

Oil-Expert.net

DGF

Deutsche  Gesellschaft für Fettwissenschaft e.V.

Oil-Expert.net

Standard Program for Fat Chemists

**Product Development
Calculation, Simulation and Optimization
of Fat Blends on the Computer**

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PREFACE

The first release of OilExpert was developed 1998 by Dr. Hans Cullmann at comicon GmbH. The software was already very complex at that time and the development was only possible through a broad knowledge spectrum of Dr. Cullmann:

:

- Study of chemical process engineering (Dipl. Ing.),
- Study of chemistry (Dr. rer. nat.) and
- Study of computer science.

All this was completed by many years of practical experience in working as a laboratory manager, quality manager and product developer in a large edible oil and fat refinery.

Over the years, OilExpert has been developed by several programmers to the present release 6.5.0 and was renamed to *Oil-Expert.net*. *Oil-Expert.net* has now over 100,000 lines of source code and there are more than 500 days of development and programming needed. *Oil-Expert.net* works with modern algorithms such as genetic algorithms. To make it easier for users and developers *Oil-Expert.net* has a completely object-oriented structure.

Today *Oil-Expert.net* is used by many well-known companies in the area of edible oil and food industry all over the world.

In June 2018 the comicon GmbH has closed business activities. The automation software - SFC Automation, Peak-O-Mat and cConnect - is now supported by LAIX Technologies. The copyrights to the software *Oil-Expert.net* are passed to Dr. Cullmann Consulting. Dr. Cullmann Consulting is now responsible for the customer support and further developments. In marketing and sales Dr. Cullmann Consulting is supported by Deutsche Gesellschaft fuer Fettwissenschaft e.V. and LAIX Technologies.

Please have a look on the website www.oil-expert.net, there is the newsletter no. 5 with new functions of release 6.5.0.

SHORT DESCRIPTION

Oil-Expert.net is a successor of OilExpert, covering and supporting the whole product development cycle in the latest release especially the development of recipes for fat refineries, margarine factories and the confectionery & chocolate area. Particularly if working with edible fats and oils it is possible to move a large part of laboratory work to the PC by calculation, simulation and optimization recipes and parameters.

The benefits are:

- Simplification and cost control in product development
- Workflow from the idea to the first delivery
- Audit Trail
- All important data are stored in a database and are available at any time
- Integrated recipe management with multi-level assemblies
- Great cost savings of regarding lab tests and analysis – minimization of lab costs
- Significant time savings
- Cost optimization – searching for a recipe with the lowest price
- Faster reaction to customer requests and internal process changes
- Fast response regarding to questions about possible recipes
- Quick and flexibel reaction on changes of the market eg commodity prices

Oil-Expert.net is intuitive, based on modern algorithms and easy to use.

SERVICES OVERVIEW

Oil-Expert.net consist overall of 6 modules and is multi-client capable. The access of the clients is controlled by the user management.

Basic modules for Product Development

The product development module consists of further sub-modules, containing apart from the project management also the workflow, recipe and user management.

Master Data Management is used to maintain analytic and component data. You can modify the supplied data and supplement them by your own. The 'Solubility Factors' for the calculation of the Solid Fat Content can be easily determined in the laboratory.

You can use the **Workflow Management** is to manage and control the projects. It contains approval and release mechanisms.

Project Management is used to store regarding particular projects – beginning with the initial idea up to the procedural instructions for the production. In each project, all project-related data are stored in a project container and are retrievable through intelligent search algorithms.

With the help of a "**Search Engine**", not only project data but also similar products can be found easily. Before a new project is initiated, the database can be trawled for possible matches with the required specifications of the new product.

The integrated **Recipe Management** operates on the basis of so-called assemblies. A recipe for margarine contains e.g. the following components: fat, vitamin, dye, water and packaging. Thus, changes can be reduced to a minimum.

User Management allows to define "roles" and can control the access down to the level of dialogs. Therefore it is possible to define which buttons are available in which roles or not.

Database includes more than just project data. It contains also the basic data that come along with standard products, such as edible oils, palm products, lauric fats etc. "Solubility Factors" necessary to calculate the Solid Fat Content are also supplied. MS ACCESS, SQL-Server or ORACLE can be used as database.

