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# Purification of Phenol from Hydroxyacetone and 2-Methylbenzofuran by Rectification

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**Abstract**—This paper presents structural relationships of phase equilibrium diagrams and azeotropic properties, and resulting evaluation of optimum process conditions for removal of hydroxyacetone (HA) and 2-methylbenzofuran (2-MBF) from phenol. It is demonstrated that the concentration region of HA separation from phenol is absolutely different from that for 2-MBF, which makes the task of HA and 2-MBF removal from phenol by distillation requiring installation of at least two highly selective extractive distillation columns operating with significant steam consumption.

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The advent about 20 years ago of various types of carbonate plastics produced by the phenol/acetone process has generated the demand for high-purity phenol.

To attain conditions meeting requirements for the extra quality phenol (so-called "carbonate purity") and to remove from phenol two key admixtures: hydroxyacetone (HA) and 2-methylbenzofuran (2-MBF), it proved necessary to complicate the traditional rectification scheme by introducing two azeotropic extractive rectification columns and installing more efficient plates in a series of columns. These measures allowed to solve, while not cardinally, the problem of purification from HA and 2-MBF: Phenol of required quality is manufactured at most enterprises, but it is too expensive; moreover, the quality of the product is unstable and deteriorated by any deviations in the composition of product flows delivered to separation.

The above circumstances forced researchers to search for approaches to cardinally solving the problem of phenol purification. In essence, this means to decide between two ways to further enhancing the efficiency of distillation columns: complication of rectification scheme and prevention of 2-MBF formation in a catalytic phenol purification unit (chemical purification).

In the present paper we focus on the first approach, specifically phenol purification by rectification. Correct analysis of the reasons for inefficient operation of the rectification unit required detailed research into the phase equilibria in HA–water, HA–phenol, HA–$\alpha$-methylstyrene (AMS), and HA–cumene systems and azeotripic properties. The results of earlier studies of some of the mentioned systems in a narrow concentration range satisfied neither researchers nor practical people, since, first, they failed to explain the reasons for deterioration of phenol quality and, second, contradicted the practice of exploitation of separation columns for the products in question. The results of our present work give insight into a whole series of previously unclear facets of the rectification stage.

## Physicochemical Properties of Systems Containing HA and 2-MBF

### *Critical literature Review*

Linek and Wichertle [1] have studied the phase equilibria in HA–water, HA–phenol, HA–AMS, and HA–cumene systems at HA concentrations higher than 0.4 wt %. In this HA concentration range, one cannot determine whether the systems exhibit azeotropic properties and, as a consequence, to reveal thermodynamic and topologic characteristics of the liquid–vapor equilibrium diagrams and the distillation lines. Furthermore, in [1] substances of 95–98 wt% purity were used; the equilibrium phases in systems with a very low concentration of one of the components were analyzed by refractometry and densimetry, and the

**Table 1.** Physicochemical characteristics of compounds studied

| Component | $n_D^{20}$ | bp, °C | $d_4^{20}$, g cm$^{-3}$ |
|---|---|---|---|
| Phenol | 1.5426 | 181.8 | 1.063 |
| AMS | 1.5437 | 165.4 | 0.913 |
| Cumene | 1.4915 | 152.4 | 0.862 |
| HA | 1.4295 | 145.5 (decomp.) | 1.082 |
| 2-MBF | 1.5495 | 197.5 | 1.054 |

concentration range studied allowed no thermodynamic consistency testing of the resulting data; consequently, they may involve considerable errors.

Aristovich et al. [2] reported phase equilibrium data water–HA and phenol–HA–water systems, but did not studied phenol–HA phase equilibria and made use of old, unreliable, and unchecked azeotropic characteristics for constructing phase diagrams for phenol–AMS and water–AMS binary systems [3–5]. As a result, the structure of fields and distillation lines in the diagrams for phenol–HA–water and phenol–AMS–water ternary systems and, consequently, wrong conclusions as to the conditions for separation of pure phenol from its mixture with water, HA, and AMS. Based on the results of the research on rectification purification of phenol from HA, reported in [2], maintenance people can choose wrong operational conditions for isolation of pure phenol.

