

Live calculations, functions and calculation procedures on properties of ion-exchange resins

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The paper describes network open interactive calculations on properties of the ion-exchange resins applied for water treatment, corresponding functions and calculation methods for topical programming calculation tools.

Information on properties of ion-exchange resins is supplied to users in two forms: as protected calculation programs of water treatment plants (CADIX, IxCalc and other) on CD-ROMs and as “open” technical documentation on paper or on the Internet sites. The advantages and limitations of these publication forms were discussed in [1]. The first way (protected programs on disks) can be called publications by stretching a point. As a rule, a user runs a program installed on a disk or downloaded from the Internet and it enables him (her) to enter initial data and get a result: no intermediate data or formulae used for the final results are available. Such “closed” informational technology is not convenient for the company developing the ion-exchange resins, too: if a software engineer leaves the company it becomes difficult or sometimes impossible to make changes or supplements into the program (a “nightmare” of inherited software [2]). It is also worth to note that such programs are difficult to learn. Even an experienced specialist in water treatment and advanced user have to spend much time (several months) and force to master such programs as CADIX, IxCalc and other. After mastering the program a specialist often “gets hooked” on it and can’t change it for more advanced calculation tools. The limitation of the second technology of technical information publication is that one can’t calculate by it at once entering initial data, it is a “dead” technology.

The publication technology for technical information that enables us to calculate directly was developed at Moscow Power Engineering Institute (www.mpei.ru) and Trieru company (www.trie.ru).

http://twt.mpei.ac.ru/TTHB/1/RH/1200-hclcfr_ban.pdf - Windows Internet Explorer

http://twt.mpei.ac.ru/TTHB/1/RH/1200-hclcfr_ban.pdf



ENGINEERING DATA SHEET (HCl, Co-flow regeneration)

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These data provide information to calculate the sodium leakage and operating capacity of AMBERJET 1200 Na used for water demineralisation with co-flow regeneration with hydrochloric acid. The properties of AMBERJET 1200 Na are described in the Product Data Sheet PDS 0354 A.

These data are valid for Amberjet 1200 H but the results obtained refer to the Na form and must be corrected for the reversible swelling between the Na and H forms.

Note : Sodium leakage values are expressed as a percentage of the equivalent mineral acidity (EMA).

The value obtained in meq/L must be converted to mg/L as Na and eventually to a conductivity value, using the graph supplied in the Memento of Ion Exchange published by Rohm and Haas.

SODIUM LEAKAGE

The average sodium leakage is obtained by multiplying the basic leakage value from Table 1 by the correction factor A from Table 2.

$$\text{Leak} = \text{Leak}_0 \times A$$

HCl g/L	Leakage % EMA (Leak ₀)
50	3.9
60	3.0
70	2.5
80	2.0
100	1.5
120	1.2
150	0.9

Na %	Factor A
10	0.15
20	0.30
30	0.50
40	0.75
50	1.00
60	1.30
70	1.70
80	2.20
90	2.80
100	3.60

Figure 1. Information on the ion-exchange resin on the Internet

Figure 1 shows a part of technical process bulletin of ion-exchange resin Amberjet 1200 Na produced by Rohm and Haas¹ available on the Internet as a pdf-file, which one can read and print but can't calculate by it. This file can be also found on the site of developing company or on the calculation site of department "Technology of water and fuels" of MPEI (see Fig. 2) clicking the hyperlink "description of the resin".

¹ Today the company is an affiliate of Dow Chemical (www.dow.com)