SERVICES OVERVIEW

Module for the calculation and simulation of oil and fat blends

Oil-Expert.net calculates the analytical values for given recipes including the Solid Fat Content with consideration of the mutual 'solubilities'.

Oil-Expert.net calculates the specifications which can be reached on the basis of a predefined blend.

Module for price optimization

Oil-Expert.net calculates possible blends with predefined specifications and recipes. It calculates the blend with the lowest price based on the daily prices of the raw materials.

Module for 'Recalculation'

Oil-Expert.net calculates possible recipes based on given analytical values (Solid Fat Content, fatty acids) of a sample or specification using the entered raw material data or those existing in the database.

Module for calculation of Solid Fat Content of interesterifications

Oil-Expert.net calculates the Solid Fat Content of interesterifications based on the fatty acid composition of a defined fat blend.

Module for import/export

Oil-Expert.net has an integrated interface – OE-Connect – to import and export data from external sources.

Working with *Oil-Expert.net*

The handling of *Oil-Expert.net* is Windows-compliant, requiring only basic Windows expertise.

Extensions

Oil-Expert.net can be extended by customer-specific functions or can be integrated in a function scheme of other programs (eg LIMS, QM-Module, ERP or Raw Material Optimization).

OIL-EXPERT.NET – CALCULATION FUNCTIONS FOR FAT BLENDS

Calculation of the analytical parameters of fat blends:

- Solid fat content considering to the solubility behaviour of edible oils and fats such as rapeseed oil, sunflower oil, coconut oil, palmkernel oil and palm oil.
- Fatty acid composition
- Triglycerides
- Iodine and saponification value
- Tocopherol content
- Sterol content
- Other analytical values, e.g. the sum of saturated fatty acid, sum of mono-unsaturated fatty acids, etc. (The list of analytical values is expandable with own data).

Product development on the computer by simulation

Instead of countless test blends and corresponding analyses, it's possible to develop new products with special properties by simulation on the PC using *Oil-Expert.net*. The laboratory work is limited to the verification of the results.

All parameters of fat blends mentioned above can be calculated according to your requirements. The analytical values of the components can be changed temporarily for special calculations, eg in order to allow the processing of faulty batches into production quickly.

Price optimization of fat blends

The composition of a recipe can be automatically optimized, taking the prices of raw materials into account and keeping a fixed specification (eg Solid fat Content, fatty acids). The result is the recipe with the lowest price.

Determination of fat recipes based on analytical parameters

Oil-Expert.net can calculate possible basic components based on the analytical values coming from a fat sample or a blend.

For this you need the results of a previous analysis during which at least Solid fat Content and fatty acids composition were determined. In Cases of doubt, it might also be necessary to have the results for triglycerides, tocopherols and sterols.

The raw materials to be used can either be predefined in the form of a list or searched for from all available components using the optimization algorithm.

OIL-EXPERT.NET – CALCULATION FUNCTIONS FOR FAT BLENDS

Verification of the putity of oils and fats

Oil and fat purity is verified by the comparison with extensive data material included in the delivery of the program. In case of certain oils, such as peanut oil, it is even possible to identify the origin.

Calculation of the Solid Fat Content of interesterifications

Given the fact that the fatty acids are randomly distributed over all triglycerides during chemical interesterification, it is theoretically possible, to calculate the Solid Fat Content from the fatty acid composition.

Requirement is a sufficient number of data records of known interesterifications (at least 100 records). This allows calculating the Solid Fat Content of interesterifications directly by entering the fat blend or the fatty acid spectrum.

Development of specifications

By calculating the analytical parameters in fat blends, it is possible to easily and quickly verify specifications or create new ones.

Search engine

A comfortable search engine allows to recover data quickly and safely.

Example: We look for a fat with Solid Fat Content N20 = 20-30 and N30 = 7-10. After starting the the query editor, the search engine shows all data sets complying with the criteria in the form of a table.

