Solid Fat Content Calculation for fat Blends and Interestifications

Preface

This newsletter is again about the calculation of the Solid Fat Content (SFC), a very important key figure in product development in the field of oils and fats. The SFC values are so important because they reflect the melting behavior in the mouth. The melting behavior does not only depend on the solid fat content at a certain temperature, but also on the slope of the SFC curve. Because the SFC values / curve are so important for product development, there are now two new features:

- There is a serious change in the mixture of fats and oils, but this has no effect on the processing or calculation of the SFC values. Up until now, the version number of the associated component was increased every time the data for calculating the SFC values was changed. As of the new version, this is no longer the case. You can read the explanation for this in the section *Factors for the SFC calculation*.

- There have been major changes to the prediction of the SFC values for interesterifications, both in the software and in the data. There are now approx. 130 data sets of measured transesterifications that we have gathered from existing information in the literature and the internet. In addition, we have done research work in the algorithms and in the expansion of the processing and calculation and invested a lot of time. You can find out more about the extensions and changes in the section *SFC prediction of interesterifications*.

First we would like to point out our demo version.

Demo Version

We would be happy to provide you with a full-featured demo version. The demo version can be used for three months. If necessary, the term can be extended.

The demo version not only offers all functions of the full version, the data generated with the demo version can still be used with the full version. The database is compatible with both the demo and the full version.

And it's that quick and easy (time required approx. 15 minutes):

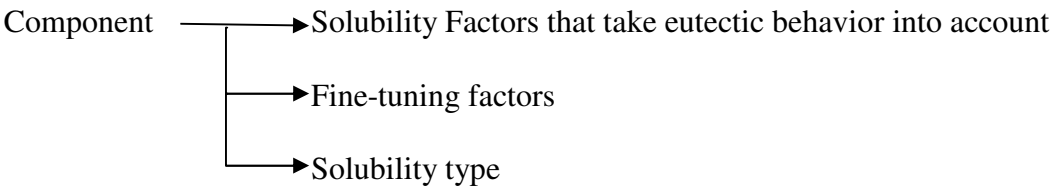
- Request download link info@oil-expert.net
- Download the software package from our website
- Install Oil-Expert software
- Start Oil-Expert.net and enter the registration code
- Finished!

The software is supplied with around 40 standard components and some example projects. Using the example projects and the PDF manual, you can quickly and easily learn how to work with Oil-Expert.net. If you have any questions, please do not hesitate to contact us - by email, phone, Skype or any other medium of your choice.

