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THE COMPUTER ASSISTED SYNTHESIS FOR OPTIMAL HEAT EXCHANGER NETWORK AT STYRENE POLYMERISATION

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In this paper a synthesis of an optimal heat exchanger network has been studied to realize the required thermal regime at styrene bulk polymerisation in a continuous operation. The synthesis is realized using a method based on the balance calculations, and supposes: the thermal balance over each chemical reactor, the heat exchanger calculations and the determination of the optimal heat exchanger network. The calculation of the heat exchangers involves the selection of the exchanger type, the choice of the thermal agents and the cost calculation. The optimal heat exchanger network can be obtained by selecting the heat exchanger for each reactor, which corresponds to the technological criterions and has the minimum total cost.

Key words: heat exchanger, network synthesis, styrene polymerisation, and thermal regime

Introduction

The heat exchanger network synthesis has two main objectives: the determination of the maximum heat amount which can be recovered from process, respectively, the obtaining of the heat exchanger network realizing the minimum cost.

The synthesis of the heat exchanger networks is the well-tested problem from those of the synthesis of different subsystems, like separation sequence synthesis or reactor systems. Gundersen and Naess [1], in an ample detailed review, note more than 200 papers in this field. Further, Gundersen [2] is referring at 30 papers on the same topic. Jezowski [3, 4] presents and analyses 142 works for the synthesis of heat exchanger networks. Recently, some papers present synthesis methods for retrofitting flexible or multi-period heat exchanger networks [5] and, respectively, heat exchanger networks under uncertainty [6]. In order to systematize such a literature, the available synthesis methods of heat exchanger networks are classified in two groups: methods based on the balance calculation and methods using the optimising techniques.

The methods using the optimising techniques solve the heat exchanger network synthesis problem like a formal optimising problem, by mathematical instruments, while the methods based on the balance calculation avoid the mathematical techniques and involve the knowledge of the problem, the thermodynamics laws and the logical judgments.

In this work, a method based on balance calculation for synthesizing optimal heat exchanger networks is presented. The method is applied to the optimal heat exchanger network synthesis which realizes the required thermal regime at the styrene bulk polymerisation in a continuous operation.

The optimal heat exchanger network, by its capacity and thermal regime, belongs to a system containing an optimal industrial reactor network. The realization of the pre-established thermal regime, during the styrene bulk polymerisation, is a very difficult problem, which is unsolved yet. The difficulty is due to a very complicated reaction system having a large number of reaction components and reactors. To those, the special behaviour of the polymer during polymerisation must be added, when the conversion and temperature is changing. The temperature increase complicates the problem because of strong exothermal reaction and its influence upon the polymer properties.

From the above considerations, it results the necessity of an optimal system synthesis of heat exchangers to realize the required thermal regime for the polystyrene production.

The synthesis algorithm supposes the thermal balance over each reactor, the calculation of the heat exchangers and the determination of the optimal heat exchanger network. This algorithm was implemented in MathCAD 2000 Professional. In the modelling and in the optimisation of the heat exchangers, all required parameters have been established. The optimal heat

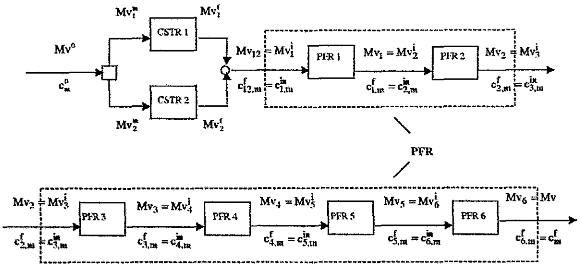


Fig.1 Reactor network for polystyrene production by bulk polymerisation

exchanger network for the styrene polymerisation has been obtained taking into consideration the technical and economical criterions, the technical criterions are the most important. For given initial conditions and specified thermal regime, the optimal network contains five coil heat exchangers. The results of the system synthesis of heat exchangers attest the viability of the optimal reactor network obtained preliminarily for polystyrene production, in which the thermal regime problem was solved.