Data import and update

OE-connect allows inporting, exporting and/or updating data (Specifications, recipes, analytical values and prices) from external sources (text files, Excel, Access, ODBC data sources). You only have to define the links and to generate a script, whereupon the data can be updated by pushing a button.

Oil-Expert.net is supplied with the data of 40 public available standard components. Company specific products can be added to the database. Existing data sets can also be changed according to your own specifications. Integrated Data (Fatty acid spectra, tocopherols, sterols, Solid Fat Content, etc.) have been compiled through years of painstaking work from open literature sources and experience.

The master data structure is hierarchical:

- Articles / fat blends
 - Components (with interesterifications as a sub component)
 - Analytical parameters
 - Triglycerides
 - Fatty acids
 - Tocopherols
 - Sterols
 - Chemical characteristics
 - Other analyses
 - Packaging
 - Expenses
 - Laboratory experiments (refining, hydrogenation, interesterification)
 - Technical tests (combinator, frying tests)
 - Operational tests in the factors(refining, hydrogenation, interesterification)

Existing data can be expanded with your own data (eg, fatty acids for special applications). Data you don't use, e.g. Analytical parameters or components can be hidden.

Factors for iodine value and saponification value are used to calculate the iodine value and saponification value of the blend from the fatty acid composition.

In the section "Key Figures" and "Other Analyses" any own parameters can be defined. Definition of new sections is also possible e.g. "Special Parameters".

OIL-EXPERT.NET IN DETAILS – BASIC MODULE: MASTER DATA

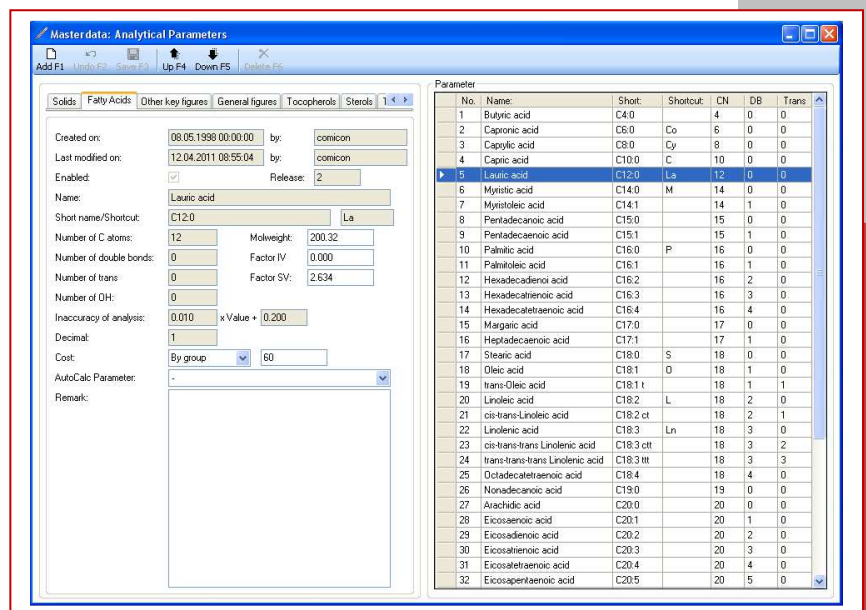
The so-called "Solubility Factors" are in the delivery of the program and are based on empirical measurements which can be determined using a NMR device on the basis of series of blends with a standard component.

Apart from the fat specific master data, the following is also available:

- **Grouping**
Grouping criteria for other master data (eg for the components: rapeseed, sunflower, soya, palm, animal, etc.)
- **Customer Data**
 - Company
 - Address
 - Contact data
 - Contact person
- **Recipes**
 - Subassemblies
- **Nutritional values**