Phase equilibrium data for systems containing 2-MBF were lacking from the literature, which prevented correct calculation of industrial columns.

### *Experimental Conditions and Characteristic of Substances Used*

In the present work, aiming at determining conditions for purification of phenol from HA and 2-MBF, we have studied liquid–vapor phase equilibria in HA–water, HA–phenol, HA–AMS, and HA–cumene at 0.2 atm, azeotropic properties of binary and ternary mixtures in the phenol–AMS–HA–water systems at 0.2 and 1 atm, as well as phase equilibria in 2-MBF–water, 2-MBF–phenol, 2-MBF–AMS, 2-MBF–cumene mixtures at 1 atm. In [6] we already showed that it is systems containing cumene, AMS, water, and phenol, whose study is necessary to develop theoretical principles of purification of phenol from HA and 2-MBF.

It experiments we used specially purified materials. Their physicochemical characteristics are presented in Table 1. The purity was controlled by the refractive index $n_D^{20}$, boiling point, density $d_4^{20}$, and chromatography.

Liquid–vapor equilibria in homogeneous mixtures were studied on a modified Gillespie device [4] and in heterogeneous mixtures, on a Sventoslavskii ebulliometer [4]. Azeotropic properties of heterogeneous mixtures were studied by the rectification method. A rectification column with an efficiency of 30 TP, connected with a monostator [7, p. 492] and equipped with a modified head for collecting a stratifying vapor condensate. For the still liquor to boil uniformly, magnetic stirring was applied. The collected vapor condensate was homogenized with isopropanol.

The compositions of equilibrium phases were determined by chromatography. The HA-containing mixtures were analyzed using a glass packed column. The relative error was no larger than 2%.

Since HA decomposes above 145°C, phase equilibria in binary systems were determined at the pressure 0.2 atm, at which the temperature of the mixtures was no higher than 135°C. In view of the fact that commercial phenol is most commonly isolated at a nearly atmospheric pressure, the azeotropic properties of HA-containing mixtures were also additionally studied at atmospheric pressure.

### *Experimental Data on Phase Equilibria*

The liquid–vapor equilibrium data that can be used to determine conditions for purification of phenol from HA and 2-MBF are listed in Tables 2 and 3. Correctness of these data was tested for thermodynamic consistency by the Redlich–Kister method [8].

All the HA-containing systems studied are homogeneous, and the phase equilibrium data for them point to:

– lack of azeotropes in the HA–water system;

– presence of positive azeotropes (with a minimum point) in the HA–AMS and HA–cumene systems;

– presence of a negative azeotrope (with a maximum boiling point) in the phenol–HA system.

The compositions of azeotropic mixtures of minimum boiling points were confirmed additionally by rectification on a 30-TP column.