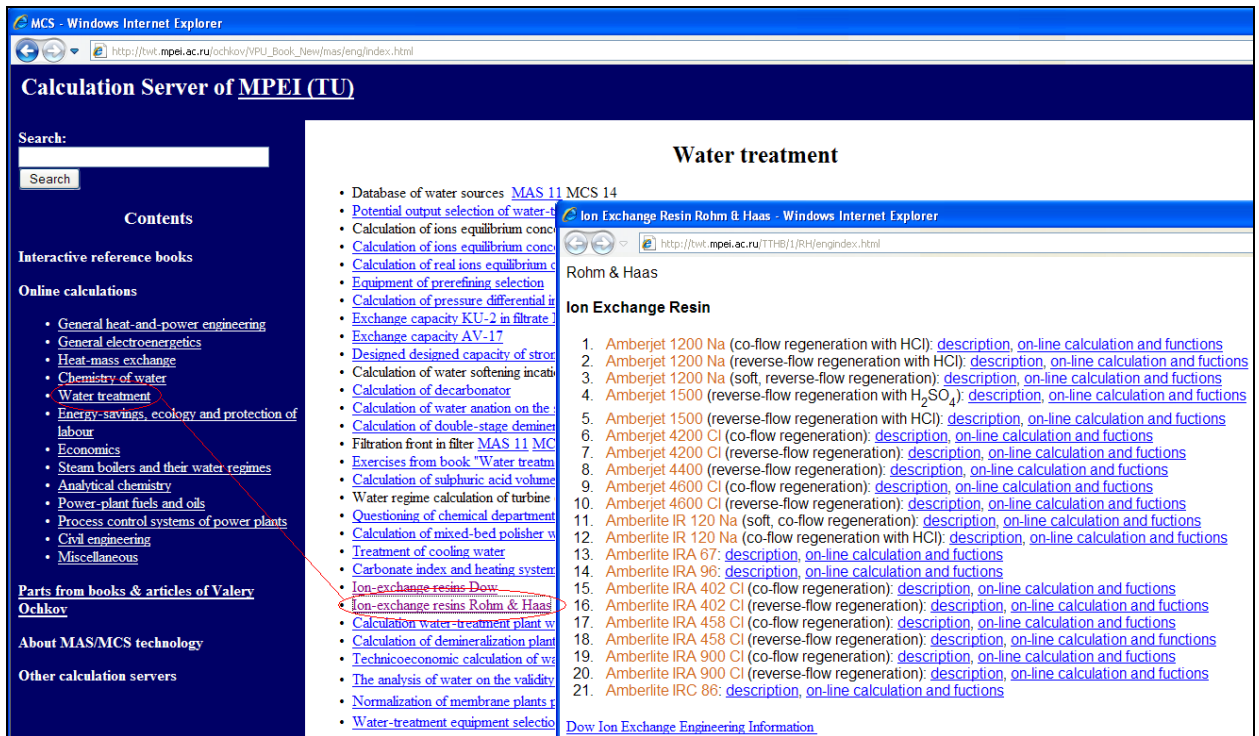


Figure 2. Calculation site of MPEI – Trieru

There is another hyperlink, “on-line calculations and functions”, to the right of the first one: clicking it one can go to the page shown on Figure 3.

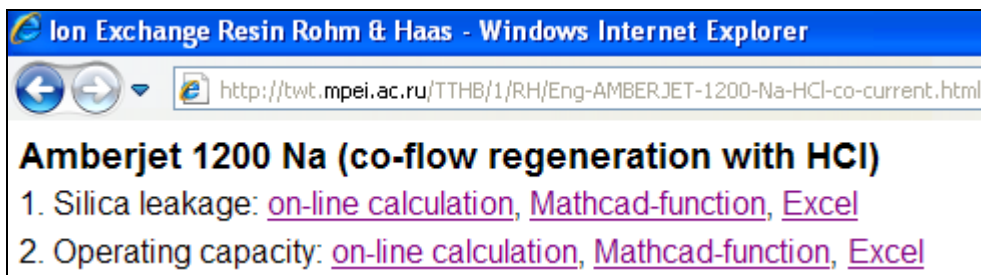


Figure 3. Site containing references on calculations

It enables a user to calculate automatically such important technological parameters of the resin as leakage of the removed ion and the operating capacity. Figure 4 shows interactive open network calculation of the resin parameters described in the technical process bulletin (see Fig. 1): it was done corresponding interpolation of the table points and the result is given by the entered data. If a consumer of the informational services (designer of water treatment equipment or operational staff) needs not only a single calculation (see Fig. 4) but also the corresponding function (calculation method) which could be inserted into a large calculation project he (she) has an opportunity to download required program parts and insert them into his (her) own calculation. Today the most popular tools for engineering calculations are considered to be mathematical package Mathcad and spreadsheet Excel².

² Excel spreadsheet is designed primarily for accounting estimate but a lot of engineers “get hooked” on this program and can’t change it for more convenient computer calculation worksheets.