Factors for the SFC Calculation

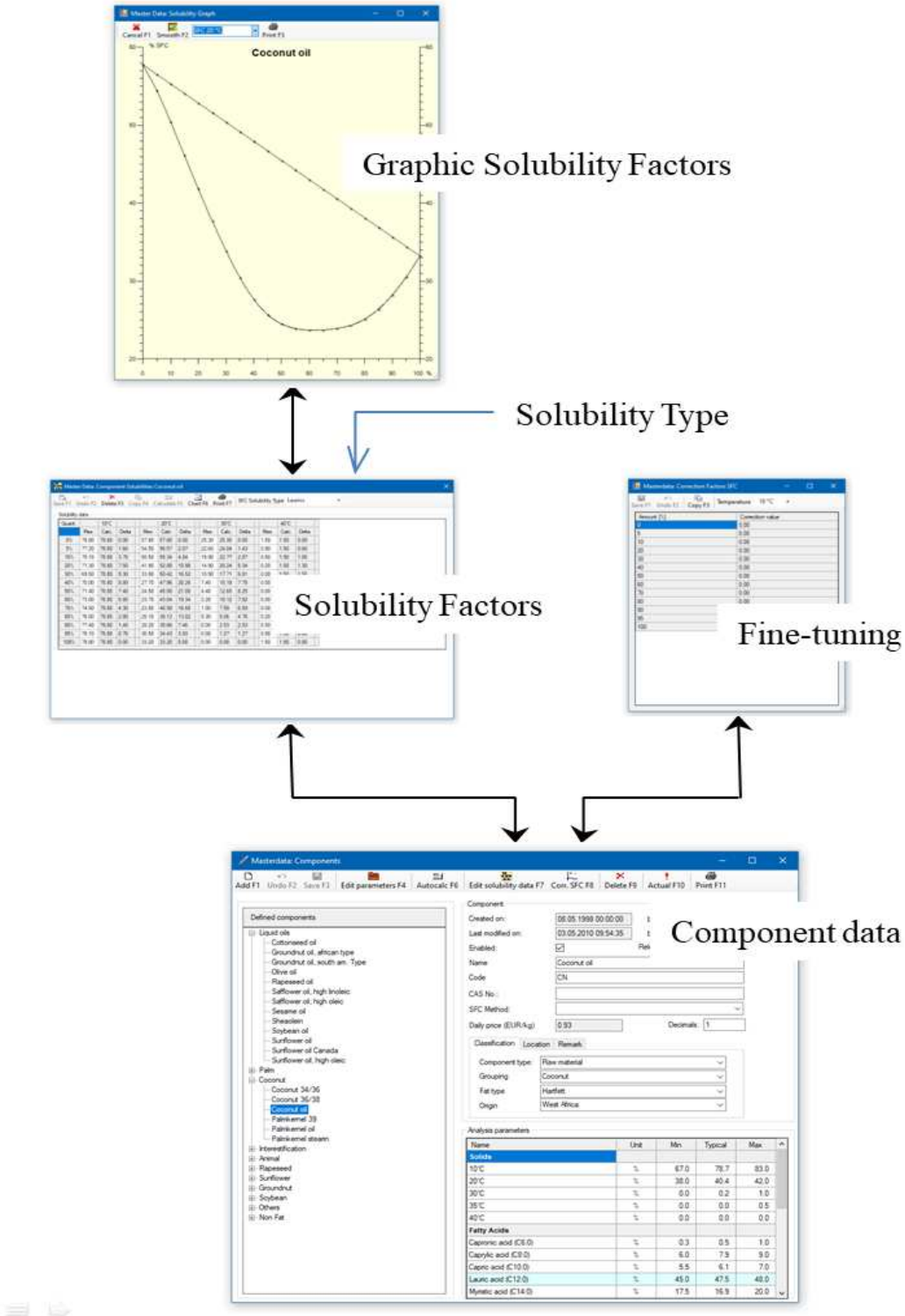
A number of factors are required to calculate the SFC values of fat mixtures (see Newsletter 8). Two of these factors, which take eutectic behavior into account and factors for fine-tuning, are directly related to the respective components. Each time the factors are changed, the version number of the component is therefore increased. Changing the solubility type also increases the version number. The solubility type - Liquid oil, Laurics, etc. - is used to summarize components with the same eutectic behavior for the calculation, e.g. liquid oils. Otherwise the calculated SFC values would be too low, as rapeseed oil, for example, has no solubility for sunflower oil. The assignment of the solubility type prevents the calculation of solubilities if the solubility types are the same.

As of the new version, when the solubility data are changed, the version number is no longer increased. The reason is as follows: for each component there can only be one valid set of factors for solubility! Regardless of whether you are using earlier or more recent versions of the component. Each component is therefore always associated with only one set of factors:



Change data - who changed what, when - of course, are retained.

The following figure shows the relationships based on the dialogues provided for this purpose. All other factors - e.g. global correction factors - are not tied to individual components.



SFC Prediction of Interestifications

Introduction

There are various approaches to predicting the SFC values of interesterifications. The first approach is through Gibbs free energy. The two references given in the footnote provide more information on this procedure [1] [2].However, this requires the Gibbs free energy of all components.

In contrast, we use a statistical approach to estimate the SFC values. With chemical interesterification it is the case that after complete interesterification all fatty acids are statistically distributed over the triglycerides. It should therefore be possible to estimate the SFC values of the interesterification from the proportions of the individual fatty acids in the interesterification mixture. In order to use statistics sensibly, however, a lot of data is required. Because of this, this procedure failed in the past. We have now gathered around 130 data sets of transesterifications from the literature and the internet. That sounds like a lot at first, but it is just enough to prove how this method works. In practice, therefore, even more data records are required that each user can add himself.

The application of statistical methods to these 130 data sets also exposed another problem - the reliability of the data. There are four possible types of errors that play a role in the calculations:

- Inaccuracy of the measured values (SFC values, fatty acids)
- Incomplete interesterification
- Wrong recipes (e.g. Palm oil instead of Palm stearin)
- Differences in the SFC values and the fatty acids of the raw materials used

The inaccuracy of the measured values has only a negligible effect on the results. The completeness of the interesterification is more. A 90% interesterification will probably also result in corresponding deviations in the SFC values. We could not prove this, however, as this information is missing in all examinations. Incorrect information about the recipe, e.g. palm oil instead of palm stearin, rarely occurs, but the calculation has a major impact on the result
.