**Table 2.** Liquid–vapor phase equilibria in HA-containing binary systems at 0.2 atm

| Luquid composition, $X_1$, mol % | System | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | HA (**1**)–cumene (**2**) | | HA (**1**)–α-methylstyrene (**2**) | | HA (**1**)–phenol (**2**) | | HA (**1**)–water (**2**) | |
| | $T_b$ mixture, °C | Vapor composition, $Y_1$, mol % | $T_b$ mixture, °C | Vapor composition, $Y_1$, mol % | $T_b$ mixture, °C | Vapor composition, $Y_1$, mol % | $T_b$ mixture, °C | Vapor composition, $Y_1$, mol % |
| 0.00 | 99.07 | 0.000 | 111.50 | 0.00 | 131.84 | 0.00 | 60.02 | 0.00 |
| 4.40 | | | | | 133.00 | 4.40 | | |
| 10.00 | 86.35 | 42.45 | 103.90 | 30.86 | 132.80 | 11.89 | 60.85 | 3.95 |
| 20.00 | 84.25 | 47.70 | 99.52 | 46.62 | 131.20 | 28.96 | 61.72 | 5.91 |
| 30.00 | 83.92 | 48.20 | 96.85 | 56.04 | 128.00 | 55.00 | 62.81 | 7.68 |
| 40.00 | 83.82 | 48.50 | 95.24 | 62.14 | 125.00 | 70.00 | 64.36 | 9.87 |
| 48.50 | 83.80 | 48.50 | | | | | | |
| 50.00 | 83.80 | 48.50 | 94.33 | 66.29 | 120.00 | 81.80 | 66.57 | 12.94 |
| 60.00 | 83.85 | 48.55 | 93.89 | 69.23 | 115.00 | 89.00 | 69.61 | 17.47 |
| 70.00 | 84.00 | 48.70 | 93.73 | 71.54 | 110.50 | 93.66 | 73.72 | 24.43 |
| 72.30 | | | 93.74 | 72.30 | | | | |
| 80.00 | 84.59 | 49.48 | 93.81 | 74.10 | 105.05 | 97.01 | 79.25 | 35.78 |
| 90.00 | 87.55 | 59.06 | 94.50 | 79.38 | 101.13 | 98.93 | 86.92 | 56.18 |
| 100.00 | 98.45 | 100.00 | 98.45 | 100.00 | 98.45 | 100.00 | 98.45 | 100.00 |

**Table 3.** Liquid–vapor phase equilibria in 2-MBF-containing binary systems at 1 atm

| Luquid composition, $X_1$, mol % | System | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | 2-MBF (**1**)–cumene (**2**) | | 2-MBF (**1**)–AMS (**2**) | | 2-MBF (**1**)–phenol (**2**) | | 2-MBF (**1**)–water (**2**) | |
| | $T_b$ mixture, °C | Vapor composition, $Y_1$, mol % | $T_b$ mixture, °C | Vapor composition, $Y_1$, mol % | $T_b$ mixture, °C | Vapor composition, $Y_1$, mol % | $T_b$ mixture, °C | Vapor composition, $Y_1$, mol % |
| 0.00 | 152.42 | 0.00 | 166.20 | 0.00 | 181.65 | 0.00 | 100.00 | 0.00 |
| 3.82 | | | | | | | 99.67 | 3.82 |
| 10.00 | 160.81 | 0.12 | 172.70 | 0.64 | 186.40 | 1.59 | 99.67 | 3.82 |
| 20.00 | 173.94 | 1.42 | 181.71 | 3.74 | 192.24 | 6.65 | 99.67 | 3.82 |
| 30.00 | 187.54 | 6.93 | 190.32 | 11.64 | 197.36 | 16.39 | 99.67 | 3.82 |
| 40.00 | 198.51 | 19.88 | 196.80 | 24.92 | 200.92 | 30.16 | 99.67 | 3.82 |
| 50.00 | 204.94 | 39.29 | 200.59 | 41.49 | 202.76 | 45.82 | 99.67 | 3.82 |
| 55.00 | 206.40 | 49.73 | 201.56 | 49.99 | 203.09 | 53.61 | 99.67 | 3.82 |
| 58.14 | | | | | 203.14 | 58.14 | | |
| 59.67 | 206.87 | 59.67 | | | | | | |
| 60.00 | 206.87 | 59.67 | 202.03 | 58.17 | 203.11 | 61.06 | 99.67 | 3.82 |

**Table 3.** (Contd.)

| Luquid composition, $X_1$, mol % | System |  |  |  |  |  |  |  |
|---|---|---|---|---|---|---|---|---|
|  | 2-MBF (**1**)–cumene (**2**) |  | 2-MBF (**1**)–AMS (**2**) |  | 2-MBF (**1**)–phenol (**2**) |  | 2-MBF (**1**)–water (**2**) |  |
|  | $T_b$ mixture, °C | Vapor composition, $Y_1$, mol % | $T_b$ mixture, °C | Vapor composition, $Y_1$, mol % | $T_b$ mixture, °C | Vapor composition, $Y_1$, mol % | $T_b$ mixture, °C | Vapor composition, $Y_1$, mol % |
| 63.50 |  |  | 202.12 | 63.50 |  |  |  |  |
| 70.00 | 205.75 | 76.27 | 201.85 | 72.70 | 202.40 | 74.37 | 99.67 | 3.82 |
| 80.00 | 203.19 | 87.83 | 200.74 | 84.33 | 201.03 | 85.18 | 99.67 | 3.82 |
| 90.00 | 200.26 | 95.30 | 199.19 | 93.24 | 199.33 | 93.59 | 106.25 | 5.20 |
| 100.00 | 197.51 | 100.00 | 197.51 | 100.00 | 197.51 | 100.00 | 197.51 | 100.00 |