Problem formulation

The optimal heat exchanger network has been synthesized on an optimal reactor network, obtained also by computer assisted synthesis [7]. This network is presented in *Fig.1*.

The considered reactor network represents an industrial system, it produces 2000 polystyrene tones /year. The thermal regime is in the 80 °C – 200 °C range, according to the production scale technologies [8, 9].

The reactor network for the styrene bulk polymerisation, in a continuous system, contains eight reactors, working in isothermal conditions, as follows:

- Two continuous stirred tank reactors, CSTR1 and CSTR2, with parallel connection, operate at 80°C. These provide the required capacity of the polymerisation system.
- Other six plug flow reactors (PFR) provide the required conversion, of 97%, and 641 numerical average polymerisation degrees. These operate in isothermal conditions for temperatures of 100°C for PFR1 and PFR2, 150°C for PFR3, 180°C for PFR4 and PFR5, and 200°C for PFR6.

In the specified conditions, the problem solved in this paper is formulated as follows: one gives the reaction mixture containing styrene, polystyrene and initiating agent, each one having a specified initial temperature, the required exit temperature, the specific heat and the flow rate and, also, a set of thermal agents for heating and cooling and their properties (enthalpies, working temperature). The heat exchanger network bringing the reaction mixture at desired temperature is synthesizing and the annual cost for operating and investment charge is minimizing.

Since the reaction mass follows a pre-established way by the reactor network, the heating or cooling is realized only with thermal agents who can be associated between them.

Synthesis algorithm

The synthesis problem is decomposed in sub-problems treating each reactor with a distinct thermal regime. As long as, both of the continuous stirred tank reactors for pre-polymerisation (*Fig.1*) work in the same condition regarding feed and temperature, it is enough a single calculation. Also, the plug flow reactors working in the same conditions, in a series arrangement, it can be considered as a single reactor. Thus, one treats together the plug flow reactors, PFR1 and PFR2, working at 100°C, and PFR4 and PFR5 working at 180°C. For each considered reactor, the design calculation of the heat exchangers realizes the required heat transfer using the available thermal agents. The agent can be at its first use or can be a thermal agent which was heated /cooled in other heat exchanger, by taking-up or transfer of the excess heat of the reaction mass from other reactor.

From the above considerations, it results that the algorithm of the optimal heat exchanger network synthesis has the following steps:

- *The effectuation of the thermal balance* over each reactor in order to determine the needed heat to be transferred and the sense of the heat transfer leading to heating or cooling of the reaction mass.
- *The calculation of the heat exchangers* involving the selection of the heat exchanger and of the thermal agents, taking into account the technological characteristics of the polymerisation and the heat amount to be transferred. For the selected heat exchangers, one calculates the flow rate, the overall heat transfer coefficient, the heat transfer surface area and the coil length. Finally, for one year operation (8000 hours), the cost of the heat exchangers and of the thermal agents is calculated.
- *The determination of the optimal heat exchanger network* consisting in the selection, for each reactor, of the heat exchanger which respects the technological criterions and has the minimum total cost (operating cost and investment charge). The obtained network by the *interconnection* of the selected heat exchangers is the network realizing the required thermal regime for a total minimum cost and, consequently, this is the optimal network.

Thermal balance over reactors

The thermal balance has been realized over each reactor having a distinct thermal regime in the polymerisation system. One considers the steady state. The energy conservation law is: the amount of inlet heat plus the generated heat are equal to the outlet heat.