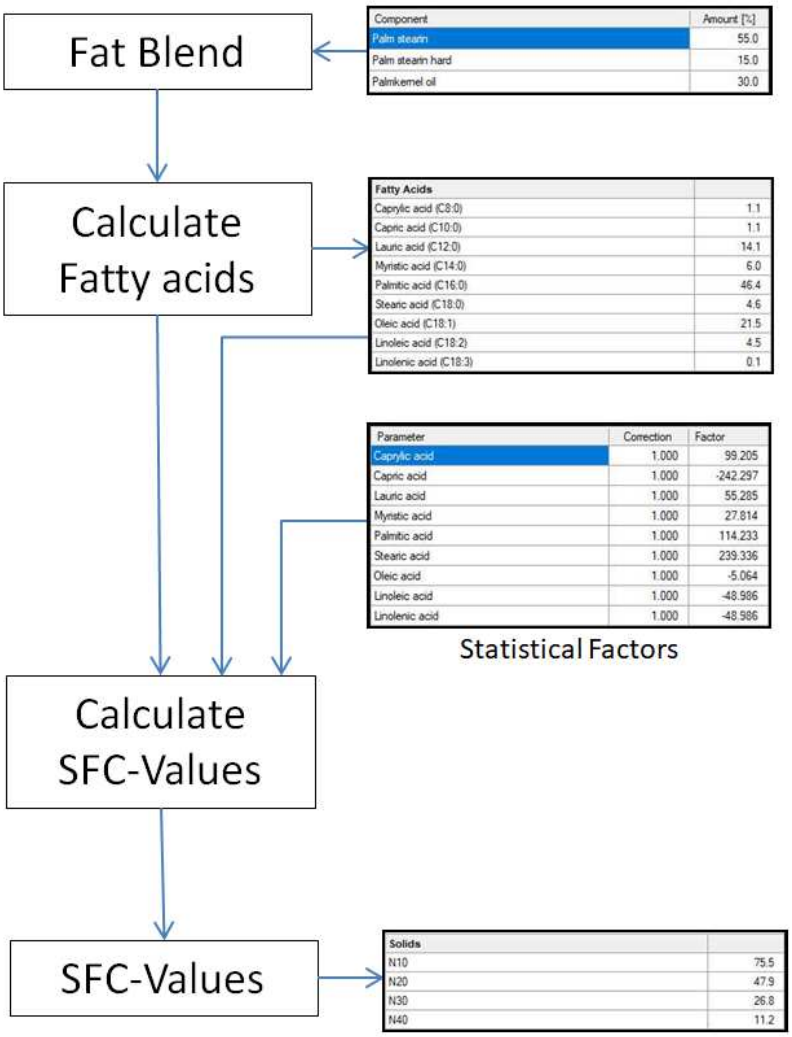
[1] Teles dos Santos, Moises and Gerbaud, Vincent and Le Roux, G. A.
C. *Modeling and simulation of melting curves and chemical interesterification of binary blends of vegetable oils.* (2013) Chemical Engineering Science, vol. 87 . pp. 14-22. ISSN 0009-2509

[2] Teles Dos Santos, Vincent Gerbaud, Galo Antonio Carrillo Le Roux. Solid Fat Content of Vegetable Oils and Simulation of Interesteri_cation Reaction: Predictions from Thermodynamic Approach. Journal of Food Engineering, Elsevier, 2014, vol. 126, pp.198-205.