The azeotropic properties of all ternary mixtures in the phenol–cumene (AMS)–HA–water systems were studied at 0.2 and 1 atm. The resulting data were reported in [6].

We did not study the composition of the HA–phenol azeotrope at atmospheric pressure because of the high probability of HA thermolysis.

It was established that the HA–phenol azeotrope shows no tendency for degeneration as the pressure increases. According to the second Vrevskii law [8], as the pressure increases, in systems with negative deviations from ideality the azeotrope is enriched with a component whose vaporization point is lower that those of the other components of the system. The same picture is observed with HA whose vaporization point is lower than that of phenol. We constructed distillation line diagrams and identified rectification fields determining conditions for complete purification of phenol from HA (Fig. 1).

In Fig. 1, the directions of distillation lines are shown by arrows. The shaded surface borded by special points (phenol and cumene–water, cumene–HA, and phenol–HA azeotropes) separates rectification fields on the quaternary system. Figure 1 shows three figurative points corresponding to the composition of products coming to the rectification stage in different technologies.

Point *1* falls below the separating surface and correspond to a mixture containing ≤ 3 wt % of cumene; the distillation lines are directed toward the phenol–HA azeotrope. In this case, phenol is impossible to purify from HA, which is confirmed by industrial practice.

Point *2a* falls on the intercept of the phenol–cumene–water surface and the separating surface

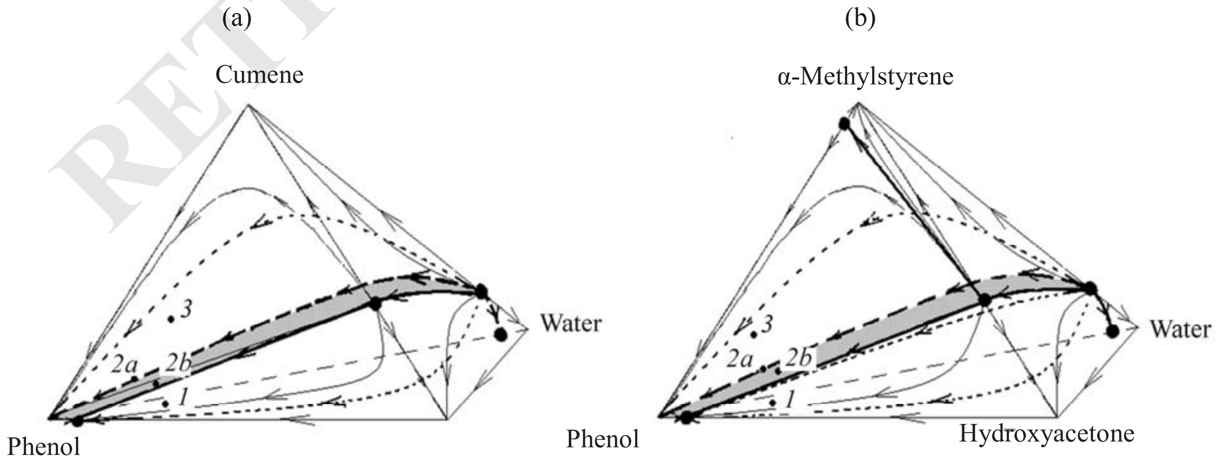

**Fig. 1**. Distillation line diagrams in the systems (a) cumene–water–phenol–HA and (b) AMS–water–HA (concentrations are in mol %).