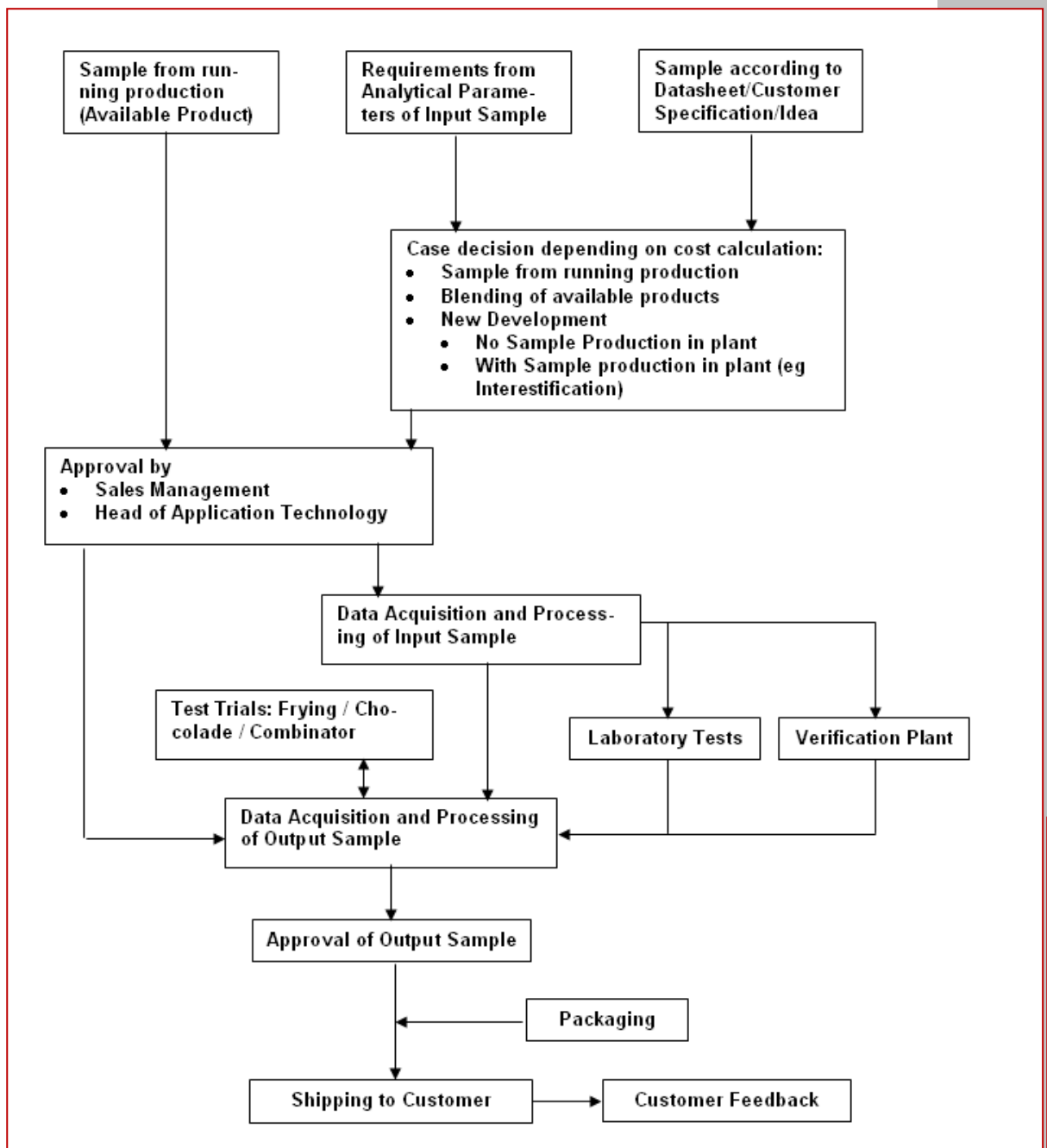
All master data are subject to version control. When changing a data set a new version is created. This way it is easy to trace the changes regarding author, subject and time of change.

For editing the corresponding master data you can use dialogs, (an example of the processing of fatty acids is shown in the figure below).



OIL-EXPERT.NET IN DETAILS – BASIC MODULE: WORKFLOWMANAGEMENT

This workflow controls the process of product development (see illustration). It contains the functions for the approval of sample inquiries and the release of outgoing samples and specifications. Of course, these mechanisms can be turned off, if desired.