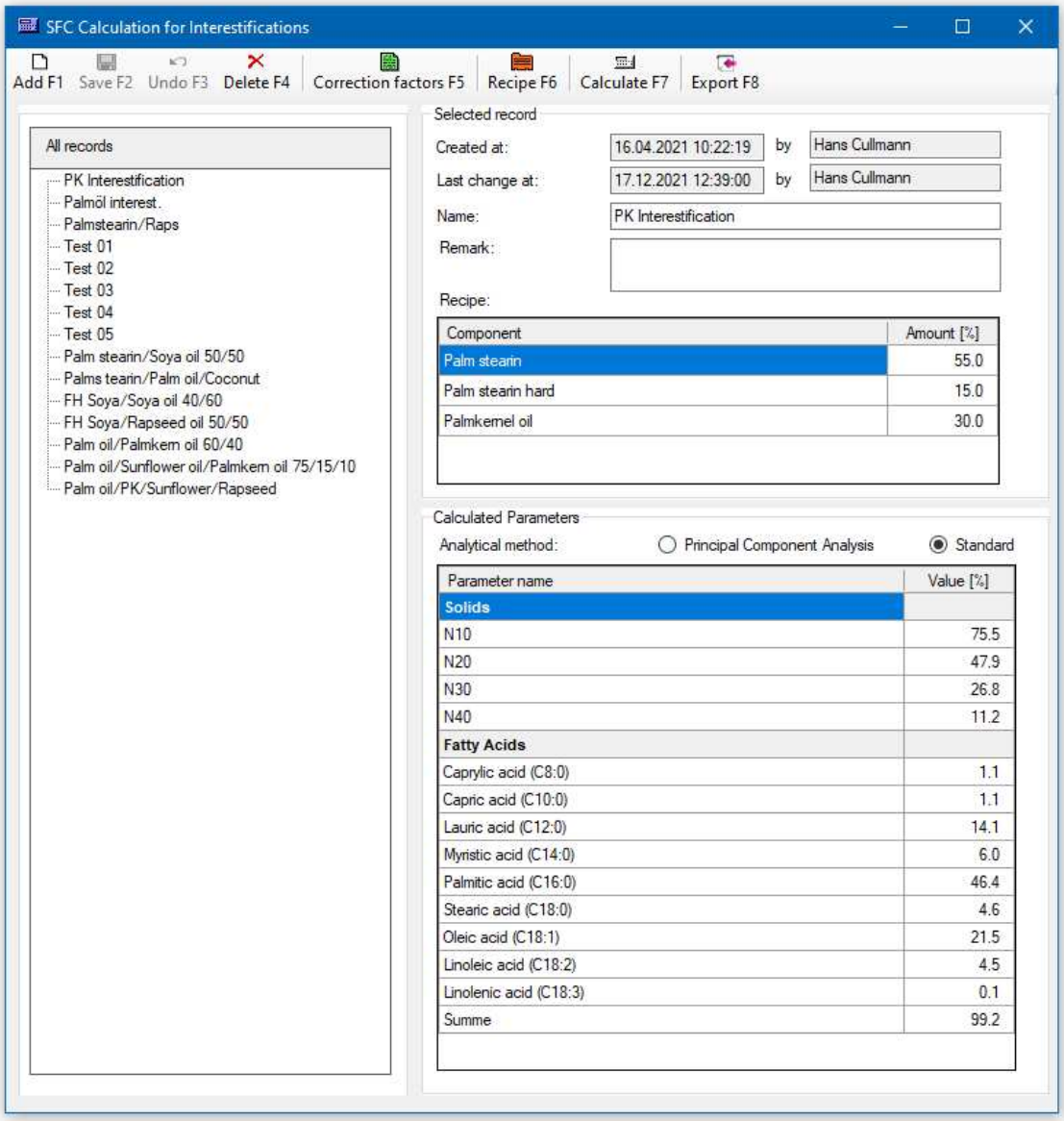
Much larger deviations arise from differences in the raw materials. You have to know that e.g. palm oil or palm stearin from previous studies had significantly different SFC values and fatty acids. Of course, this is particularly noticeable when you use older data. The specified SFC values still match the fatty acid spectra. Only if you use the corresponding recipe you will get different SFC values as well as different fatty acid spectra. We will show this when discussing the results. But first a few considerations about the procedure and how the calculation works.

How it works

As already mentioned, it is a statistical process. This means that before you can start the calculation, a statistical analysis of a lot of the existing data must be carried out. The order of the calculations is shown in the following figure:



On the basis of the fat mixture, the fatty acid spectrum is first calculated and the SFC values are calculated from the fatty acid spectrum with the help of statistically determined factors. For each fatty acid there is a statistical factor with which the proportion of the respective fatty acid is multiplied. The only thing the user has to do is to enter the recipe. The software calculates all other data up to the SFC values. There is an easy-to-use dialog for this (see below). As of the new version, it is also possible to export the interesterification as a component.



Determining the statistical factors is much more difficult. This is what the next section will look at.

Determination of the statistical Factors

The aim is to establish a relationship between the fatty acid spectrum and SFC values. To do this, it must first be clarified which fatty acids are relevant.