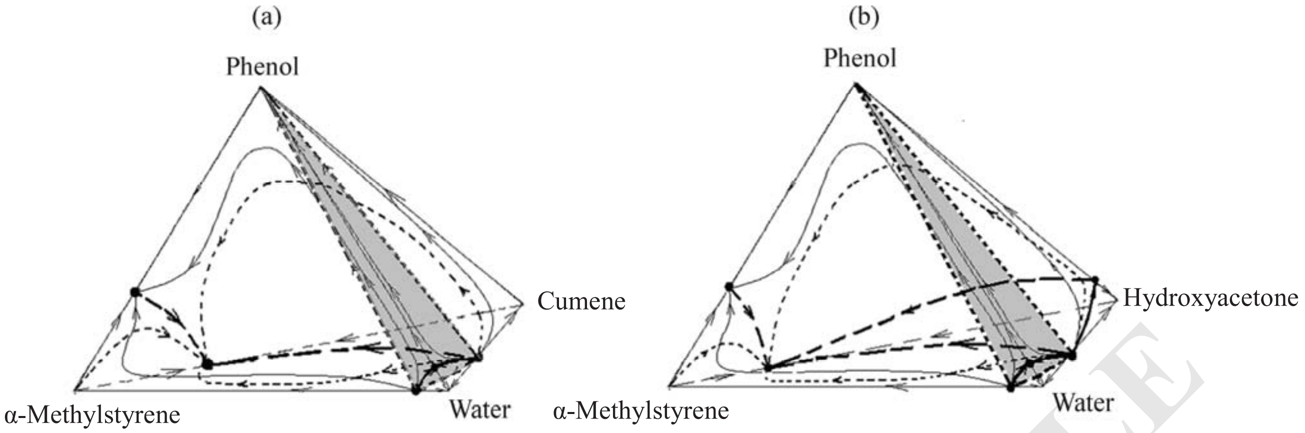

**Fig. 2.** Distillation line diagrams in the systems (a) cumene–water–phenol–2-MBF and (b) AMS–water–phenol–HA–2-MBF (concentrations are in mol %).

between the phenol–cumene–water azeotrope– cumene–HA azeotrope and phenol–HA systems; the distillation lines are directed toward phenol. In this case, phenol can be purified from HA.

Point *2b* falls on the separating surface, the separating lines are directed toward the phenol–HA azeotrope, implying that phenol is impossible to purify from HA.

Point *3* falls above the separating surface, and the distillation lines all are directed toward pure phenol. It is these conditions that allow phenol to be best purified from HA. However, if rectification is performed on columns with a limited number of theoretical plates and/or their efficiency is insufficient for a concrete load, complete purification of phenol from HA may prove impossible.

Research on systems containing 2-MBF showed that the 2-MBF–water system is heterogeneous and the 2-MBF–phenol, 2-MBF–AMS, and 2-MBF–cumene systems are homogeneous.

The resulting phase equilibrium data point to the presence of positive azeotropes (with a minimum boiling point) in the 2-MBF–water system and of negative azeotropes (with a maximum boiling point) in the 2-MBF–phenol, 2-MBF–AMS, and 2-MBF–cumene systems.

We constructed distillation line diagrams and identified rectification fields determining conditions for complete purification of phenol from 2-MBF (Fig. 2).

As seen, the separating surface of the cumene (AMS)–water–phenol–2-MBF quaternary systems is confined by special points: water–2MBF azeotrope, cumene (AMS)–water azeotrope, and phenol.

The field in which effective purification of phenol from 2-MBF is possible is by the intersept of the following surfaces:

– separating surface,

– surface formed by phenol, water, and 2-MBF–water azeotrope,

– surface formed by phenol, water, and cumene–water azeotrope,

– surface formed water and cumene–water and 2-MBF–water azeotropes.

The resulting data provide convincing evidence to show why effective purification of phenol from 2-MBF in industrial conditions cannot be provided by varying a single parameter, say by increasing water feed.