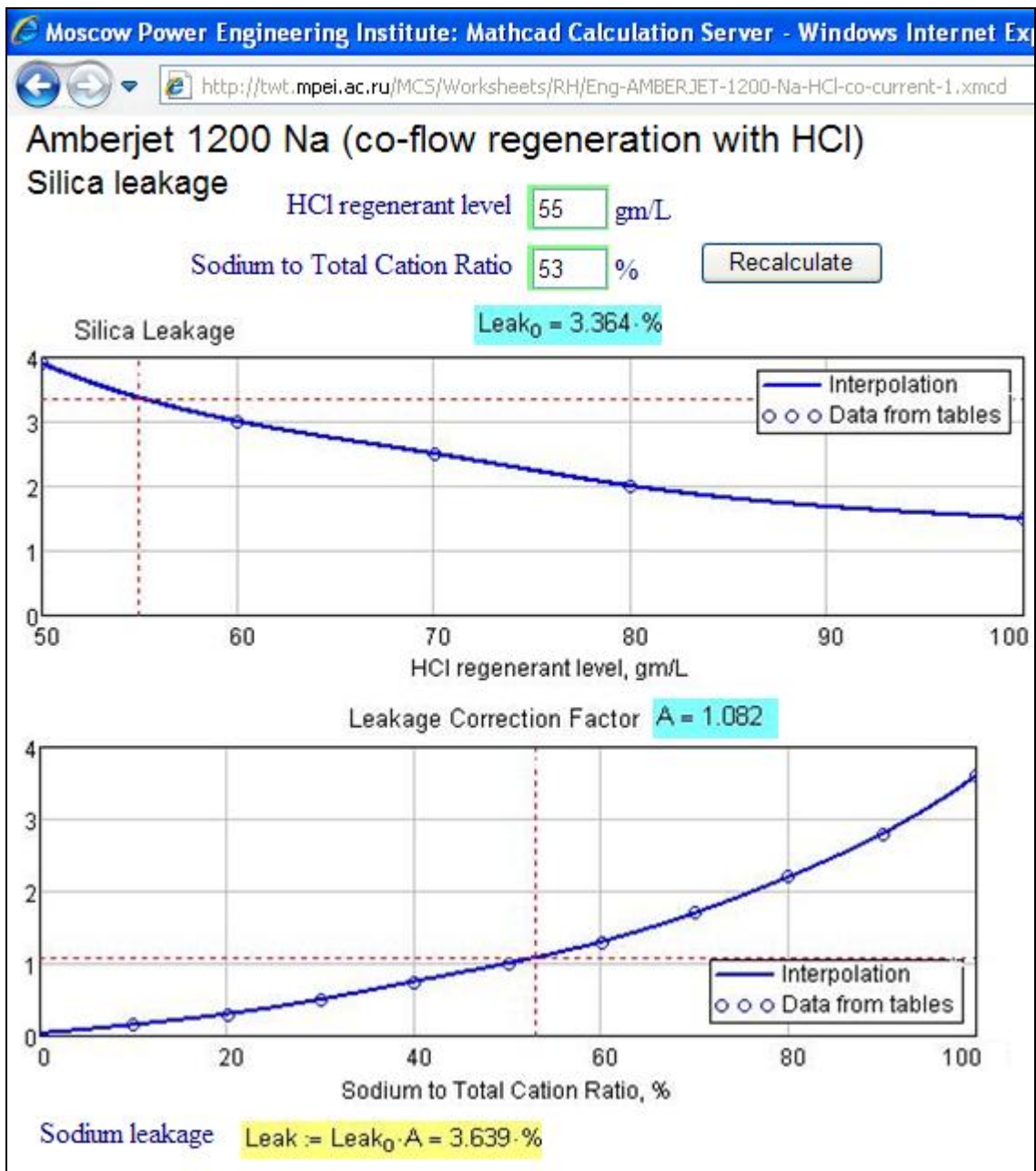


Figure 4. On-line calculation of the ion-exchange resin properties

Figure 5 shows the Mathcad function and Figure 6 shows the similar procedure downloaded from the site shown on Figure 3. The calculation created in Mathcad (Fig. 5) compare favorably with that developed in Excel (Fig. 6).

Mathcad - [AMBERJET-1200-Na-HCl-co-current-1.xmcdz]

File Edit View Insert Format Tools Symbolics Window Help

Normal Arial 10 B I U

▼ Silica leakage of Amberjet 1200 Na (HCl, co-flow regeneration)

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Leak-1200Na-HCl(co-flow)(GHCl,Na/Kt) := "Silica leakage of Amberjet 1200 Na (HCl, co-flow regeneration)"
GHCl ←  $\frac{G_{HCl}}{\frac{gm}{L}}$ 
Tab1 ←  $\begin{pmatrix} 50 & 60 & 70 & 80 & 100 & 120 & 150 \\ 3.9 & 3 & 2.5 & 2 & 1.5 & 1.2 & 0.9 \end{pmatrix}$ 
return "GHCl-?" if GHCl < min[(Tab1T)(0)] ∨ GHCl > max[(Tab1T)(0)]
Leak0 ← interp[cspline[(Tab1T)(0), (Tab1T)(1)], (Tab1T)(0), (Tab1T)(1), GHCl]
Na/Kt ←  $\frac{Na/Kt}{\%}$ 
Tab2 ←  $\begin{pmatrix} 10 & 20 & 30 & 40 & 50 & 60 & 70 & 80 & 90 & 100 \\ 0.15 & 0.3 & 0.5 & 0.75 & 1 & 1.3 & 1.7 & 2.2 & 2.8 & 3.6 \end{pmatrix}$ 
return "Na-?" if Na/Kt < 0 ∨ Na/Kt > 100
A ← interp[cspline[(Tab2T)(0), (Tab2T)(1)], (Tab2T)(0), (Tab2T)(1), Na/Kt]
return Leak0 · A · %