OIL-EXPERT.NET IN DETAILS – BASIS-MODULE: PROJECT MANAGEMENT

Project management is used to manage the complete product development cycle. Each project comprises the following steps:

- Input sample / specification / idea
- Analysis / Determination or definition of analytical parameters
- Laboratory tests
 - Blending
 - Hydrogenation
 - Interesterification
 - Refining (deacidification, bleaching, deodorization)
 - Tests for chocolate applications
 - Frying tests
 - Tests for margarine applications (eg combiner)
- Output sample
- Creation of specifications
- Recipe
- Production instructions

All data pertaining to a project are saved together in a “Project Folder” – a kind of “Project container”.

Definitions

- **Input sample:** These are mainly customer samples but also those samples from a competitor or raw material samples. A project has at least one input sample but can also contain any number of input samples. In some cases the fat has to be isolated from the input sample (eg margarine) before determining the analytical values.
Instead of an input sample, you can also use a description (eg an idea), or a customer specification sheet containing the necessary specifications.
- **Analytical Parameters:** These parameters include all data describing a product. The following grouping of the parameters is proposed (as an example for fat oils and fats), but can be modified at any time:
 - **Quality Parameters**
Colour, ffa, POV, anisidine value, smoke point, water, oxidation stability, polar parts, soap, taste, etc.

OIL-EXPERT.NET IN DETAILS–BASIS-MODULE: PROJECT MANAGEMENT

- **Physical Parameters**
Refraction index, solid fat content, melting point, etc.
- **Chemical Parameters**
Iodine value, saponification value, etc.
- **Fatty acid spectrum**
- **Triglyceride composition**
- **Tocopherol/Sterol content**
- **Miscellaneous Parameters**

The number of groups and parameters as well as their assignment can be changed or expanded at any time.

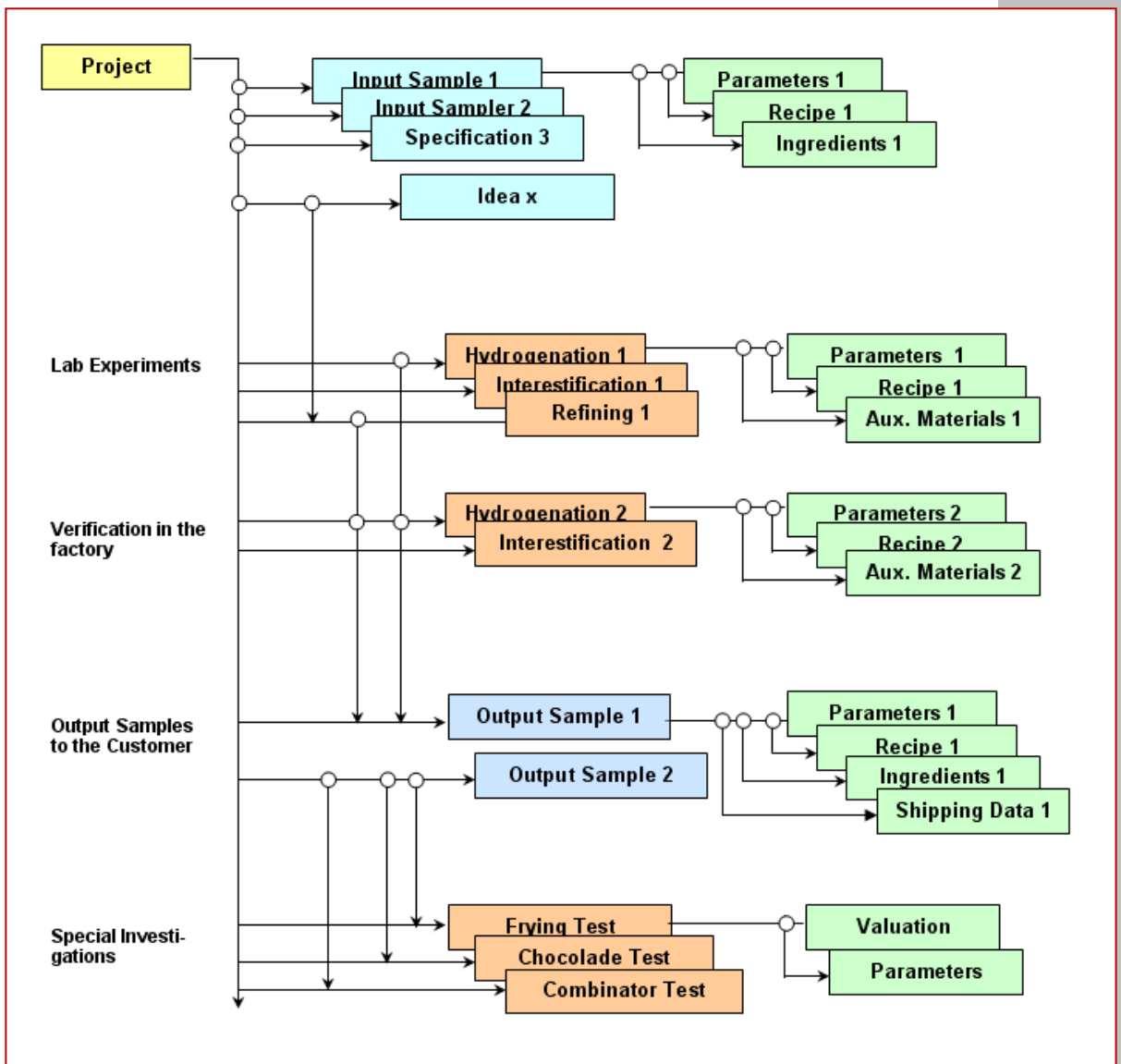
- **Laboratory tests:** All tests required in to get one or more output samples based on the data and the analytical parameters of the input sample, containing as much equivalent properties as the input sample as possible. The following processing options are predefined (expandable by the user):
 - Blending of several oils and fats, hydrogenated or interesterified fats for example
 - Hydrogenation
 - Interesterification
 - Enzymatic interesterification
 - Fractionation
 - Refining
 - Deacidification
 - Bleaching
 - Deodorization
 - Frying tests / Tests for chocolate applications / tests for margarine applications