Sometimes, when the products to be separated contain very little cumene (1–3 wt %), the task to remove 2-MBF from phenol is at all unsolvable. At high cumene contents (~28 wt %) and involuntarily low water contents, phenol is much more difficult to purify from 2-MBF just because of the low water concentration.

## Optimal Conditions for Purification of Phenol from HA and 2-MBF

Analysis of the structural regularities in the phase equilibrium diagrams shows that the best technology for purifying phenol from HA is azeotropic extractive rectification with the use of a combined separating

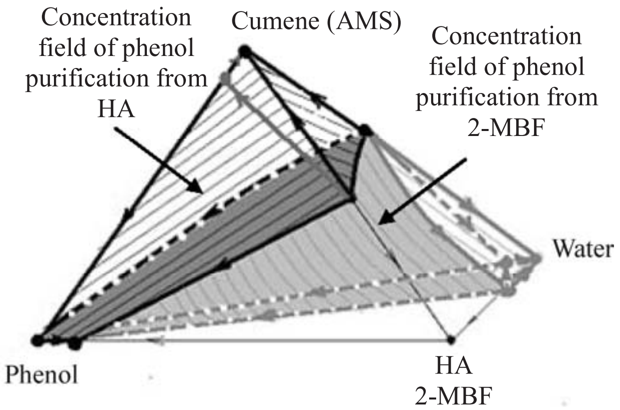

**Fig. 3.** Concentration fields of purification of phenol from HA and 2-MBF.

agent, specifically a mixture of cumene, AMS, and water. The principal condition is to maintain a definite ratio of the weight concentrations of hydrocarbons (cumene and AMS) and water in the mixtures to be separated.

As follows from the phase equilibrium diagrams, the practically required level of phenol purification from 2-MBF is provided by azeotropic extractive reactivication with the use of water as the azeotropic agent. However, this can be accomplished if the water, cumenea (AMS), and 2-MBF weight ratio is maintained higher or equal to the weight ratio of water in its azeotropes with cumene (AMS) and 2-MBF.

Therewith, the task to purify phenol simultaneously from HA and from 2-MBF using a single separating column is impossible to solve even theoretically. Both HA and 2-MBF require extremely individual conditions (column operating mode). As clearly seen from the diagram in Fig. 3, the concentration fields for purifying phenol from HA and 2-MBF are quite different. To remove HA, rectification should be performed in a cumene (AMS)–rich region and maintain a definite weight ratio of cumene (AMS) and water in the mixtures to be separated. To remove 2-MBF, rectification should be performed in a water-rich region, maintaining definite weight ratios of water and cumene (AMS) and water and 2-MBF. The concentration range for purification of phenol from HA is by vertices: cumene (AMS), phenol, and cumene–HA, phenol–HA, and cumene–water azeotropes. The concentration field for purification of phenol from 2-MBF is confined by vertices: water, phenol, and water–2-MBF and cumene–water. For simultaneous purification of phenol from HA and 2-MBF the concentration ranges should intersect or overlap, which is impossible (see Fig. 3). The concentration ranges for purification of phenol from HA and 2-MBF do not overlap each other but only adjoin along the line passing through the phenol–cumene–water ternary system from the binary cumene–water azeotrope to the phenol vertex (intersection lines between the separating surfaces of the phenol–cumene(AMS)–water–HA and phenol–cumene (AMS)–water–2-MBF systems). Thus, the lack of a common concentration field does not allow, even theoretically, simultaneous purification of phenol from HA and 2-MBF.

Clear evidence for these conclusions is provided by the practice of exploitation of industrial columns, when varied conditions did not lead and could not lead in principle to effective simultaneous removal of HA and 2-MBF.

The digrams in Figs. 1–3 provide illustrative and convincing evidence showing that phenol is extremely difficult to purify from HA and 2-MBF by rectification and requires installation of at least two columns for high-efficiency extractive rectification with significant steam consumption.

Complete purification of phenol from HA and 2-MBF on real industrial columns is practically impossible because of unstable compositions of column feed flows, i.e. because of the difficulty (and not infrequently impossibility) of maintaining flow compositions in the required concentration range, as well as due to restricted efficiency of columns.