Fatty Acids
Caprylic acid (C8:0)
Capric acid (C10:0)
Lauric acid (C12:0)
Myristic acid (C14:0)
Palmitic acid (C16:0)
Stearic acid (C18:0)
Oleic acid (C18:1)
Linoleic acid (C18:2)
Linolenic acid (C18:3)

This results in a total of nine fatty acids that must be taken into account when calculating the factors (see table on the left). If necessary, additional fatty acids can be added or fatty acids that are not required can be removed from the calculation. A factor is determined for each of these fatty acids. The SFC value is obtained by multiplying the fatty acid proportions by the factors. The SFC value for the respective temperature is therefore a function of the fatty acid content.

Mathematically, the system to be solved can be represented as a linear system of equations with 9 unknown (fatty acids) and 130 equations (interesterifications).

$$\begin{pmatrix} C_{8:0}\,\%_{(1)} & C_{10:0}\,\%_{(1)} & C_{12:0}\,\%_{(1)} & C_{14:0}\,\%_{(1)} & C_{16:0}\,\%_{(1)} & \dots & C_{18:3}\,\%_{(1)} \\ C_{8:0}\,\%_{(2)} & C_{10:0}\,\%_{(2)} & C_{12:0}\,\%_{(2)} & C_{14:0}\,\%_{(2)} & C_{16:0}\,\%_{(2)} & \dots & C_{18:3}\,\%_{(2)} \\ C_{8:0}\,\%_{(3)} & C_{10:0}\,\%_{(3)} & C_{12:0}\,\%_{(3)} & C_{14:0}\,\%_{(3)} & C_{16:0}\,\%_{(3)} & \dots & C_{18:3}\,\%_{(3)} \\ \vdots & \vdots & \vdots & \vdots & \vdots & & \\ C_{8:0}\,\%_{(130)} & C_{10:0}\,\%_{(130)} & C_{12:0}\,\%_{(130)} & C_{14:0}\,\%_{(130)} & C_{16:0}\,\%_{(130)} & \dots & C_{18:3}\,\%_{(130)} \end{pmatrix} \bullet \begin{pmatrix} F_{C8:0} \\ F_{C10:0} \\ F_{C12:0} \\ F_{C14:0} \\ \vdots \\ F_{C18:3} \end{pmatrix} = \begin{pmatrix} N10_{(1)} \\ N10_{(2)} \\ N10_{(3)} \\ N10_{(4)} \\ \vdots \\ N10_{(130)} \end{pmatrix}$$

$$\mathbf{A} \quad \bullet \quad \mathbf{x} \quad = \quad \mathbf{b}$$

Here, C8: 0% is the percentage of the individual fatty acids and FC8: 0 is the specific factor of the fatty acid. N10 is the SFC value at 10 ° C for each of the n equations. So a linear system of equations with n = 9 unknowns and m = 130 equations has to be solved. For each SFC value - 10 ° C, 20 ° C, 30 ° C and 40 ° C - a 130 x 9 system of equations must be solved. After the factors have been successfully determined, the SFC value, e.g. for 10 ° C, can be calculated as follows:

$$N10 = C_{8:0}\,\% \times F_{C8:0} + C_{10:0}\,\% \times F_{C10:0} + C_{12:0}\,\% \times F_{C12:0} + C_{14:0}\,\% \times F_{C14:0} + C_{16:0}\,\% \times F_{C16:0} + \dots + C_{18:3}\,\% \times F_{C18:3}$$

That's the theory. In practice, however, there are some difficulties in solving the equation systems.

- It is an "overdetermined" system of equations, ie. there are many more equations than unknowns (130 to 9)
- It is a 'sparsely populated' system of equations, ie. many positions in the matrix are zero or have only very small values (<1).
- The values in the matrix are subject to more or less large errors.

Therefore standard methods (such as Gauss-Seidel) cannot be used, there is no exact solution. We have therefore chosen the Kaczmarz method [3] [4] for the iterative solution of linear systems of equations of the form Ax = b. Where A is a solvable and overdetermined matrix, b is the given solution and x is the solution vector.

With this method we have achieved useful results. During the investigations it was found that the stearic acid has a significant influence on the SFC values. This influence is so great that we have defined two different factors, one for low levels and one for higher levels. The limit was set at 10% stearic acid.

