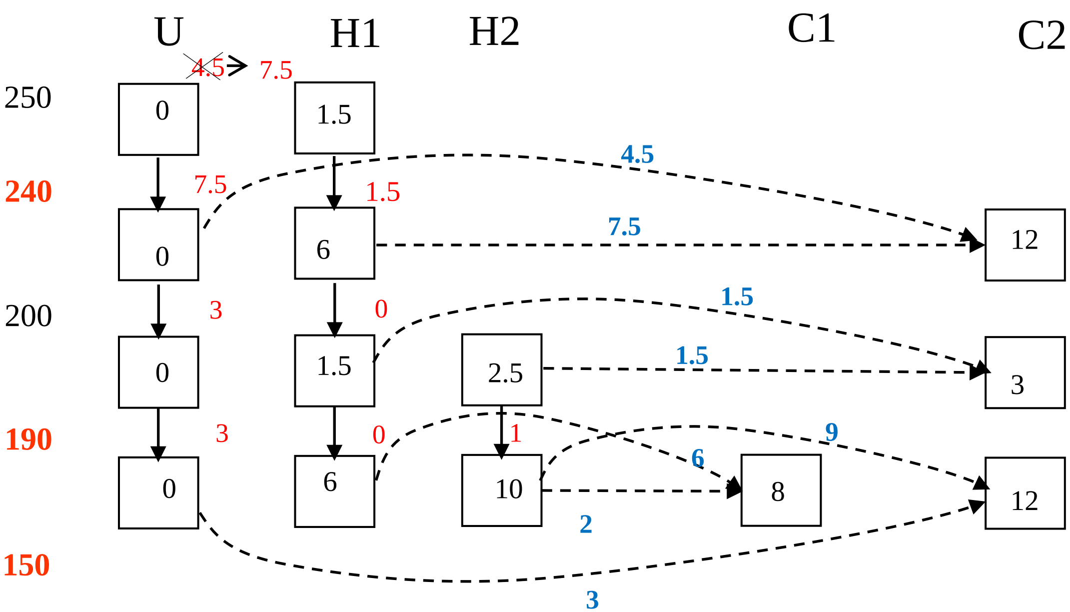
TRANSSHIPMENT

We finish in interval 4 using H1 first with C1, then H2-C1 followed by H2-C2 and then U, which is now been augmented

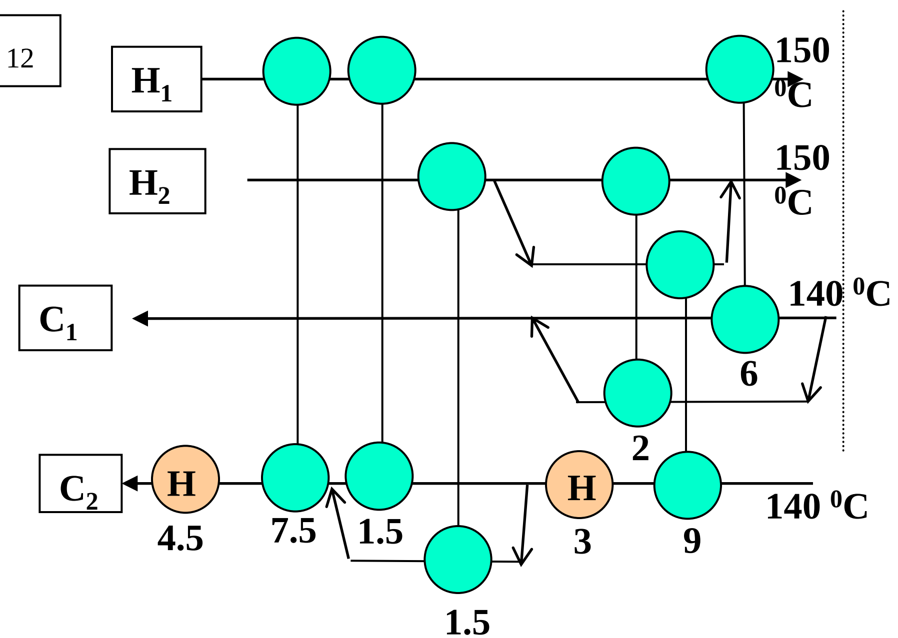


We obtain the same utility!!!

TRANSSHIPMENT



The resulting suggested network is very complicated

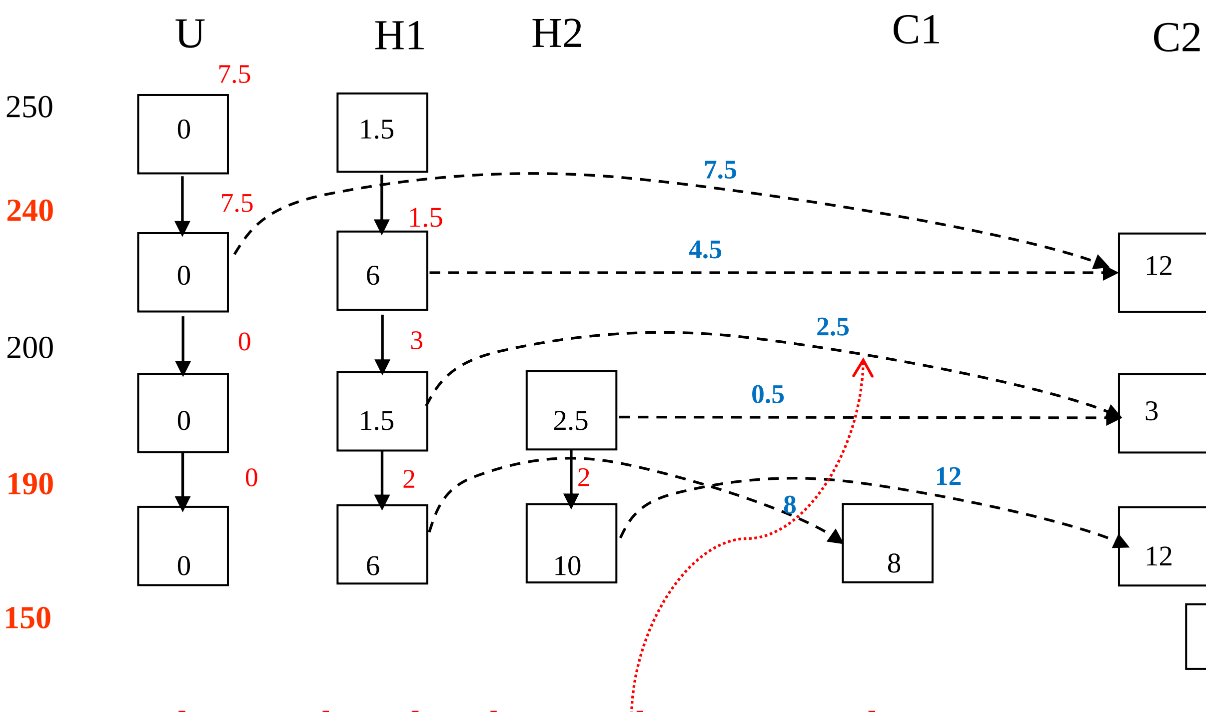


The flowsheet can be simplified.

-The heater in C2 can be moved to higher temperatures and merged with the other, allowing removal of the split in C2.

