

PerCalc

User Guide



PerCalc

A web based calculation program for alkyds and polyesters

Welcome to PerCalc, a powerful web based calculation program. PerCalc makes it possible to manage complex calculations on alkyds and polyesters based on theoretical data. It also manage to handle urethane modifications created by isocyanate functionalities and ring-opening polymerization by cyclic esters like caprolactone monomers.

PerCalc is made for hydroxyl rich formulations and allows you to theoretically vary different parameter values in order to check and optimize various formulations. However it is important to stress that these theoretical formulations need to be confirmed in lab trials. Parameters like purities of raw materials, lab set-ups and procedures can have a decisive influence on final results.

Note: PerCalc is not designed to calculate acid rich formulations.

Where to find it:

Website: <https://percalc.perstorp.com/>

User name and password are provided by Perstorp

Confidentiality assurance statement:

All generated data in the program is handled and stored locally on the users computer. Perstorp assure that we have no access to any calculations, formulations or added products created by the user.

Technical Overview

PerCalc is an web application hosted in the Microsoft Cloud Environment, Azure. The web application is using https for secure communication between the client and the application. The application is verified for Chrome, version 60 and above, and Internet explorer version 11. No other browsers are supported and will therefore not work.

Data Storage

The PerCalc database holds information about shared official product library and user information such as user name, login id, password and when the user has been logged in to PerCalc.

All PerCalc calculations are executed in the web clients browser. When data is saved by the user in PerCalc, a file with the data is stored locally in the user's local IT-environment. Therefore the PerCalc user is responsible for managing backups of locally saved data.

Disclaimer

For any use of the application Perstorp can not be held responsible direct, indirect, economic, consequential or consequential damages arising from the use of the application results in. All calculations in PerCalc are theoretical and needs to be verified in lab trials.

Enjoy PerCalc!

Starting screen for PerCalc

Material	(gram)	(moles)	(ea)	(eb)	(wt% / y)	(Price/kg)
Neopentyl glycol	0.00	0.0000	0.0000	0.0000	0.00	0.00
Adipic acid	0.00	0.0000	0.0000	0.0000	0.00	0.00
Select a product						
Total	0.00	0.0000	0.0000	0.0000		0.0

Acid number (mg KOH/g)	Hydroxyl number (mg KOH/g)	Molecular weight (g/mole)	Acid number GEL (mg KOH/g)	Alkyd constant	
0.0 Enter value	0.0	0	0.0	0.000	Can not calculate
Oil length (%)	Hydroxyl excess (%)	Functionality	Produced water (g)	Yield	Calculate
0.0	0.00	0.000	0.00	0.00	Save

For more info, go to www.Perstorp.com/PerCalc

Your calculation space

Material	(gram)	(moles)	(ea)	(eb)	(wt% / y)	(Price/kg)
Neopentyl glycol	0.00	0.0000	0.0000	0.0000	0.00	0.00
Adipic acid	0.00	0.0000	0.0000	0.0000	0.00	0.00
Select a product						
Total	0.00	0.0000	0.0000	0.0000		0.0

Acid number (mg KOH/g)	Hydroxyl number (mg KOH/g)	Molecular weight (g/mole)	Acid number GEL (mg KOH/g)	Alkyd constant	
0.0 Enter value	0.0	0	0.0	0.000	Can not calculate
Oil length (%)	Hydroxyl excess (%)	Functionality	Produced water (g)	Yield	Calculate
0.0	0.00	0.000	0.00	0.00	Save

The upper part of the view contains information about the raw materials in the current batch, i.e. name, the amount in grams and moles, ea. (equivalents carboxylic acid groups), eb. (equivalents hydroxyl groups), weight percentage per yield and price per weight.

How to select products (raw materials)

Available raw materials will be selected in the curtain menu when clicking on "Select a product". Products are grouped in four categories:

- Polyols
- Acids (also includes anhydrides and isocyanates)
- Oils & Fatty acids
- Hydroxy acids (also includes cyclic esters)

Basic information about selected products can be found when hovering above the name of selected product.

Material (gram)

Neopentyl glycol 0.00

Select a product

Product type: Polyol
Abbreviation: NEO
Molecular weight: 104.15
Functionality: 2

Total 0.00

A selected product can be deleted by clicking on the cross on the right of row.



How to calculate

When products (raw materials) have been chosen calculation parameters have to be set.

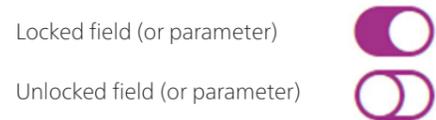
Acid number (mg KOH/g)

0.0 Enter value

Important to remember:

It is always required to set a value in the field for Acid number:

In the fields with a lock/unlock button you can choose whether you want to set values or if you want them to be calculated.
 Note: Only dots, not decimal, can be used when setting values.