Table 1 Reactor network characteristics for polystyrene production by bulk polymerisation

Reactor position in the network	Inlet flow for reactor	Outlet flow for reactor	Average concentration on reactor								Conversion degree in the j reactor	Final conversion degree
	Mv^i_j (l/s)	Mv_j (l/s)	$c_{j,1}$ (mol/l)	$c_{j,2}$ (mol/l)	$c_{j,3,0}$ (mol/l)	$c_{j,3,1}$ (mol/l)	$c_{j,3,2}$ (mol/l)	$c_{j,4,0}$ (mol/l)	$c_{j,4,1}$ (mol/l)	$c_{j,4,2}$ (mol/l)	X_j	X_f
1	3.9×10^{-2}	0.110	7.187	5.285×10^{-3}	9.69×10^{-9}	1.96×10^{-5}	7.91×10^{-2}	4.72×10^{-3}	0.522	3.01×10^{3}	0.350	0.350
2	3.9×10^{-2}	0.110	7.187	5.285×10^{-3}	9.69×10^{-9}	1.96×10^{-5}	7.91×10^{-2}	4.72×10^{-3}	0.522	3.01×10^{3}	0.350	0.350
3	0.110	0.126	5.19	8.638×10^{-4}	6.875×10^{-9}	1.79×10^{-5}	0.104	5.1×10^{-3}	0.588	3.88×10^{3}	0.166	0.458
4	0.126	0.141	4.25	3.99×10^{-5}	5.515×10^{-9}	1.655×10^{-5}	0.106	5.265×10^{-3}	0.558	6.05×10^{3}	0.199	0.566
5	0.141	0.152	3.31	1.05×10^{-6}	7.035×10^{-9}	1.65×10^{-5}	0.078	4.765×10^{-3}	1.335	8.825×10^{3}	0.248	0.674
6	0.152	0.167	2.205	3.735×10^{-10}	7.12×10^{-9}	1.38×10^{-5}	0.055	4.84×10^{-3}	2.065	1.18×10^{4}	0.449	0.820
7	0.167	0.255	1.112	1.195×10^{-9}	7.07×10^{-9}	1.375×10^{-5}	0.055	4.08×10^{-3}	2.265	1.185×10^{4}	0.583	0.925
8	0.255	0.465	0.458	2.39×10^{-9}	7.00×10^{-9}	1.365×10^{-5}	0.055	2.595×10^{-3}	1.61	8.225×10^{3}	0.600	0.970

For a *j* reactor, the inlet heat is the sum of the reaction mixture heat and polymerisation reaction heat (strong exothermal, ΔH=671,238 J/kg [10]).

Inlet heat in *j* reactor:

$$Q^i_{st,j} = Mw_{st} \cdot cp_{st,j} \cdot t^i_j \tag{1}$$

$$Q^i_{pst,j} = Q^e_{pst,j-1} \tag{2}$$

$$Q^i_{pob,j} = Mw_{pob} \cdot cp_{pob,j} \cdot t^i_j \tag{3}$$

$$Qr_j = Mw_{st} \cdot \left(X_j - X_{j-1} \right) \cdot \Delta H \tag{4}$$

Outlet heat from *j* reactor:

$$Q^e_{st,j} = Mw_{st} \cdot \left(1 - X_j \right) \cdot t^e_j \tag{5}$$

$$Q^e_{pob,j} = Mw_{pob} \cdot cp_{pob,j} \cdot t^e_j \tag{6}$$

$$Q^e_{pst,j} = Mw_{st} \cdot X_j \cdot cp_{pst,j} \cdot t^e_j \tag{7}$$

The transferred heat is:

$$Q^{tr}_j = \left| Q^i_j - Q^e_j \right| \tag{8}$$

Obviously, for $Q^i_j > Q^e_j$ it is necessary the cooling, and for $Q^i_j < Q^e_j$ the heating of the reaction mass.

The thermal balance over the reactors of the optimal synthesis network for the polystyrene production by bulk polymerisation has been realized by the *Eqs.(1)-(8)*. For the first reactor, the heat losses have not been considered because these favour the cooling. For the other reactors, the heat losses have been 1% of the inlet heat. The flow of the reaction mass components and the conversion of each reactor are presented in *Table 1*. The specific heats for the inlet and outlet streams were taken from the available literature [10, 11].

The results of the thermal balance over the optimal reactor network for the styrene bulk polymerisation are presented in *Table 2*.