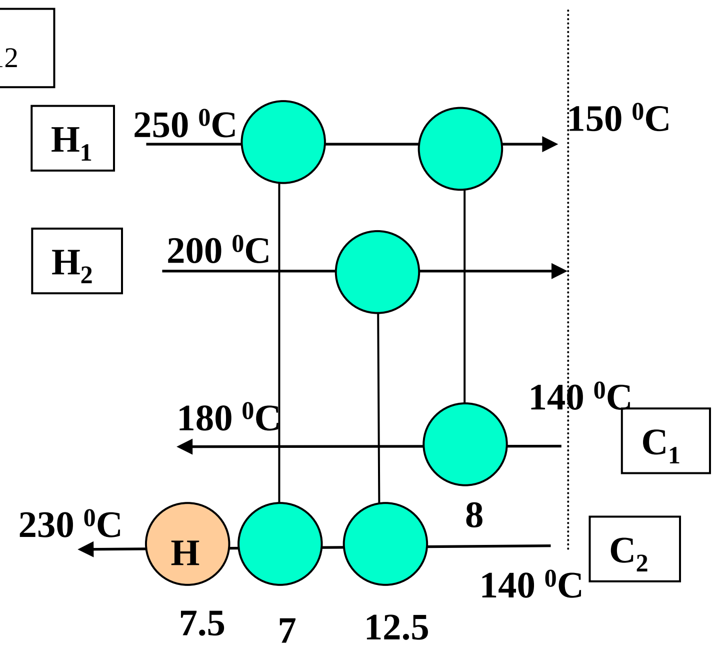
-The split in H2 and C1 cannot be removed simply by inspection

TRANSSHIPMENT



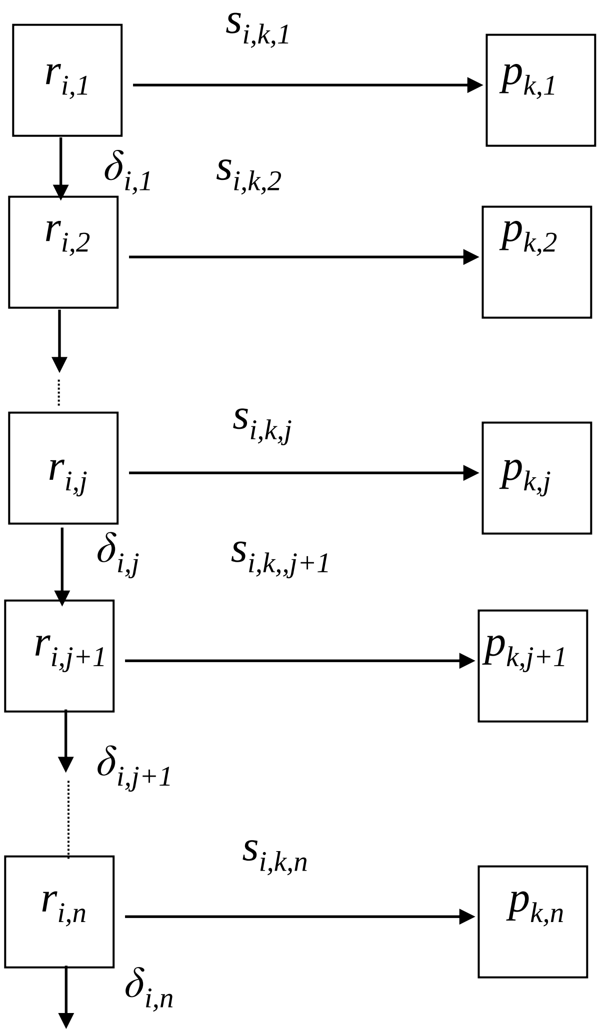
The PDM network is less complicated

No splitting takes place because hot H1 cascades 3 units to supply the 2.5 in the 3rd interval



We conclude that we need to minimize the number of matches between streams

COUNTING MATCHES



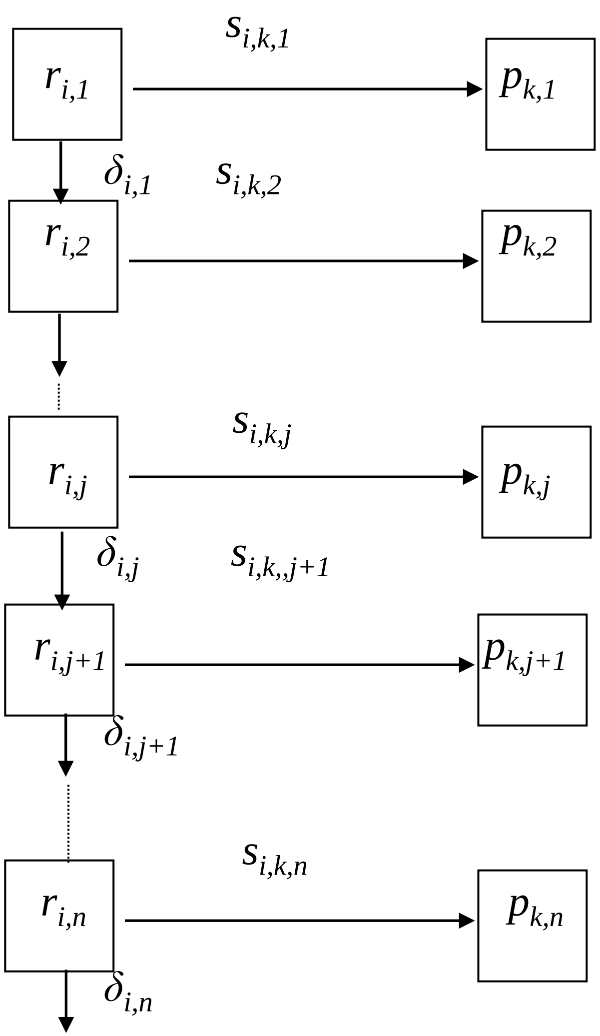
We would like to have a model that would tell us the $s_{i,k,j}$ such that the number of units is minimum. We now introduce a way of counting matches between streams. Let $Y_{i,k}$ be a binary variable (can only take the value 0 or 1).

Then we can force $Y_{i,k}$ to be one using the following inequality

$$\sum_j s_{i,k,j} - \Gamma Y_{i,k} \leq 0$$

indicating therefore that heat has been transferred from stream i to stream k in at least one interval.