## Analysis of Industrial Technologies of Phenol Purification from HA and 2-MBF

In the technology in which the cumene content in cumene hydroxide (CHP) decomposition products is about 12 wt %, two azeotropic extractive rectification columns with two different azeotropic agents are used.

In the column for separating the acetone and phenol flows, phenol is purified from HA by means of a combined separating agent fed together with the column feed. The weigh ratio of the mixture of cumene and AMS and water should be the same as azeotropic to meet the principle condition for purification of phenol from HA. The practice of industrial exploitation show that the phenol flow outgoing from the azeotropic extractive rectification column is designed to contain 0.0008–0.001 wt % of HA. To purify phenol from 2-MBF, this technology makes use of water as the azeotropic agent in the column for afterpurification of phenol from hydrocarbons and 2-MBF; water is fed into the condensate in a quantity sufficient for the concentration of water on plates in the most part of the column to be higher than 90 mol %. This ensures the required degree of phenol purification from 2-MBF. The experience of industrial exploitation gives evidence showing the phenol flow outgoing from the phenol afterpurification column in the designed conditions contains no more than 0.0003–0.0005 wt % of hydrocarbons and 2-MBF. It is this technology that ensures the required level of phenol purification from HA and 2-MBF.

In the technology in which the cumene content in CHP decomposition products is 28–30 wt %, a single azeotropic extractive rectification column is used for purifying the phenol flow from HA and 2-MBF. Since, as follows from the above analysis, phenol cannot be simultaneously purified from HA and 2-MBF, water should be fed into the condensate for complete separation of cumene and AMS from phenol. As a result, phenol is purified from 2-MBF but incompletely purified from HA.

If cumene and AMS are distilled incompletely, which occurs when an organic phase is fed into the condensate, the resulting still phenol flow is purified from HA but contains more 2-MBF. The reason is that the latter is in principle impossible to distill from a water-free mixture of products. The experience of industrial exploitation of this technology shows that the phenol flow outgoing from the column for distillation of hydrocarbons contains much HA (~0.01 wt %) even in the designed conditions, not to mention the cases when the column is operated at increased load levels or when deviations from the designed mode occur, which is not a rare case. In this connection at the stage of catalytic phenol purification 2-MBF is formed in expectedly large amounts, and, consequently, multireactor catalytic purification with a long contact time is required.

In the technology in which the cumene content of CHP decomposition products is no more than 3 wt %, the phenol flow is almost impossible to purify from HA by rectification, and 2-MBF is removed on the cumene and AMS after distillation column at a low water concentration; as a result, afterpurification of phenol from HA and 2-MBF is required. The operational mode of the AMS after distillation column is far from that required for azeotropic extractive rectification.

In the column for separation of the acetone and phenol flows the concentrations of cumene and AMS are low and the concentration of water is high; as a result, the weight ratio of the acetone and phenol to water is much lower than azeotropic. According to the established structural regularities (see Fig. 1, point 1), the phenol flow will inevitably contain the HA amount that enters the column with the feed, i.e. all HA will stay in the column still bottom together with phenol, thus leading to an inadmissibly high concentration of 2-MBF at the stage of catalytic purification of phenol, which further raises a virtually unsolvable problem of removal of 2-MBF from phenol. Nevertheless, the established theoretical regularities allowed us to find a nonstandard solution of the problem of phenol purification from HA at a low concentration of cumene in the products to be separated [9].

The above-presented theoretical foundations for the purification of phenol from HA and 2-MBF by rectification, on the one hand, make it possible to determine optimal conditions for manufacturing high-purity phenol and, on the other, form the basis for calculation of multicomponent rectification columns. In the absence of our data on phase equilibria and azeotropic properties of systems containing HA and 2-MBF, there has been clear inconsistency between the calculated characteristics of columns and the practice of their industrial exploitation. Correct calculation of rectification columns proved possible even after the calculated binary interaction parameters for the NRTL equation [10, p. 180], presented in Table 4, were taken into account.