Table 2 Thermal balance results over each reactor of the network for polystyrene manufacturing by bulk polymerisation

Reactor	Inlet heat (W)	Outlet heat (W)	Transferred heat (W)	Sens of the heat transfer
CSTR working at 80°C	$9.45\cdot10^{3}$	$4.97\cdot10^{3}$	$4.48\cdot10^{3}$	Cooling
CSTR working at 80°C	$9.45\cdot10^{3}$	$4.97\cdot10^{3}$	$4.48\cdot10^{3}$	Cooling
PFR working at 100°C	$2.03\cdot10^{4}$	$1.25\cdot10^{4}$	$7.76\cdot10^{3}$	Cooling
PFR working at 150°C	$1.78\cdot10^{4}$	$2.05\cdot10^{4}$	$2.77\cdot10^{3}$	Heating
PFR working at 180°C	$3.27\cdot10^{4}$	$2.95\cdot10^{4}$	$3.18\cdot10^{3}$	Cooling
PFR working at 200°C	$3.19\cdot10^{4}$	$3.39\cdot10^{4}$	$1.98\cdot10^{3}$	Heating

Heat exchangers calculation

The selection of the heat exchangers and of the thermal agents is based on the thermal balance results.

Due to the difficulty of the heat transfer between the reaction mass and the thermal agent, the coil heat exchangers have been considered. Because the heat amount transferred into the reactor network is small, a jacket heat exchanger is not necessary.

Since the reaction mass has a very high viscosity in the last reactor (PFR6), the Reynolds number is small and the heat transfer rate is reduced, therefore electrical heating has been chosen.

In the continuous stirred tank reactors, being connected in parallel, the temperature is 80 °C, one can use water of different temperatures as cooling agent. For the variants with high outlet water temperatures from reactors, for instance, 50°C for inlet temperature and 60°C for outlet temperature, even if the water consumption is larger and the coil length is also larger, there is the advantage of a small temperature variation into the reaction mass and its properties are unchanged.

In the plug flow reactors PFR1 and PFR2, the inlet temperature of the reaction mass is 80°C and outlet temperature is 100°C. Consequently, the cooling agent for reaction mass is the water with different temperatures.

The plug flow reactor working at 150°C (PFR3), according to the thermal balance, needs the heating. As

Table 3 The calculation results for the heat exchanger design realizing the needed thermal regime in a CSTR

Thermal agent	Inlet temperature (^0C)	Outlet temperature (^0C)	Transferred heat (W)	Overall heat transfer coefficient $(W/m^2 \cdot K)$	Mass flow rate of thermal agent (kg/s)	Heat transfer surface area (m^2)	Coil length (m)	Total annual cost (u.c.)
Cooling water	15	30	$4.48 \cdot 10^3$	638.1	0.0713	0.359	7.15	$4.11 \cdot 10^8$
	15	40		536.1	0.0428	0.497	9.86	$2.47 \cdot 10^8$
	25	40		676.0	0.0713	0.395	7.85	$4.11 \cdot 10^8$
	25	50		565.7	0.0428	0.568	11.3	$2.47 \cdot 10^8$

heating agent steam of different pressures or Dowtherm A is used.

The plug flow reactors (PFR4 and PFR5) working at 180 °C, needs cooling. Due to the high temperatures, one proposed boiling water under pressure of 1 bar or 2 bar, as cooling agent.

Conclusively, for each reactor from the synthesis network, the amount of heat to be transferred, the heat exchanger type and the available thermal agents have been established.

Hereinafter, for each reactor, the needed thermal agent flow rate, the overall heat transfer coefficient, the heat transfer surface area, the coil length and the total cost have been calculated.

Investment charge can be calculated with the relation:

$$C_j = \alpha \cdot A^{\beta} \tag{9}$$

where A is the heat transfer surface area, α and β are specific constants for the heat exchanger type: α =145 and β=0,65-0,95 [12, 13].

The operating cost is $CO_j = Mw \cdot cu \cdot nh$, where *cu* represents the unit cost for the thermal agent and *nh*=8000 the hours number of operating a year.