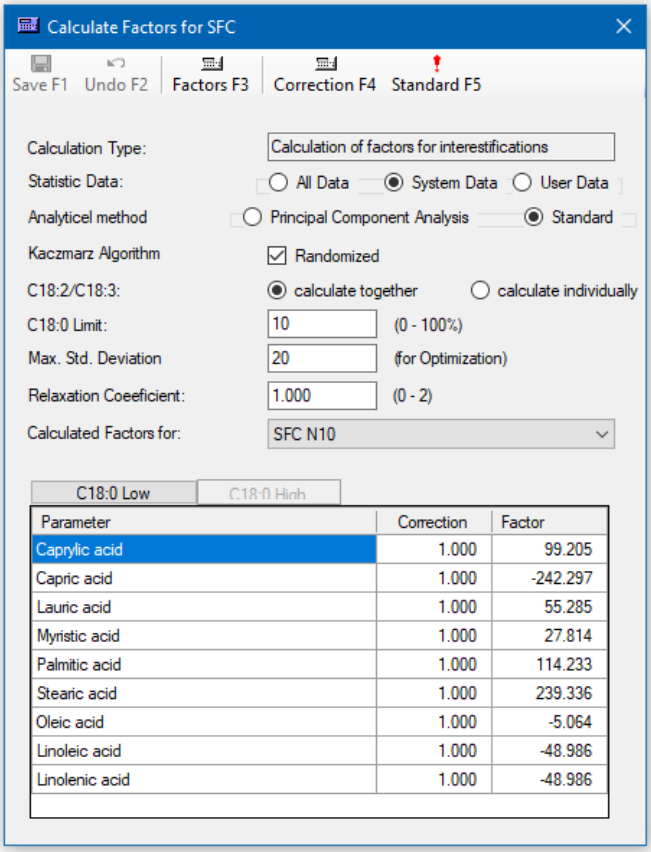
In addition, we tried out a relatively large number of options in order to get reproducible and plausible results. You can try out these options yourself or use our standard settings. The setting options are best explained using the dialog (see next page).

In addition to the familiar buttons for *Save* and *Undo*, there are three more:

- *Factors*
  After actuation, the calculation of the factors takes place with the set conditions. Depending on the CPU and main memory of the PC, this can take from 10 seconds to a few minutes.
- *Correction*
  If necessary, special correction factors can be calculated after the factors have been calculated. With these factors, the factors for calculating the SFC value are corrected by multiplication. Correction factor = 1 means no correction. The calculation time is similar to the calculation of the factors.
- *Standard*
  With this function the correction factors are set to 1.

[3] S. Kaczmarz: *Angenäherte Auflösung von Systemen linearer Gleichungen*. Bull. Internat. Acad. Polon. Sci.Lettres A, pages 355-357, 1937.

[4] J. Snoeijer, *Iterative image reconstruction algorithms for diagnostic medicine*, Bachelor-Thesis, University of Groningen, pages 30-33, 2014



Parameter	Correction	Factor
Caprylic acid	1.000	99.205
Capric acid	1.000	-242.297
Lauric acid	1.000	55.285
Myristic acid	1.000	27.814
Palmitic acid	1.000	114.233
Stearic acid	1.000	239.336
Oleic acid	1.000	-5.064
Linoleic acid	1.000	-48.986
Linolenic acid	1.000	-48.986

Dialog for calculating the interesterification factors

The parameters for the calculation are very numerous. In the dialog shown above, standard settings have been selected with which the best results have been achieved. Below is a brief overview of the parameters.

Statistic Data
These data are the known transesterifications that are used to calculate the SFC factors and that were entered either by us or by the user. You can select between:

- All Data
  All available data sets are used.
- System data
  Only data sets that have been entered by us will be used.
- User Data
  Only data sets entered by the user are used.

Analytical Method
There are two ways to calculate the factors. The default setting is *Standard*.

- Standard Procedure
  In this way of working, the factors for all fatty acids are calculated separately. If necessary, C18: 2 and C18: 3 can be combined. In the standard procedure, however, a distinction is made between fatty acid spectra with a high and low content of C18: 0. The limit value can be defined for C18: 0 (see below).
- Principal Component Analysis
  In this process, various fatty acids that behave similarly are grouped together. E.g.:
  - C8:0 + C10:0 + C12:0
  - C14:0 + C16:0
  - C18:2 + C18:3

  Unfortunately, this has not proven to be very successful in practice. The principal component analysis is still available, however, because better results may be achieved with other data configurations and more data sets.

Kaczmarz Algorithmn
If this checkbox is activated, a randomized algorithm is used, a variant of the method which converges more quickly in the case of overdetermined systems of equations.