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▲ Silica leakage of Amberjet 1200 Na (HCl, co-flow regeneration)

G_{HCl} := 55 $\frac{gm}{L}$ Na/Kt := 53% Leak-1200Na-HCl(co-flow)(G_{HCl},Na/Kt) = 3.639%

Figure 5. Mathcad function on the ion-exchange resin properties

	A	B	C
1	Amberjet 1200 Na (co-flow regeneration with HCl)		
2	Silica leakage		
3			
4	HCl regenerant level	55	gm/L
5	Sodium to Total Cation Ratio	53	%
6	Basic leakage	3,444	%
7	Leakage Correction Factor A	1,0730	
8	Silica leakage	3,6956	%

Figure 6. Excel calculation on the ion-exchange resin properties

It is plainly visible so we can easily modernize it, develop, to build other calculations on its basis. Among other things, Mathcad enables us to use dimensions that mitigate the risk of errors significantly. The data obtained in Mathcad (Fig. 4 and 5) and in Excel (Fig. 6) vary slightly. The difference results from that it was used interpolation of table points in Mathcad (linear – Fig. 4 or spline – Fig. 5) and approximation by cubic polynomial in Excel. This discrepancy can be neglected remembering that, as a rule, obtained values are changed to 10-20% in practical calculations (so called engineering “margin of safety”). Furthermore, it should be noted that technical characteristics of the resin (capacity, leakage value and other) depend on more parameters, not only on composition of the source water and regeneration characteristics. Operating capacity of the resin also depends on form of the column, number of regenerations carried out, presence of the constituents which cause fouling of the ion-exchange resins, etc. So it makes no sense to “split hairs” in the calculations shown on Fig. 4, 5, and 6.

Today MPEI and Trieru coordinate the work on information and calculation provision at power engineering branch with the American corporation Knovel (www.knovel.com). Knovel publishes online reference books and monographs, which help researchers and engineers to solve their everyday and long-range problems. A great number of leading universities³ and companies including Dow Chemical Company subscribe to Knovel informational service.

³ Moscow Power Engineering Institute subscribes to Knovel since October 2010.

The screenshot shows the Knovel website interface in a Windows Internet Explorer browser. The search bar contains 'water t' and has a dropdown menu showing 'water treatment'. The search results page displays 'Number of Titles Retrieved: 1020' and 'Page: 1 of 34'. The main heading is 'You searched for (water treatment) within Your Subscription Titles:'. Below this, several search results are listed, each with a book cover image, a 'Search Within' button, and a table of sections with their corresponding content types.

Sections	Content Type
4.5.2 Synthesis of Water Treatment Trains	Text
4.5.1 General Considerations Involved in Selection of Water Treatment Processes	Text
8.1.2 Application of Conventional Oxidants in Water Treatment	Text
12.2.1 Application of Membrane Filtration to Drinking Water Treatment	Text
15.5.1 Uses of PAC in Water Treatment	Text

Sections	Content Type
Appendix A. Properties and Characteristics of Water Treatment Chemicals	Text
23.1 Water Treatment Plant Site Selection	Text
23.2 Arrangement of Water Treatment Plant Facilities	Text
11.1 Water Hardness and Softening Treatment	Text
18.1 The Role of the Architect in Water Treatment Plant Design	Text

Figure 7. Knovel site

Figure 7 shows the Knovel site representing information on monographs and reference books at water treatment (found 1020 sources which contain words “water treatment” in the titles or in the texts) on a user demand. This information is supplemented with corresponding calculation component described in this paper.

Besides, the last Mathcad version, Mathcad 15, enables us to connect with Knovel site directly using Knovel item from Tools menu. This results from strategic partnership of PTC company (www.ptc.com is an owner of Mathcad) and Knovel Corporation. Although, we pitifully have to state that companies developing mathematical packages and engineering calculators are not interested in evolvment of on-line calculations by Internet calculation servers, which do not demand installation of corresponding programs on personal computers as it is shown on Fig. 4. It is profitably for developers if users buy their

rather expensive programs even for simple one-time calculation by a ready-made program downloaded from the Internet (Fig. 5 and 6). And this advantage for developers often goes against world IT trend. Meanwhile, MPEI calculation server works and supplies users with calculations in the area of power engineering.

References

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2. V. Ochkov, G. Yankov. “Reference book + site” complex and the problem of knowledge transfer. // Trudi Akadenenergo. No 1, 2009
3. V/ Ochkov. Development of “Electronic Encyclopedia of Power Engineering”- informational contribution into industry and educational processes// Teploenergetika. No 7, 2007.