MATHEMATICAL MODEL



The complete model would be:

$r_{U,1}$ =Minimum utility from previous model ($\delta^{*}_{U,0}$)

$$Min \sum_i \sum_k Y_{i,k}$$

$s.t$

$$\delta_{i,0} = 0 \quad \forall i$$

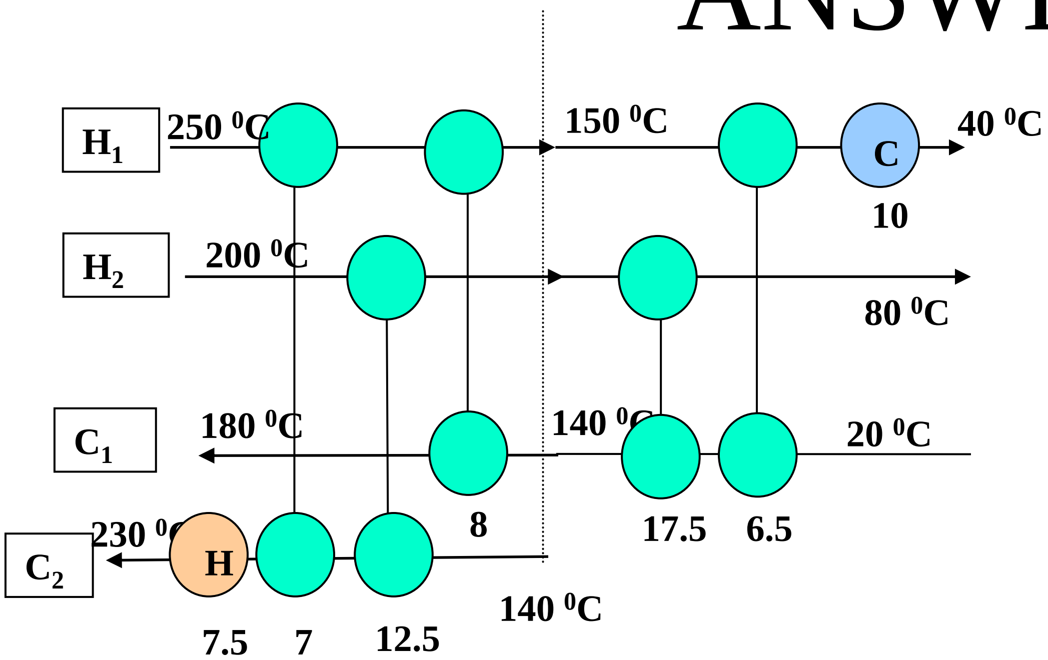
$$\delta_{i,j} = \delta_{i,j-1} + r_{i,j} - \sum_k s_{i,k,j} \quad \forall i, \forall j = 1,\ldots m_I$$

$$p_{k,j} = \sum_i s_{i,k,j} \quad \forall k, \forall j = 1,\ldots m_I$$

$$\sum_j s_{i,k,j} - \Gamma Y_{i,k} \leq 0 \quad \forall i, \forall k$$

The model can only be solved above and below the pinch separately. Why???

ANSWER



We are minimizing the number of matches. We saw already that more than one exchanger can exist if all regions (above and below the pinch) are considered.

Example: H1-C1 has one match above the pinch and one match below the pinch. If solved ignoring the pinch (one region for the whole problem), then it would count these two exchangers as one match.

When solved separately, it would give the right number.

THUS, this model will ONLY give the right answer (Matches= Exchangers) if run in each region separately

GAMS MODEL

$$z = Min \sum_i \sum_k Y_{i,k}$$

$s.t$

$$\delta_{i,0} = 0 \quad \forall i$$

$$\delta_{i,j} = \delta_{i,j-1} + r_{i,j} - \sum_k s_{i,k,j} \quad \forall i, \forall j = 1,\dots m_I$$

$$p_{k,j} = \sum_i s_{i,k,j} \quad \forall k, \forall j = 1,\dots m_I$$

$$\sum_j s_{i,k,j} - \Gamma Y_{i,k} \leq 0 \quad \forall i, \forall k$$

GAMS MODEL

```
SETS
      I   hot streams above pinch   / U, H1,H2 /
      K   cold streams above pinch  / C1,C2 /
      J   temperature intervals / J0*J3 / ;

 SCALAR GAMMA /10000/;

 TABLE R(I,J)  load of hot stream I1 in interval K
          J1     J2      J3        J4
    U    7.5     0        0         0
    H1   1.5     6       1.5        6
    H2    0      0       2.5       10;

TABLE P(K,J)  load of cold stream K1 in interval J
               J0    J1    J2      J3
     C1        0      0     0       8
     C2        0     12     3      12   ;


VARIABLES
      S(I,K,J)  heat exchanged hot and cold streams
      D(I,J)  heat of hot streams flowing between intervals
      Y(I,K)  existence of match
      Z       total number of matches  ;

 POSITIVE VARIABLE S
 POSITIVE VARIABLE D
 BINARY VARIABLE Y   ;

 EQUATIONS
      MINMATCH       objective function-number of matches
     HSBAL1(I,J)      heat balances of hot stream I in INTERVAL J ne 1
      HSBAL(I,J)      heat balances of hot stream I in INTERVAL 1
     CSBAL(K,J)       heat balances of cold stream J1 in K
      HTINEQ1(I,K)    heat transferred inequalities;

 MINMATCH .. Z =E= SUM((I,K), Y(I,K));
 HSBAL1(I,J)$(ORD(J) NE  1)  .. D(I,J)-D(I,J-1)+ SUM(K,S(I,K,J)) =E= R(I,J);
 HSBAL(I,J)$(ORD(J) EQ  1)  .. D(I,J)+SUM(K,S(I,K,J)) =E= R(I,J);
 CSBAL(K,J)..   SUM(I, S(I,K,J)) =E= P(K,J) ;
 HTINEQ1(I,K) ..   SUM(J, S(I,K,J))-GAMMA*Y(I,K)  =L= 0  ;

 MODEL TSHIP /ALL/ ;
 SOLVE TSHIP USING MIP MINIMIZING Z;
 DISPLAY S.L, D.L, Y.L,Z.l;
```

TRANSSHIPME

SOLUTION

VARIABLE S.L

	J1	J2	J3
U .C2	**7.500**		
H1.C2	**4.500**	**0.500**	**10.000**
H2.C1			**8.000**
H2.C2		**2.500**	**2.000**

---- VARIABLE D.L

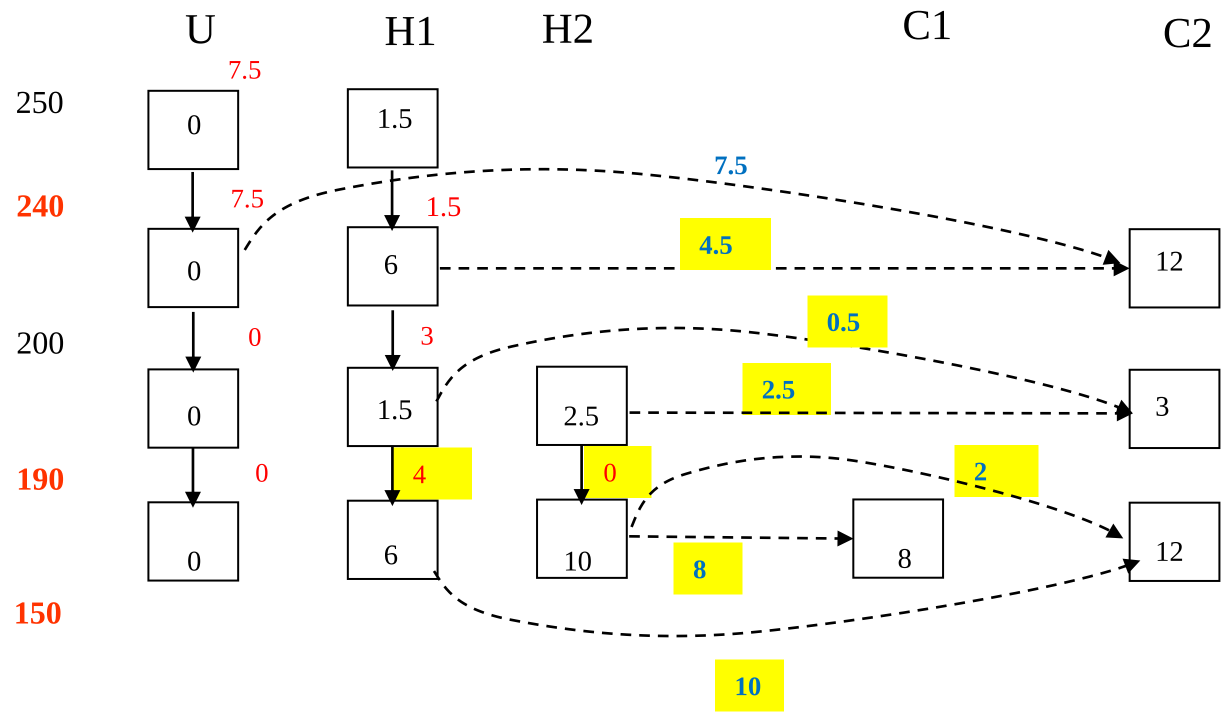
	J0	J1	J2
U	**7.500**		
H1	**1.500**	**3.000**	**4.000**