Each project can be assigned any number of laboratory tests.

- **Output sample:** These are the samples, developed using the analytical parameters and characteristics from the input sample. Any number of output samples can be assigned to a project. The output sample must not necessarily be delivered to the customer. For each output sample, the following shipping information is recorded: date of shipment, shipping type (courier, freight forwarding, etc.), costs, a reference to the forwarder/courier.
- **Recipes:** The recipe is divided into fat assemblies and other assemblies. The sum of all fat recipe components is always 100%. All data are normalized to 1000 kg.

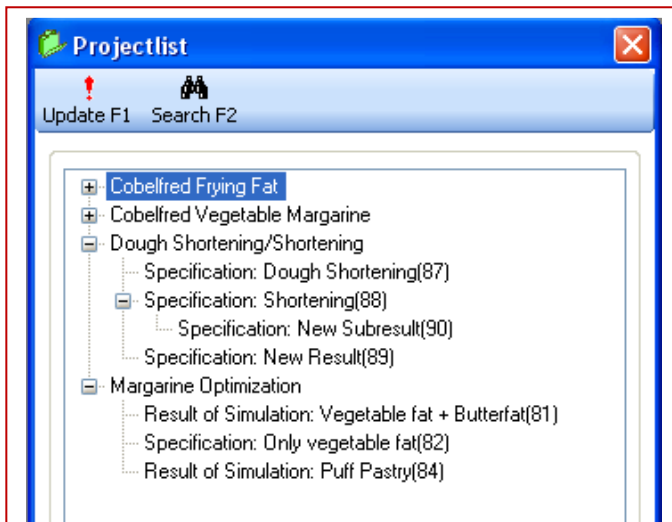
Data structure

The complex data of a project are presented as a tree structure (see illustration). This allows the optional assignment of any input sample, laboratory test and output sample. Every part of the tree structure can get any analytical data, recipes, additives etc. assigned. Each project obtains a unique identification number, which can be identified in all branch nodes of the tree. This allows for example to find a particular sample on the basis of given analytical values and to map the whole project due to the project identification number.