**Table 4.** Binary interaction parameters for the NRTL equations for HA- and 2-MBF-containing systems

| System | Binary interaction parameters | | | |
|---|---|---|---|---|
| | $\tau_{12}$ | $\tau_{21}$ | $G_{12}$ | $G_{21}$ |
| HA (**1**) –cumene (**2**) | 1.203 | 1.645 | 0.739 | 0.662 |
| HA (**1**) – AMS (**2**) | 1.949 | 0.013 | 0.524 | 0.996 |
| HA (**1**) – phenol (**2**) | –0.798 | –0.291 | 1.341 | 1.113 |
| HA (**1**) – water (**2**) | –1.335 | 3.023 | 1.313 | 0.540 |
| 2-MBF (**1**) – cumene (**2**) | –2.139 | 0.093 | 2.353 | 0.964 |
| 2-MBF(**1**) – AMS(**2**) | –1.917 | 0.908 | 2.088 | 0.706 |
| 2-MBF(**1**) – phenol(**2**) | –1.838 | 1.418 | 2.037 | 0.578 |
| 2-MBF(**1**) – water (**2**) | 1.492 | 2.793 | 0.593 | 0.376 |

It should be noted that all approached to rectification separation of products containing HA and 2-MBF, including azeotropic extractive rectification, turned out to be quite power-consuming, insufficiently efficient, input intensive, and costly. In particular, azeotropic extractive rectification, while solving in part the problem of removal of HA and 2-MBF, increased considerably the waste water volume of the phenol process. These reasons made designers [11–14] to rule out many rectification approaches used in the overwhelming majority of industrial phenol/acetone technologies. First of all, to solve the problem cardinally, technologies that exclude 2-MBF formation at the stage of catalytic purification of phenol were developed [11–14]; moreover, these technologies allow a much more facile operation of azeotropic extractive rectification columns and reduced steam consumption. The developed approaches made it possible complete purification from HA and 2-MBF in all technologies differing from each other by cumene contents, not only at the rectification stage, but also at the stage of catalytic purification of phenol, which ensures stable production of a carbonate-purity phenol. We have to admit that the concept of phenol purification from HA and 2-MBF by rectification and azeotropic extractive distillation is useful but outdated and passing stage of the development of the phenol process. Obviously, the new concept and strategy will become prevailing with time. Evidence for this statement is provided by the appearance of works analogous the above-cited ones, specifically [15], as well as the appearance of a series of the so-called "bypass" patents [16] whose authors make an attempt, following [11–14], to solve the problem of removing HA before the products are delivered to the rectification unit.

Nevertheless, since most industries still uses the traditional technology for rectification and purification of phenol, neglecting the theoretical basis and approaches to controlling and optimizing the rectification stage is not recommended.

## CONCLUSIONS

(1) The results of detailed research into the phase equilibria and azeotropic properties of binary systems containing cumene, AMS, phenol, water, HA, and 2-MBF, allowed us:

– to reveal the impropriety of traditional approaches to rectification of the listed products in industrial technologies and to suggest a theoretically substantiated technology of azeotropic extractive rectification;

– to find out the reasons for varied contents of HA in the phenol flow at varied contents of cumene (1–28 wt %) in the separated products;

– to obtain evidence showing that the content of HA in phenol is determined by the content of cumene in the separated products, forming the following order in terms of HA nondistillable from phenol:

1–3 wt % cumene >> 26–30 wt % cumene
>> 10–13 wt % cumene.

(2) The azeotropic extractive rectification applied in the traditional technology to remove HA and 2-MBF from phenol was a forced approach, but it proved to be extremely power-consuming and insufficiently efficient.

(3) With the advent of technologies that exclude 2-MBF formation at the stage of catalytic purification of phenol, the stage of product rectification in the phenol process is considerably facilitated and eliminates the need in a costly aqueous extractive purification of phenol from 2-MBF.

(4) Our obtained data on the phase equilibria and properties of HA- and 2-MBF-containing systems point the way to reducing the content of HA in the flow directed to catalytic purification, in the framework of traditional technologies for separation of products of the phenol process.

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