---- VARIABLE Y.L

	C1	C2
U		**1.000**
H1		**1.000**
H2	**1.000**	**1.000**

---- VARIABLE Z.L = 4.000

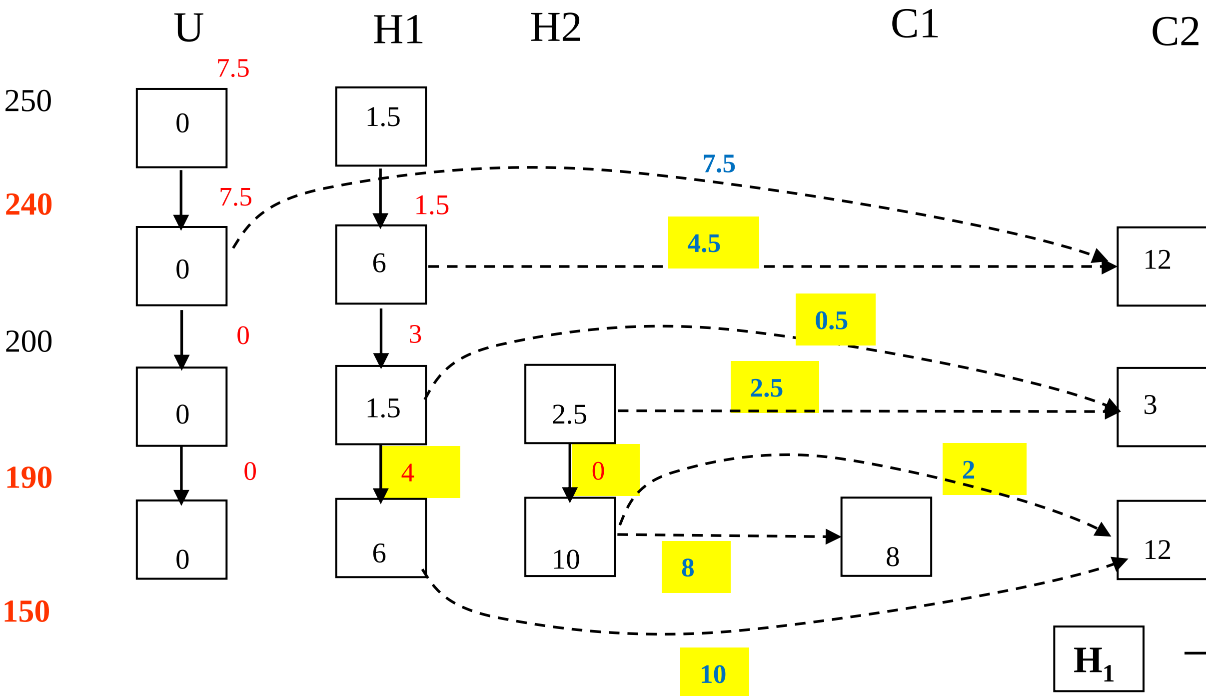
EXECUTION TIME = 0.0001 SECONDS



This result is different from the one given by the PDM.

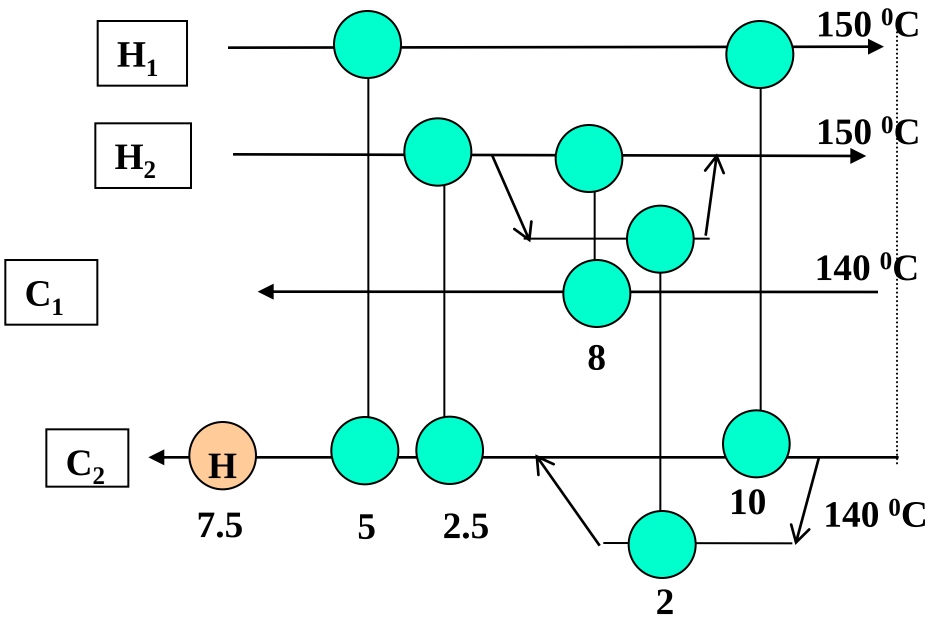
However, it predicts correctly the number of exchangers.

TRANSSHIPMENT



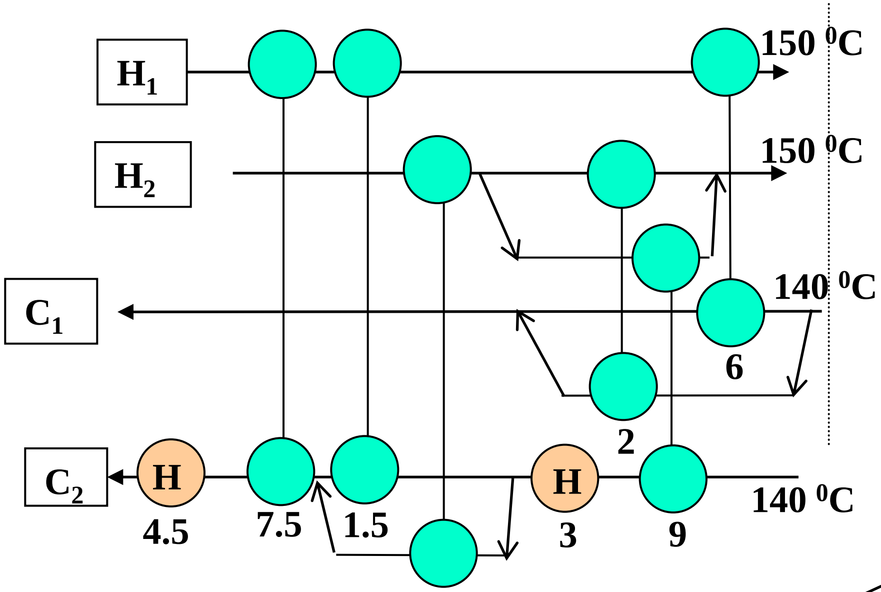
Splitting of C2 takes place because hot H1 and H2 give to C2 in the last interval. H2 values cannot be moved to a sequential arrangement because the cascade is zero.