C18:2/C8:3
Here you can select whether the two fatty acids C18: 2 and C18: 3 should be included in the calculation of the factors. Choosing this option is useful for two reasons.

- The two fatty acids behave very similarly in interesterification.
- There are only a few data sets with C18: 3> 1%.

This option is only possible with the standard procedure, not with the principal component analysis. The two fatty acids are combined there anyway.

C18:0 Threshold
This value can be used to set the percentage of the fatty acid C18: 0. This percentage divides the data sets into those with a Low and a High content of C18: 0. So far, a value of 10% has proven to be optimal. For other data configurations and more data sets, a different value may be useful.

In the standard procedure, two calculations are carried out each time. On the one hand for interesterification recipes with a low C18: 0 content, on the other hand for recipes with a high C18: 0 content. The C18: 0 content is determined automatically. When calculating the SFC values for interesterification, the selection of the factors takes place automatically based on the C18: 0 content determined.

With a limit value (threshold) of 0%, the factors are calculated for all data records, with 100% no calculation is carried out. This function is also only available for the standard method, not for the principal component analysis.

The table shown below in the dialog shows the factors for C18: 0 Low, you can switch over by clicking on the C18: 0 High button. Then the factors for C18: 0 high can be seen.

Max. Standard Deviation for Optimization
During the optimization, the factors are determined twice. After the first run, all data sets are separated whose standard deviation is smaller than the maximum value. A second run is started with these data records. This leads to significantly better results (see the following tables).

No Optimization

115 Records PCA	Temp.	Std. Dev.
	N10	7,94
	N20	9,02
	N30	8,79
	N40	8,39
	Average	**8,54**
85 Records Low	Temp.	Std. Dev.
	N10	6,66
	N20	7,45
	N30	7,21
	N40	7,48
	Average	**7,20**
30 Records High	Temp.	Std. Dev.
	N10	5,99
	N20	6,80
	N30	6,98
	N40	5,21
	Average	**6,25**

With Optimization

68 Records PCA	Temp.	Std. Dev.
	N10	6,82
	N20	6,10
	N30	4,89
	N40	2,31
	Average	**5,03**
47 Records Low	Temp.	Std. Dev.
	N10	5,84
	N20	5,22
	N30	3,79
	N40	2,08
	Average	**4,23**
21 Records High	Temp.	Std. Dev.
	N10	4,05
	N20	4,46
	N30	3,95
	N40	1,76
	Average	**3,56**

The maximum value for the standard deviation was set to 15 in the investigations carried out.

You can see two things from the two tables:

- The standard deviations are significantly lower after the optimization - that is, after the data sets with high standard deviations have been eliminated.
- The number of records processed as well.

However, there is a lower limit to the number of data records, at least 20 data records must be included in the calculation. Therefore, the maximum value of the standard deviation cannot be reduced arbitrarily, in the present case not lower than 15. This is probably possible with more data sets.

Relaxation Coefficient

Relaxation coefficients are used to achieve faster convergence with inconsistent systems of equations. The relaxation coefficient is a multiplicative factor, i.e. a value of 1 has no influence on the convergence.

There is a separate coefficient for each temperature of the SFC values. It can be changed after selecting the SFC value in the selection box below. However, we have not yet tried it out in practice.

Selection box for SFC-Values

With this selection box, an SFC value can be selected in order to display the factors in the table below or to enter the respective relaxation coefficient.

Results

Below are some examples of different interesterifications and a summary of the results. The calculation of the factors was carried out with the following settings:

• Analytical procedure	Standard
• Kaczmarz Algorithmn	Randomized
• C18:2/C18:3	Calculate together
• C18:0 Limit	10%
• Max Standard Deviation for Optimization	15
• Relaxation coefficient	1.0 for each temperature of the SFC values

First, two interesterifications with fully hydrogenated soybean oil are calculated. The SFC values are calculated using the factors for High C18: 0 content (> 10%). In both cases the C18: 0 content is approx. 45%. In the case of interesterification with rapeseed oil, the deviation between the target and the calculated at 10 ° C is relatively large, approx. 10%. The values at other temperatures agree well. The interesterification with coconut oil shows a greater deviation at 40 ° C. The fatty acid spectra agree well in both cases. However, only 21 data sets were available for calculating the statistical factors. More data sets will likely improve the result.