Fields possible to Lock/Unlock:

- Grams of each chosen raw material
- Moles of each chosen raw material
- Hydroxyl number
- Molecular weight
- Acid number GEL
- Alkyd constant
- Oil Length
- Yield

Note1: You can only lock one of Molecular weight, Acid number GEL and Alkyd constant at a time since their values are based on the same parameters.

Note2: Oil length can only be locked if exactly one oil or fatty acid is unlocked.

Values in the fields without lock/unlock button (except Acid number) cannot be set, only be calculated.

- ea – Equivalents of COOH
- eb – Equivalents of OH
- wt%/Y – Weight-% calculated on Yield
- Price/kg
- Hydroxyl excess (%)
- Functionality
- Produced water (g)

Calculations are made when clicking button Calculate. It can only be done when "Not calculated" is displayed above. It is displayed "Can not calculate" when no parameters have been set. When "Underdetermined" is displayed not enough fields have been locked and hence more field need to be locked. When "Overdetermined" is displayed too many fields have been locked and hence less fields need to be locked. When calculation has been completed "Calculated" is displayed above the button. All fields are then up-to-date.

Examples of calculations possible

Material	(gram)	(moles)	(ea)	(eb)	(wt%/Y)	(Price/kg)
Adipic acid	10.00	0.0684	0.1368	0.0000	10.00	0.00
Isophthalic acid	59.77	0.3596	0.7192	0.0000	59.77	0.00
Monothylene glycol	10.00	0.1411	0.0000	0.3222	10.00	0.00
Neopentyl glycol	25.25	0.2423	0.0000	0.4847	25.25	0.00
Trimethylolpropane	10.01	0.0746	0.0000	0.2238	10.01	0.00
Total	115.03	0.9060	0.8560	1.0307		0.00

Saturated polyester

Material	(gram)	(moles)	(ea)	(eb)	(wt%/Y)	(Price/kg)
Coconut Oil	38.00	0.0548	0.1645	0.1645	38.00	0.00
Pentaerythritol-mono	15.61	0.1346	0.0000	0.4585	15.61	0.00
Phthalic anhydride	38.42	0.2592	0.5184	0.0000	38.42	0.00
Trimethylolpropane	12.37	0.0921	0.0000	0.2764	12.37	0.00
Total	104.40	0.6853	0.6829	0.8994		0.00

Short oil baking alkyd

Material	(gram)	(moles)	(ea)	(eb)	(wt%/Y)	(Price/kg)
Linseed Oil	25.00	0.0284	0.0853	0.0853	25.00	0.00
Pentaerythritol-mono	13.18	0.0968	0.0000	0.3872	13.18	0.00
Phthalic anhydride	27.41	0.1849	0.3699	0.0000	27.41	0.00
Soybean Oil	35.00	0.0399	0.1197	0.1197	35.00	0.00
Trimethylolpropane	2.42	0.0180	0.0000	0.0540	2.42	0.00
Total	103.01	0.5173	0.5749	0.6462		0.00

Long oil air-drying alkyd

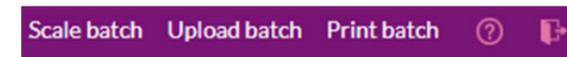
Material	(gram)	(moles)	(ea)	(eb)	(wt%/Y)	(Price/kg)
Dimethylolpropionic acid	4.20	0.0313	0.0313	0.0627	4.20	0.00
Pentaerythritol-mono	16.31	0.1198	0.0000	0.4791	16.31	0.00
Phthalic anhydride	36.93	0.2492	0.4984	0.0000	36.93	0.00
Soybean Oil	40.00	0.0456	0.1368	0.1368	40.00	0.00
Trimethylolpropane	6.00	0.0447	0.0000	0.1341	6.00	0.00
Total	103.44	0.4275	0.6665	0.8127		0.00

Waterborne baking alkyd based on Bis-MPA

Handling of batches

How to save a batch

It is possible to save both a calculated and non-calculated batch. By clicking button "Save" you will be asked to enter a batch name. Files will be saved in the folder "Downloads" from where it can be moved to a selected local folder.



How to scale a batch

It is possible scale batch size by clicking "Scale batch". Desired yield can then be selected without altering any characteristics of the batch.

How to upload a batch

By clicking "Upload batch" a batch can be directly uploaded from your "File explorer". It is then possible to continue working with a batch. Note: An uploaded batch is always based on product data valid at the time of saving the batch. It means that if the data of an added product (raw material) has been updated since saving the batch it will not be recalculated based on the new information.