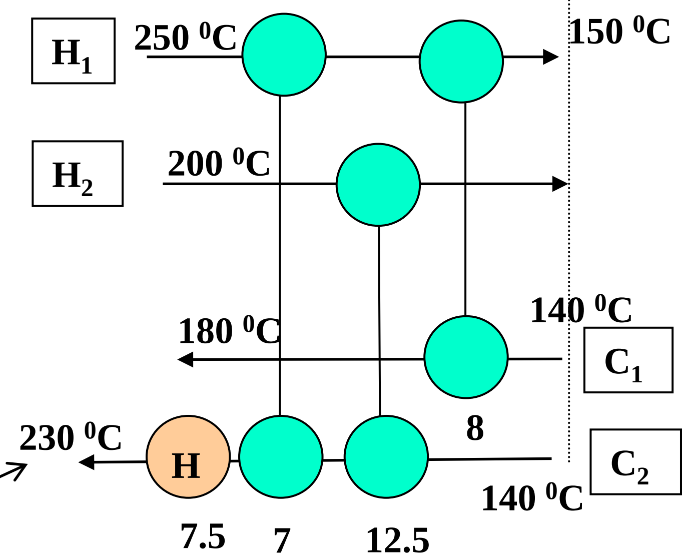
Finally, H2and C2 split at the last interval. With this solution, this cannot be changed.



Some form of limiting splitting is needed.

TRANSSHIPMENT





By ad-hoc rule

5 Matches- 8 exchangers

BAD!!!

PDM

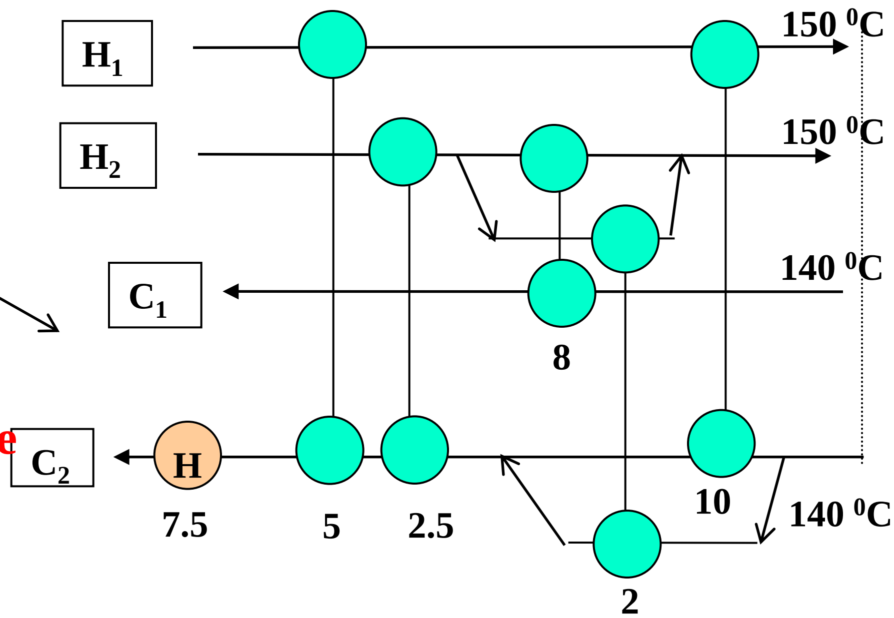
4 Matches- 4 exchangers

RIGHT ANSWER

Mathematical Programming

4 Matches- 6 exchangers

BETTER



Some way of controlling splitting AND the number of units is needed

In addition, area cost is not included

TRANSSHIPMENT

We conclude that the transshipment model

- Can calculate Minimum utility and predict the number of matches.
- The number of matches are equal to the number of exchangers, but….
- The model may (and usually does) give more exchangers, than matches.

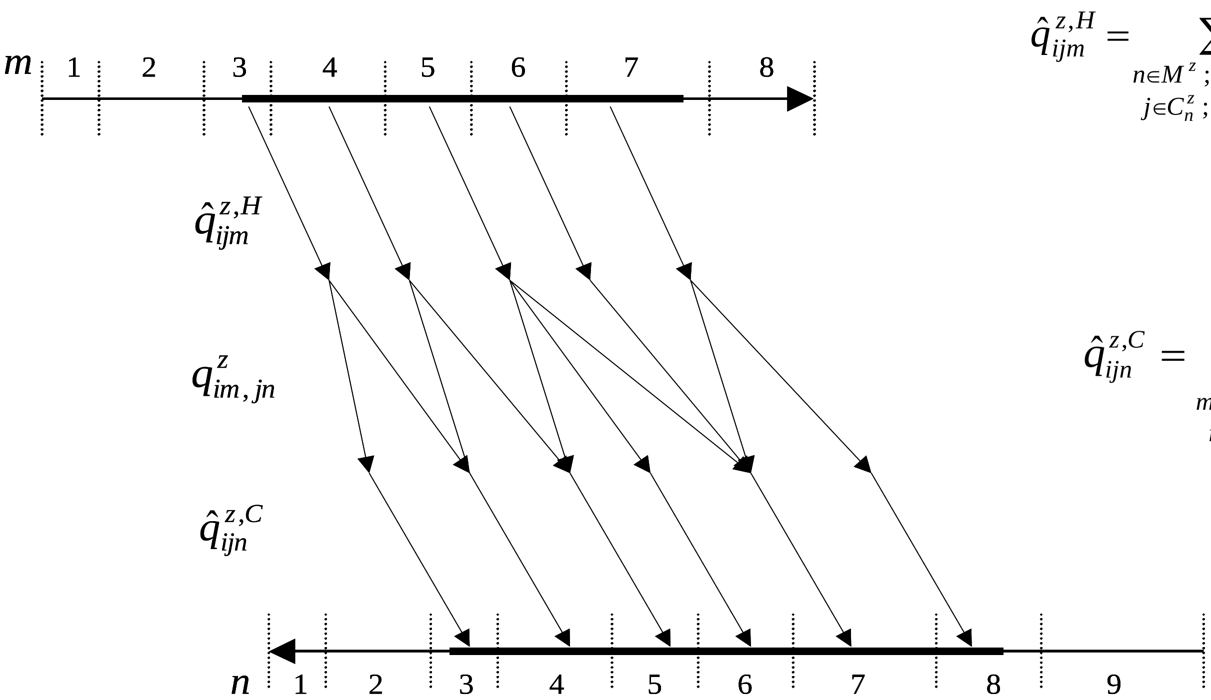
Some way of controlling splitting AND the number of units is needed as well adding area cost is needed.