Therefore, the total cost for thermal transfer to realize the needed isothermal regime into reactor is:

$$CT_j = C_j + CO_j \tag{10}$$

Table 3 presents the calculation results for the heat exchanger design using water of different temperatures, in order to realize and maintain the constant temperature of 80 °C, of the stirred tank reactor.

The plug flow reactors working at 100 °C (PFR1 and PFR2), based on the thermal balance result, both need the cooling of the reaction mass (*Table 2*). To this goal, the water with different inlet/outlet temperatures has been chosen. Being that, from stirred tank reactors results water of 40 °C and 50 °C (*Table 3*). This can be used for the reaction mass cooling from the plug flow reactors working at 100 °C.

The overall heat transfer coefficient K_{PFR12} has been calculated as function of individual heat transfer coefficient and thermal resistance of the wall. The calculation of the individual heat transfer coefficient was made using the relations obtained from literature [11-14].

Table 4 The needed characteristics for the heat exchanger design realizing the needed thermal regime in the PFR 1 and PFR 2

Thermal agent	Inlet temperature (^0C)	Outlet temperature (^0C)	Transferred heat (W)	Overall heat transfer coefficient $(W/m^2 \cdot K)$	Mass flow rate of thermal agent (kg/s)	Heat transfer surface area (m^2)	Coil length (m)	Total annual cost (u.c.)
Cooling water	15	30	$7.76 \cdot 10^3$	139.1	0.125	0.835	8.86	$7.20 \cdot 10^8$
	15	40		131.0	0.075	0.994	10.54	$4.32 \cdot 10^8$
	20	30		143.5	0.189	0.851	9.03	$1.09 \cdot 10^9$
	20	40		136.1	0.094	0.961	10.19	$5.41 \cdot 10^8$
	25	40		140.9	0.126	0.975	10.34	$7.26 \cdot 10^8$
	25	50		134.8	0.075	1.108	11.76	$4.32 \cdot 10^8$
	40	60		140.4	0.095	1.382	14.97	$5.47 \cdot 10^8$
	50	70		140.3	0.095	1.892	20.08	241.49

The needed characteristics for the heat exchangers design are presented in *Table 4*, for different cooling water types.

The thermal balance over PFR3 working at 150 °C, showed that, for a good polymerisation, it is needed to supply a heat amount of $2{,}77 \cdot 10^3$ W. To this aim, the proposed thermal agent is either steam with different temperatures or liquid Dowtherm A.

The steam flow for the heating of the reaction mass has been obtained as function of needed heat amount for the heating and steam characteristics.

In the following, the individual heat transfer coefficient for the reaction mass was calculated. The reaction mass properties were taken from literature [10], at average temperature in the reactor working at 90 °C, for a conversion degree of 67, 4%.

In these conditions, the laminar regime was obtained with very low Re_{PFR3} = 5.55. This allows considering the free convection.

Because the heat transfer coefficient for steam, used as heating agent, is much higher than that for the reaction mass, the thermal resistance for steam can be neglected.

When Dowtherm A is used as thermal agent, the thermal resistance can be also neglected.

For the required heat transfer realization, the overall transfer coefficient, the thermal transfer surface area, the coil length and the total length have been calculated. The obtained results are presented in *Table 5*.

The plug flow reactors PFR4 and PFR5 work at 180°C. The thermal balance shows that the elimination of the heat from the inside reactors is necessary, for both, $Q^{tr}_{PFR45} = 3.18 \cdot 10^3$ W. The thermal agent was the water under pressure, so that by its evaporation, the water takes up a large amount of heat. The properties of the water under pressure were taken from [11].

For the overall heat transfer coefficient determination, the individual heat transfer coefficient of the reaction mass was calculated, $\alpha_{mrPFR45}$= 147.14 W $m^{-2}K^{-1}$. The reaction mass properties are taken from [10] for 92.5 % conversion degree.