OIL-EXPERT.NET IN DETAILS – BASIS-MODULE: PROJECT MANAGEMENT

This data structure is dynamic and can also be easily found in the program (see the first figure). It can also be extended. Each node is associated with a data sheet, in which the associated data are stored (see the second figure).



Project Tree View

Datasheet

The Datasheet window displays project details on the left and two data tables on the right. The project name is 'Vegetable fat + Butterfat' and the datasheet type is 'Result of Simulation'. The component table shows the composition of the product, and the parameter table shows the simulation results for solids and fatty acids.

Component	Completely	Only Fat
Butterfat	248	29.8
PK Interesterification	280	33.6
Rapeseed oil	0	0.0
Sunflower oil	272	36.6
Water	200	-

Name	Unit	Min	Req	Max	Calc
Solids					
10°C	%	30.0	35.0	40.0	34.3
20°C	%	14.0	17.0	20.0	19.7
30°C	%	4.0	6.0	8.0	6.9
40°C	%	0.0	1.5	3.0	1.4
Fatty Acids					
Butyric acid (C4:0)	%		1.1		1.3
Capronic acid (C6:0)	%		0.6		0.6
Caprylic acid (C8:0)	%		1.0		0.9
Capric acid (C10:0)	%		1.4		1.3
Lauric acid (C12:0)	%	3.0	5.2	9.0	5.0
Myristic acid (C14:0)	%		5.1		4.9

OIL-EXPERT.NET IN DETAILS – BASIS-MODULE: SEARCH ENGINE

Another problem in terms of practical work that *Oil-Expert.net* can solve, is the finding of fat blends with certain analytical parameters out of a large amount of documented values - over many years. For this purpose a comfortable search engine is included. After entering specific criteria all products that match these criteria are found and listed.

There are three different search options:

- Search for projects using a special dialog as
 - At work / finished
 - Article number
 - Customer, etc.
- Report Generator
Targeted search for all parameters, e.g. Project ID, project name, sample numbers, components, parameters, analytical values, etc.
- „Genetic“ Search Engine
Search for products with **similar** characteristics, eg search for all products containing about 30% coconut oil with
N20 about 28%,
N30 about 12%,
C18:2 about 25% and
trans max 2%.