How to print a batch

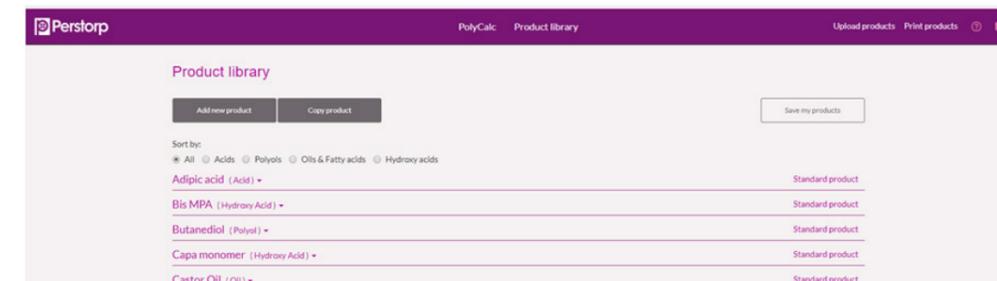
By clicking "Print batch" a printable pdf will be created. The file can be found in the folder "Downloads" from where it can be moved to folder of choice. Note: It is only possible to make a print-out of a batch which has been calculated.

Product library

Detailed information of all available products (raw materials) can be found in product library.

The products are listed in alphabetical order and are grouped in four categories:

- Polyols
- Acids (also includes anhydrides and isocyanates)
- Oils & Fatty acids
- Hydroxy acids (also includes cyclic esters)



The view of the products can be expanded to get full information of each product.

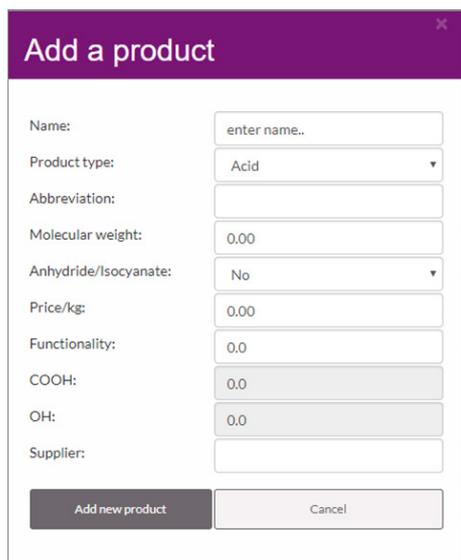
Trimethylolpropane (Polyol) - Standard product		
Anhydride/isocyanate: No	Molecular weight: 134.2	Functionality: 3
Abbreviation: TMP	Price per kg: 0	Supplier: Perstorp AB

Note: When a price is unavailable it is set to 0 by default.

Handling Product Library

Add new product

Unique products, mixtures of products or prepolymers can be added to the product library. They will always be labelled as "Added product" in contrast to "Standard product".



Adding new product to Product Library

Choice to label as "Isocyanate" is only valid for "Product type" "Acid" since Isocyanates are put in this category.

Ringclosed esters, for ring-opening polymerization, like Caprolactone monomer and Lactide monomer are defined as both "Hydroxy acid" and "Anhydride".

Functionality is always defined as the defining reactive groups for each product type. For hydroxy acids it is divided between both COOH and OH.

Note: Example of calculation of values of a mixed product:

	Weight/Part	Molecular weight	Mole	Functionality	eb
Trimethylolpropane	20	134.2	0.149	3	0.447
Neopentyl glycol	80	104.2	0.768	2	1.536

New values of the mixture:

$\Sigma 0.917$

$\Sigma 1.917$

Molecular weight: $100/0.917 = 109.1$

Functionality: $1.983/0.917 = 2.16$

Copy products

In order to make different versions of a product, which can differ in price or purity, a quick copy can be made by clicking "Copy product".

How to save added products

It is possible to save added products by clicking button "Save my products". Your personal product library will be saved as a file in the folder "Downloads" from where it can be moved to a folder of choice. File name will automatically be unique by added date.

Note: If you want to have all your added products in one saved file, you first need to upload your Product library file in the folder "Downloads", then add additional products in Product library in PerCalc, then save your products again. A new Product library file will be created in the folder "Downloads" that contains all your added products.

Upload products

Your personal product library is uploaded by clicking "Upload products"

Note1: Only one file can be uploaded at a time. Note 2: When uploading a batch containing an "Added product" your personal product library doesn't need to be uploaded in advance. Uploading of needed product is done automatically when uploading the batch.

Print product library

By clicking "Print products" a printable pdf, containing list the product library, will be created. The file can be found in the folder "Downloads" from where it can be moved to folder of choice.

Miscellaneous

More information including FAQ can be found when clicking on the question mark.