Table 5 The calculation results for the heat exchanger design realizing the needed thermal regime in the PFR3

Thermal agent	Inlet temperature (^{0}C)	Outlet temperature (^{0}C)	Transferred heat (W)	Overall heat transfer coefficient $(W/m^2{\cdot}K)$	Mass flow rate of thermal agent (kg/s)	Thermal transfer surface area (m^2)	Coil length (m)	Total annual cost (u.c.)
Steam	6	158.1	1.32	$2.77{\cdot}10^3$	138.818	0.57	6.04	$3.04{\cdot}10^7$
	7	164.2	1.33		138.818	0.51	5.39	$3.06{\cdot}10^7$
	8	170	1.35		138.818	0.44	4.70	$3.11{\cdot}10^7$
	9	175	1.36		138.818	0.40	4.27	$3.13{\cdot}10^7$
	10	179	1.37		138.818	0.37	3.92	$3.16{\cdot}10^7$
Dowtherm A	1.2	190	8.78		133.268	0.32	3.39	$1.01{\cdot}10^9$
	1.5	225	9.19		133.268	0.21	2.20	$1.06{\cdot}10^9$

Also, here the heat transfer coefficient for the water, boiling under pressure in the coil is much larger than that of the reaction mass and its value was admitted.

The calculation results for PFR4 and PFR5, including the total costs of the required heat transfer, are presented in *Table 6*.

One can assert that, for all considered reactors, the thermal resistance has the largest value for the reaction mass.

Because the last reactor (PFR6) uses electrical heating, the heat calculation cannot be any more the objective for the heat transfer optimisation.

Determination of the optimal heat exchanger network

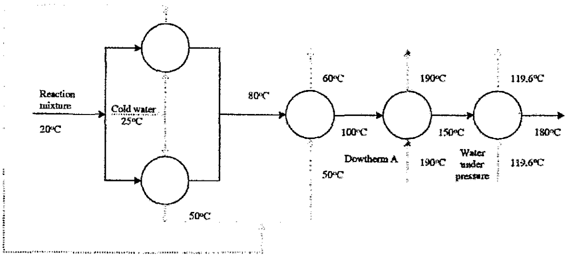
The heat exchangers realizing the required thermal transfer for each considered reactor have been chosen from the lists presented in *Tables 3, 4, 5* and *6*. For selection, the technological criterions had the maximum importance. Hereby, the temperature variations, larger than 10°C for the reaction mass, have not been accepted. Consequently, for instance, the cooling water had a higher input temperature. Also, for heating, when the thermal agent can be the steam or Dowtherm A, the Dowtherm A was chosen because this can provide a higher temperature, and, finally the required quality of the reaction mass. In the same sense, a thermal agent has been recycled even if the heat transfer surface area has been larger and, thereafter, the investment charge (heat exchanger) has been higher, due to the driving force decrease. From technological point of view, the recycling was preferred because the operating expenses have to be reduced.

The economical criterions, given by the total cost for the thermal transfer, have been used for the thermal agents' selection.

The heat exchangers and the corresponding thermal agents have been selected on the above criterions and composed the optimal heat exchanger network, because this realizes the required thermal regime under adequate technological conditions with minimum cost.

Table 6 The calculation results for the heat exchanger design realizing the needed thermal regime in the PFR 4 and PFR 5

Thermal agent	Inlet temperature (^{0}C)	Outlet temperature (^{0}C)	Transferred heat (W)	Overall heat transfer coefficient $(W/m^2{\cdot}K)$	Mass flow rate of thermal agent (kg/s)	Thermal transfer surface area (m^2)	Coil length (m)	Total annual cost (u.c.)
Water under pressure	1	99.1	0.00141	$3.179{\cdot}10^3$	120.95	0.399	4.23	$1.62{\cdot}10^7$
	2	119.6	0.00144		111.96	0.625	6.64	$1.66{\cdot}10^7$



Cost of optimizated network: $1.26{\cdot}10^9$ u.c.

*Fig.*2 Optimal heat exchanger network for polystyrene manufacturing by bulk polymerisation

The described synthesis algorithm has been implemented in MathCAD 2000 Professional. The synthesized optimal heat exchangers network is presented in *Fig.2*.