This is done in the next MILP model

TRANSPORTATION MODELS

Streams are divided in small temperature intervals

Heat can be sent to **<u>any</u>** interval of lower temperature.



$$\hat{q}^{z,H}_{ijm} = \sum_{\substack{n \in M^z;\, T_n^L < T_m^U \\ j \in C_n^z;\, i \in P_{jn}^C}} q^z_{im,jn}$$

$$\Delta H^{z,H}_{im} = \sum_{\substack{n \in M^z \\ T_n^L < T_m^U}} \sum_{\substack{j \in C_n^z \\ j \in P_{im}^H \\ i \in P_{jn}^C}} q^z_{im,jn}$$

$$\hat{q}^{z,C}_{ijn} = \sum_{\substack{m \in M^z;\, T_n^L < T_m^U \\ i \in H_m^z;\, j \in P_{im}^H}} q^z_{im,jn}$$

$$\Delta H^{z,C}_{jn} = \sum_{\substack{m \in M^z \\ T_n^L < T_m^U}} \sum_{\substack{i \in H_m^z \\ i \in P_n^C \\ j \in P_m^H}} q^z_{im,jn}$$

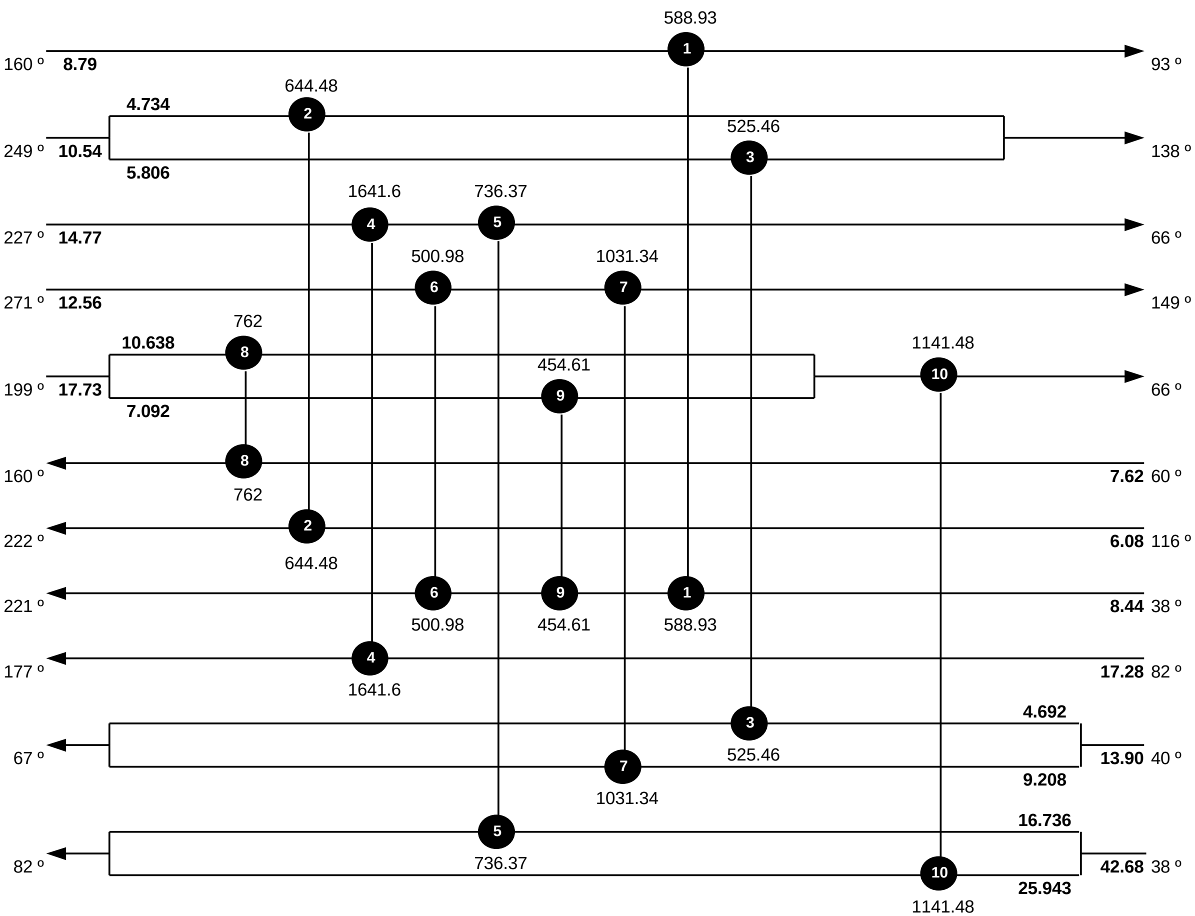
Barbaro and Bagajewicz (2005)

TRANSPORTATION MODELS

The model

- **IS LINEAR!!!!**
- **Counts heat exchangers units and shells.**
- **Determines the area required for each exchanger unit or shell.**
- **Controls the total number of units.**
- **Determines the flow rates in splits.**
- **Handles non-isothermal mixing.**
- **Identifies bypasses in split situations when convenient.**
- **Controls the temperature approximation (ΔT_{min}) when desired.**
- **Can address areas or temperature zones.**
- **Allows multiple matches between two streams**

TRANSPORTATION MODELS



10SP1

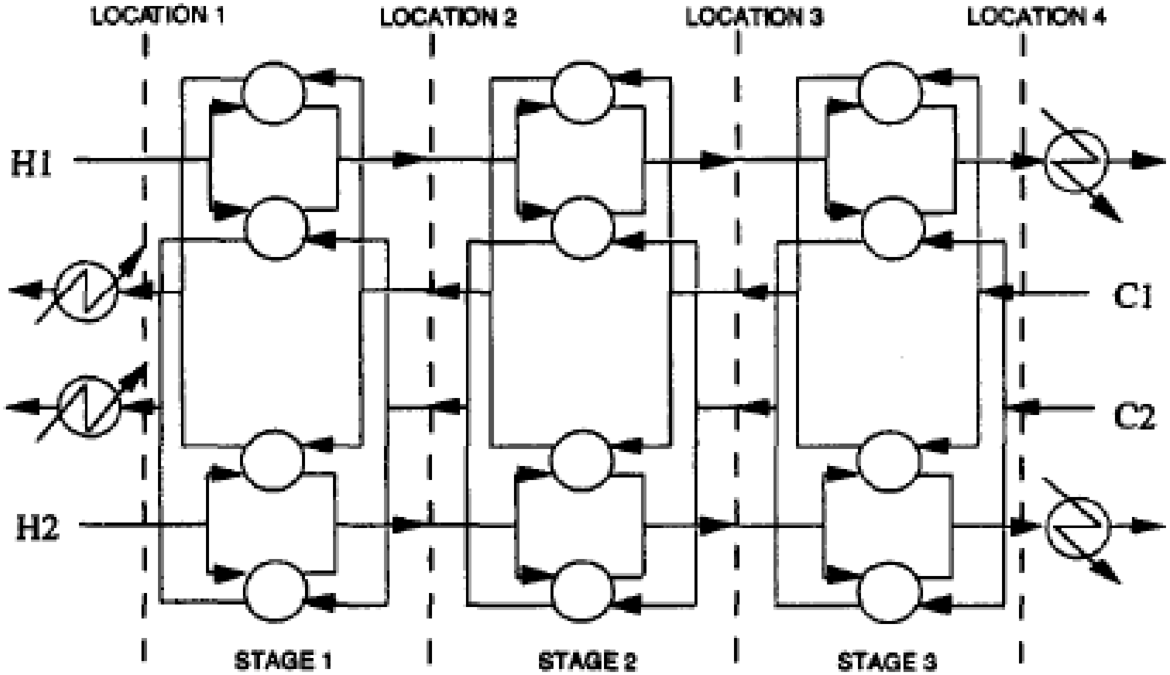
MODEL STATISTICS	
SINGLE VARIABLES	1428
DISCRETE VARIABLES	246
TIME TO REACH A FEASIBLE SOLUTION	40 s
TIME TO REACH GLOBAL OPTIMALITY	260 s