Recipe	50% FH Soybean oil 50% Rapseed oil	
	Target	Calc.
N10	43,2	53,9
N20	32,1	31,7
N30	24,0	21,4
N40	10,8	10,3
C8:0		
C10:0		
C12:0		
C14:0	0,1	0,1
C16:0	7,5	7,3
C18:0	45,3	44,7
C18:1	31,5	32,0
C18:2	9,8	9,3
C18:3	3,7	3,8
SAFA	52,9	52,1
MUFA	31,5	32,0
PUFA	13,5	13,1

Recipe	50% FH Soybean oil 50% Coconut oil	
	Target	Calc.
N10	89,6	91,0
N20	70,4	67,8
N30	37,6	41,4
N40	19,6	14,7
C8:0	3,4	3,5
C10:0	2,7	2,9
C12:0	22,5	23,2
C14:0	9,8	9,3
C16:0	10,2	9,8
C18:0	44,8	45,4
C18:1	4,1	3,9
C18:2	0,6	0,8
C18:3	0,1	0,2
SAFA	93,4	94,1
MUFA	4,1	3,9
PUFA	0,7	1,0

Interestifications with fully hydrogenated Soybean oil

The next example is a known interesterification - palm stearin / palmkernel 70/30 - a standard interesterification. If you calculate a mixture with the available data of the components, the values in the second column result. The agreement with the target values is significantly poor. This is apparently due to the fact that the palm stearin used for the calculation is much softer than that used for the real interesterification. If 20% of the palm stearin in the calculation is replaced by hard palm stearin, the calculated values are significantly improved. And one more thing, if you replace the palmkernel oil with coconut oil, you get almost the same results. Palmkernel oil and coconut oil can therefore be substituted in any ratio. This is important to know, e.g. when there are changes in the raw material market (raw material prices).

Recipe	70% Stearin 30% Palmkernel		50% Stearin 20% Hard Stea. 30% Palmkernel	50% Stearin 20% Hard Stea. 30% Coconut
	Target	Calc.	Calc.	Calc.
N10	75,9	67,2	74,8	75,4
N20	52,4	38,6	46,2	48,0
N30	25,5	19,0	25,4	27,2
N40	5,5	6,8	10,2	10,7
C8:0	1,4	1,1	1,1	2,1
C10:0	1,2	1,0	1,0	1,7
C12:0	14,1	14,4	14,4	14,1
C14:0	6,0	5,7	5,8	6,6
C16:0	43,5	42,5	46,6	47,0
C18:0	4,3	3,4	4,1	4,3
C18:1	23,0	25,4	21,5	19,1
C18:2	5,0	5,8	4,8	4,5
C18:3	0,3	0,2	0,3	0,3
SAFA	70,5	68,1	73,0	75,8
MUFA	23,0	25,4	21,5	19,1
PUFA	5,3	6,0	5,1	4,8

Palm stearin/Palmkernel oil /Coconut oil Interestifications

As a final example, interesterifications of palm stearin with liquid oils were investigated. Here, the target and actual values match relatively well - regardless of whether soybean oil, rapeseed oil or sunflower oil was used for the interesterification. However, it can also be seen that the SFC values depend on the ratio of unsaturated to saturated fatty acids. As a result, rapeseed oil gives the lowest SFC values.

Recipe	70% Stearin 30% Liquid oil	70% Stearin 30% Soybean	70% Stearin 30& Rapseed	70% Stearin 30% Sunflower
	Target	Calc.	Calc.	Calc.
N10	56,0	51,3	51,4	49,8
N20	30,0	28,8	25,3	26,8
N30	14,0	16,2	10,2	14,2
N40	3,0	5,6	1,2	4,4
C8:0				
C10:0				
C12:0	0,1	0,2	0,2	0,2
C14:0	1,1	0,9	0,9	0,9
C16:0	42,5	43,1	41,4	41,9
C18:0	4,5	3,9	3,1	3,7
C18:1	28,0	28,8	39,9	31,1
C18:2	21,5	20,3	10,6	21,3
C18:3	1,8	2,2	2,5	0,3
SAFA	48,2	48,1	45,6	46,7
MUFA	28,0	28,8	39,9	31,1
PUFA	23,3	22,5	13,1	21,6

Palm stearin/Liquid oil Interestifications

Conclusion

The investigations have shown that the SFC values of interesterifications can be estimated with statistical data. The accuracy is 3-5%, in some cases 10%, in a few cases even higher.

It is to be expected that the accuracy increases as more experimental data is available. We will inform you about this in due course.

Imprint

We would be glad to provide you with further information. Please feel free to contact one of our distributors.

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