For the initial conditions and the specified thermal regime, the network contains five coil heat exchangers, as following:

- Two heat exchangers realize the required isothermal regime (80°C) in the continuous stirred tank reactor (CSTR1 and CSTR2). These are using the cooling water as thermal agent having 25°C inlet temperature and 50°C outlet temperature.
- For the PFR1 and PFR2 requiring an isothermal regime at 100°°C, a heat exchanger recycling the resulted water from CSTR1 and CSTR2, having 50°C temperature has been used. The outlet water temperature is 60°C.
- PFR3 works at 150°C. The corresponding heat exchanger uses Dowtherm A at 190°C.
- The last heat exchanger, using cooling water at 2 bar pressure, realizes the isothermal regime, at 180°C, in PFR4 and PFR5.

One asserts that the optimal heat exchanger network cannot use the heat of the reaction mass because this has a pre-established way which cannot be modified. Also, the single thermal agent enabling the recycling was the cooling water which results from CSTR1 and CSTR2.

Conclusions

The optimal heat exchanger network realizing the required thermal regime for the reactor system at styrene production, by bulk polymerisation in a continuous system has been determined by the computer assisted synthesis. The considered system has industrial capacity and operates at the thermal regime for commercial scale. Firstly, the synthesis method supposes the thermal balance effectuation over each reactor having a distinct thermal regime. Then, the heat exchangers have been calculated and the optimal heat exchanger network has been determined.

The accurate analysis of the technological process and of the offered possibilities by system calculation allows solving the problem under optimal technological and economical conditions. The proposed heat exchanger network realizes the pre-established thermal regime under given conditions and for a minimum cost. This shows that the reactor network can be used in a practical application.

We notice that the proposed synthesis method is efficient but depends on the designer experience in the field. The designer establishes the type exchangers, the thermal agents and the accepted temperature difference, based on the knowledge of the technological process.

In the issue, the utilized synthesis method is recommended for the approached problem type of synthesis – the realizing of thermal regime for the manufacturing of the reaction mass in a known reactor network. The problem appears frequently in the industrial chemical processes and, especially, in the polymerisation process, which are strongly exothermic.

SYMBOLS

j	index for reactors
$Q^i_{st,j}$	inlet styrene heat in the j reactor, W
$Q^i_{pst,j}$	outlet polystyrene heat in the j reactor, W
$Q^i_{pob,j}$	inlet initiating agent in the j reactor, W
Mw_{st}	styrene mass flow rate, kg/s
Mw_{pob}	initiating agent mass flow rate, kg/s
$cp_{st,j}$	styrene specific heat capacity at the inlet/outlet styrene temperature, for j reactor, J/(kg·K)
$cp_{pob,j}$	specific heat capacity of the initiating agent at the inlet/outlet temperature for j reactor, J/(kg·K)
t^i_j	inlet reaction mass temperature for j reactor, °C
X_j, X_{j-1}	monomer conversion degree in j/j-i reactor
ΔH	polymerisation heat, J/kg
Qr_j	reaction heat in the j reactor, W
$Q^e_{st,j}$	outlet styrene heat for reactor j, W
$Q^e_{pst,j}$	outlet polystyrene heat for j reactor, W
$Q^e_{pob,j}$	outlet initiating agent heat for j reactor, W
t^e_j	outlet temperature for j reactor, °C
Q^i_j	inlet heat for j reactor, W
Q^e_j	outlet heat for j reactor, W
Q^{tr}_j	transferred heat for j reactor, W
A	thermal transfer surface area, m^2
C_j	investment charge for j reactor, u. c.
CO_j	operating cost for j reactor, u.c.
M_w	mass flow of thermal agent, kg/s
uc	unit cost of the thermal agent, u.c.
nh	hours number of operating a year
CT_j	total cost of the thermal transfer for j reactor, u.c.
α, β	specific constants for the heat exchanger type
CSTR	Continuous Stirred Tank Reactor
PFR	Plug Flow Reactor

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