Stages Superstructure Model

Assumptions:

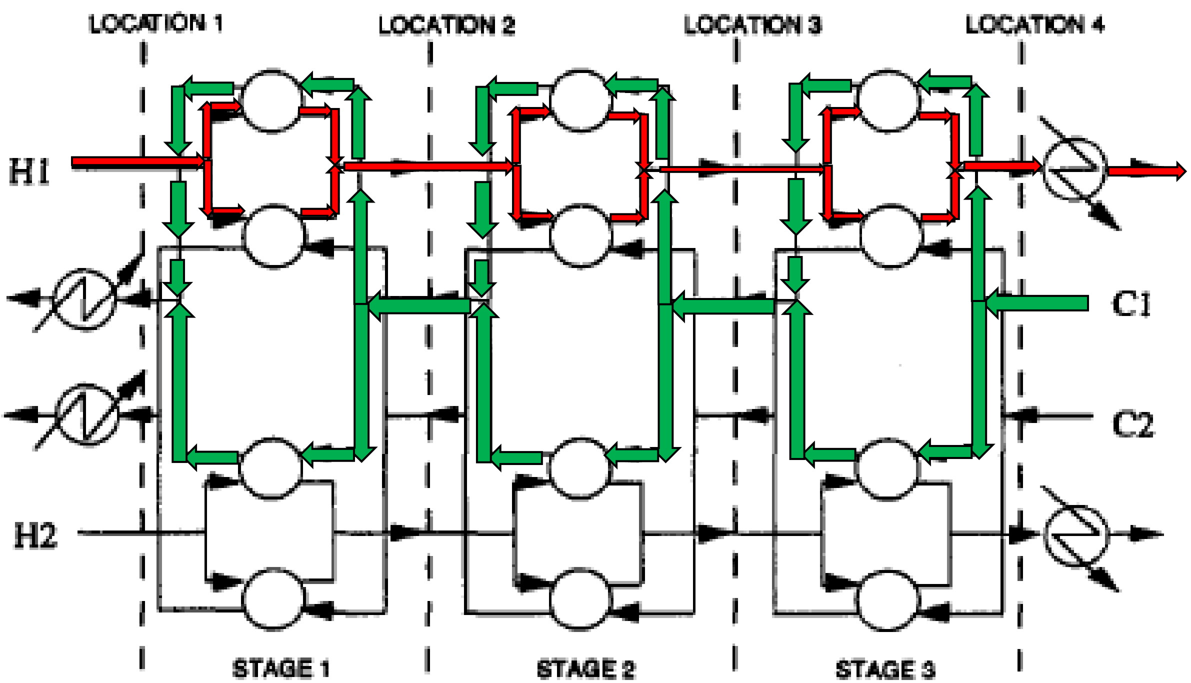
- Heating and cooling takes place at the end.
- Isothermal mixing.

Superstructure for 3 stages, two hot (H1,H2) and two cold (C1,C2) streams



Stages Superstructure Model

At each stage every hot/cold stream splits and matches with all other (cold/hot) stream. H1 and C1 are highlighted



Stages Superstructure Model

Variables

q_{ijk} Heat transferred from hot stream "*i*" to cold stream "*j*" in stage "*k*" . This heat corresponds to an exchanger!!!

$t^{H}_{i,k}$ Temperature of hot stream "*i*" in stage "*k*" (the same for all exits of heat exchangers)

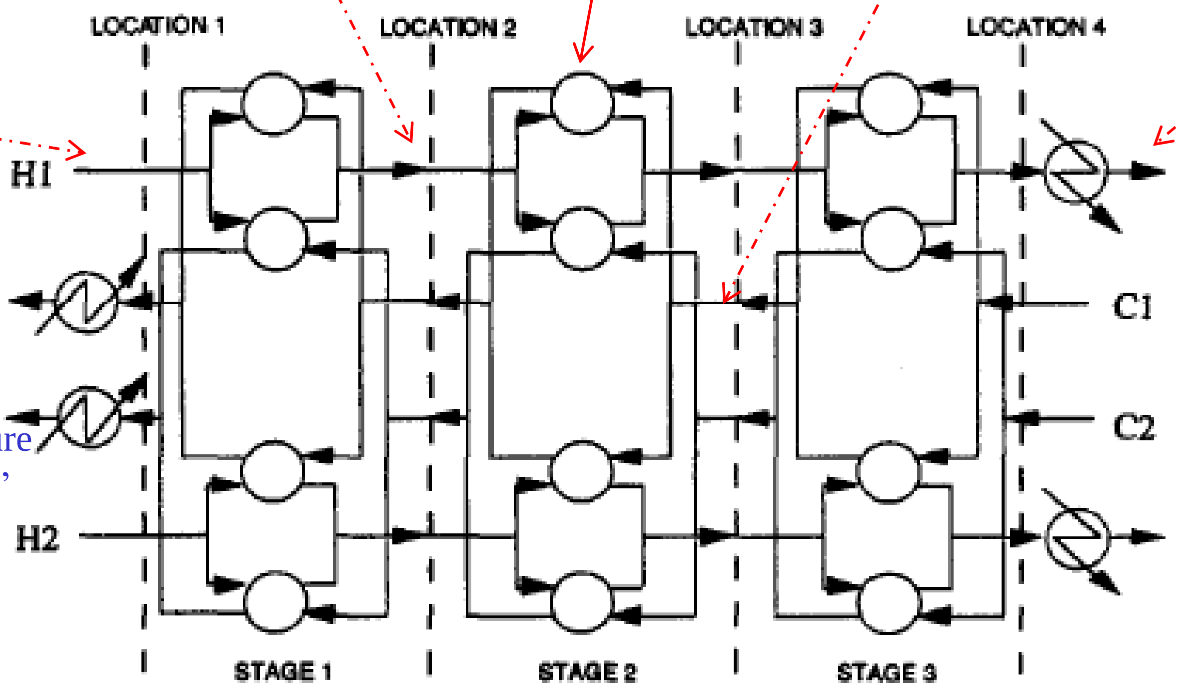
$t^{C}_{j,k}$ Temperature of cold stream "*j*" in stage "*k*" (the same for all exits of heat exchangers)

TIN^{H}_{i} Inlet Temperature of hot stream "*i*" (parameter)

$TOUT^{C}_{j}$ Outlet Temperature of cold stream "*j*" (parameter)

$TOIUT^{H}_{i}$ Outlet temperature of hot stream "*i*" (parameter)

TIN^{C}_{j} Inlet Temperature of cold stream "*j*" (parameter)



Stages Superstructure Model

Overall Heat balance for each stream.

$$(TIN_i^H - TOUT_i^H)F_i^H = \sum_{k \in ST} \sum_{j \in CP} q_{ijk} + qcu_i \qquad i \in HP$$

$$(TOUT_j^C - TIN_j^C -)F_j^C = \sum_{k \in ST} \sum_{i \in HP} q_{ijk} + qhu_j \qquad j \in CP$$

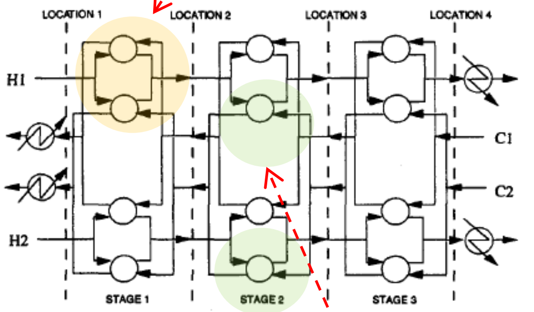
Heat load for utilities

Heat balance at each stage

$$(t_{ik}^H - t_{i(k+1)}^H)F_i^H = \sum_{j \in CP} q_{ijk} \qquad i \in HP, k \in ST$$

$$(t_{jk}^C - t_{j(k+1)}^C)F_j^C = \sum_{i \in HP} q_{ijk} \qquad j \in CP, k \in ST$$

Stage 1 exchangers involved in stage balance for hot stream H1



Stage 2 exchangers involved in stage balance for cold stream C2

Assignment of Superstructure inlet temperatures

$$TIN_i^H = t_{i1}^H \qquad i \in HP$$

$$TIN_j^C = t_{j(NOK+1)}^H \qquad j \in CP$$

NOK is the last stage

Stages Superstructure Model Equations

Feasibility

$$t_{ik}^{H} \geq t_{i(k+1)}^{H} \qquad i \in HP, k \in ST$$

$$t_{jk}^{C} \geq t_{j(k+1)}^{C} \qquad j \in CP, k \in ST$$

$$TOUT_{j}^{C} \geq t_{j,1}^{C} \qquad j \in CP$$

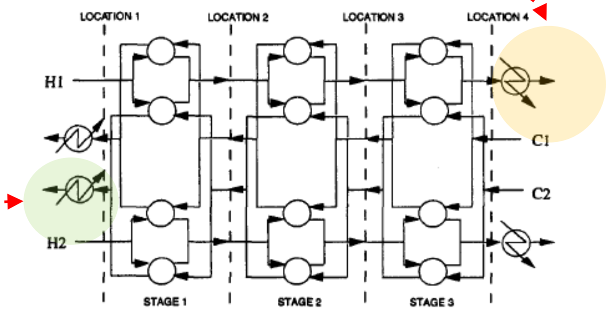
$$TOUT_{i}^{H} \geq t_{i(NOK+1)}^{H} \qquad i \in HP$$

Temperatures decrease from stage to stage

Hot and cold utility load

$$(t_{i(NOK+1)}^{H} - TOUT_{i}^{H})F_{i}^{H} = qcu_{i} \qquad i \in HP$$

$$(TOUT_{j}^{C} - t_{j1}^{C})F_{j}^{H} = qhu_{j} \qquad j \in CP$$



Logical Constraints (to count exchangers)

$$q_{ijk} - \Omega\, z_{ijk} \leq 0 \qquad i \in HP, j \in CP, k \in ST$$

$$qcu_{i} - \Omega\, zcu_{i} \leq 0 \qquad i \in HP$$

$$qhu_{j} - \Omega\, zhu_{j} \leq 0 \qquad j \in CP$$

z_{ijk}, zcu_{i} zhu_{j} are binary variables

$$q_{ijk} > 0 \qquad \Rightarrow z_{ijk} = 1$$

Stages Superstructure Model Equations

Calculation of approach temperatures

$$dt_{ijk} \le t^H_{i,k} - t^C_{j,k} + \Gamma(1 - z_{ijk}) \quad i \in HP, j \in CP, k \in ST$$

$$dt_{ij(k+1)} \le t^H_{i,(k+1)} - t^C_{j,(k+1)} + \Gamma(1 - z_{ijk}) \quad i \in HP, j \in CP, k \in ST$$

$$dtcu_i \le t^H_{i,(NOK+1)} - TOUT_{CU} + \Gamma(1 - zcu_i) \quad i \in HP$$

$$dthu_j \le TOUT_{HU} - t^C_{j,1} + \Gamma(1 - zhu_j) \quad j \in CP$$

When z_{ijk}=1, then $EMAT < dt_{ijk} \le t^H_{i,k} - t^C_{j,k}$ making $t^H_{i,k} - t^C_{j,k}$ positive and bounded from below

Limiting temperature approach

$$dt_{ijk} \ge EMAT \quad i \in HP, j \in CP, k \in ST$$

Objective function (Utility costs+ Fixed HEX installation costs)

$$O = Min\left\{ CCU \sum_{i\in HP} qcu_i + CHU \sum_{j\in CP} qhu_j + \sum_{i\in HP}\sum_{j\in CP}\sum_{k\in ST} CF_{ij}\, z_{ijk} + \sum_{i\in HP} CF_{iCU}\, zcu_i + \sum_{j\in CP} CF_{jHU}\, zhu_j \right\}$$

Notice that one could also add area cost, but the model will be nonlinear

Stages Superstructure Model Equations

- The model is linear
- One can add area cost but then more equations are needed and the model will be nonlinear.
- Using the linear model and varying the weight of the fixed costs, one can obtain solutions exhibiting different energy usage and evaluate them

Stages Superstructure Model

List of parameters and variables

Parameters

TIN = inlet temperature of stream

$TOUT$ = outlet temperature of stream

F = heat capacity flow rate

U = overall heat transfer coefficient

CCU = unit cost for cold utility

CHU = unit cost of hot utility

CF = fixed charge for exchangers

C = area cost coefficient

β = exponent for area cost

NOK = total number of stages

Ω = upper bound for heat exchange

Γ = upper bound for temperature difference

Variables

dt_{ijk} = temperature approach for match (i,j) at temperature location k

$dtcu_i$ = temperature approach for the match of hot stream i and cold utility

$dthu_j$ = temperature approach for the match of cold stream j and hot utility

q_{ijk} = heat exchanged between hot process stream i and cold process stream j in stage k

qcu_i = heat exchanged between hot stream i and cold utility

qhu_j = heat exchanged between hot utility and cold stream j

$t_{i,k}$ = temperature of hot stream i at hot end of stage k

$t_{j,k}$ = temperature of cold stream j at hot end of stage k

z_{ijk} = binary variable to denote existence of match (i,j) in stage k

zcu_i = binary variable to denote that cold utility exchanges heat with stream i