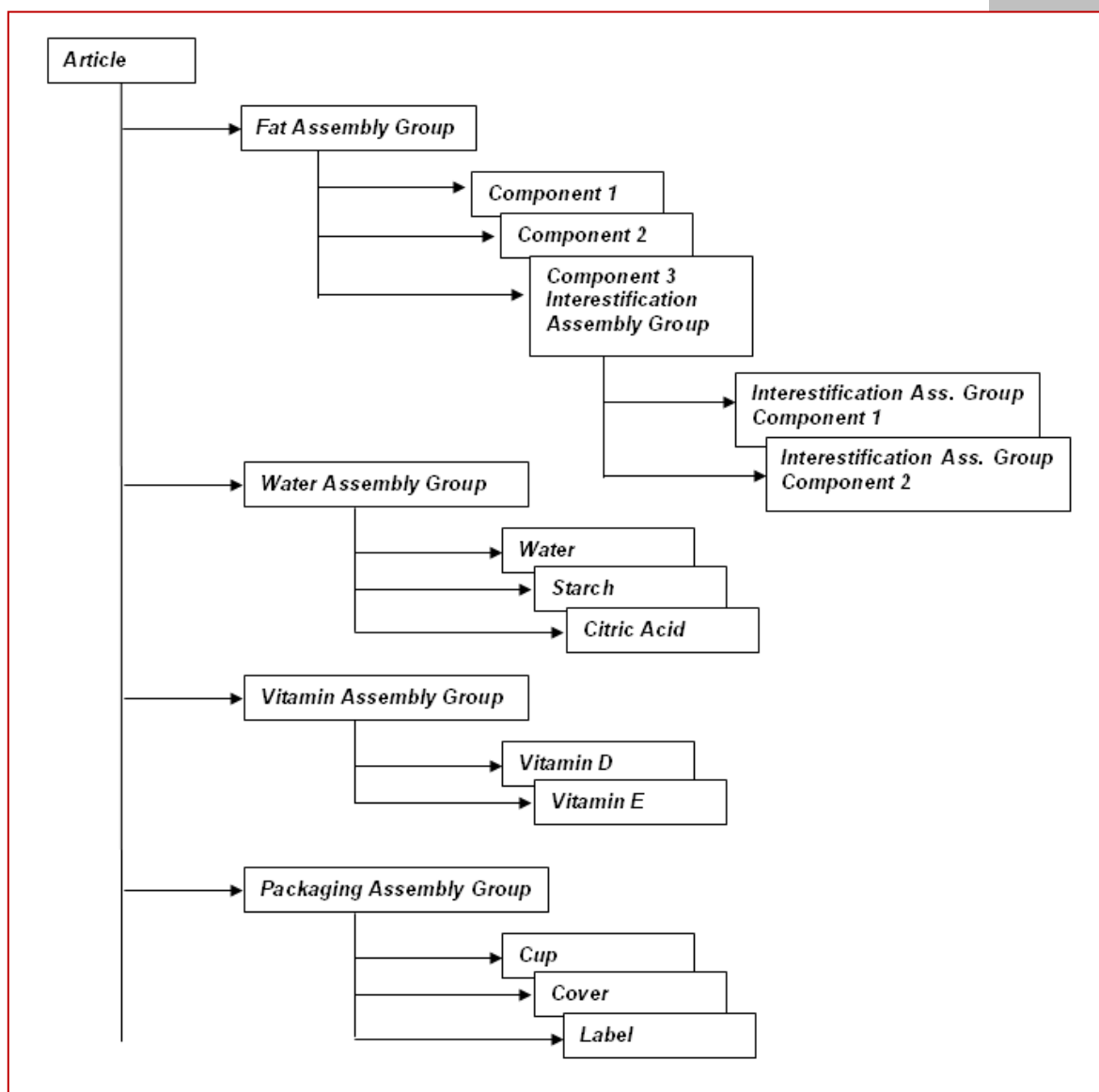
The screenshot displays two windows from the Oil-Expert.net software. The top window, titled "Experts Searching for Blends", is used for defining search queries. It shows a list of "Defined queries" on the left, with "Vegetable Margarine" selected. The main area is for "Query definition", where the description is "Vegetable Margarine". Below this, there is a table for defining search criteria with columns for "Parameter", "Component", "Operator", and "Min. value". The current criteria are: Rohstoff (Butter olein) with an equals sign operator. Below the table, a list of search criteria is shown: "[N10] inRange 22 to 28", "And [N20] inRange 10 to 15", "And [N30] <= 4", "And [PUFA] >= 20", and "And [Kokosöl] < 10". Buttons for "Add to Search (and)", "Add to Search (or)", "Add (", and "Add)" are visible. The bottom window, titled "Search Engine", shows the search parameters. It includes fields for "Datenquelle" (Sollwerte), "Fitness" (0.9500), and "Max hits" (5). Below these, it shows the "Aktuell beste Übereinstimmung" (0.9876) and the "Projekt" (Margarine Optimization). The "Datenblatt" (Vegetable fat + Butterfat) is also displayed. A table of "Components" is shown with columns for "Fat content" and "Component":

Fat content	Component
29.8	Butterfat
33.6	PK Interestification
36.6	Sunflower oil

The "Search Status" window shows a bar chart with a fitness value of 0.9876.

OIL-EXPERT.NET IN DETAILS – BASIS-MODULE: RECIPE MANAGEMENT

The administration of the formulations is managed by assemblies. In order to better understand the procedure we present an example of a margarine recipe below. Working with assemblies has the advantage that a particular module may appear in several articles. Any changes to this assembly would automatically apply to all recipes where this assembly occurs. Each module has a valid date from/to. If a recipe consists of assemblies with different validities, the validity of the recipe is calculated automatically based on the validities of all assemblies. The subassembly with the shortest validity determines the validity of the recipe.



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OIL-EXPERT.NET IN DETAILS – BASIS-MODULE: RECIPE MANAGEMENT

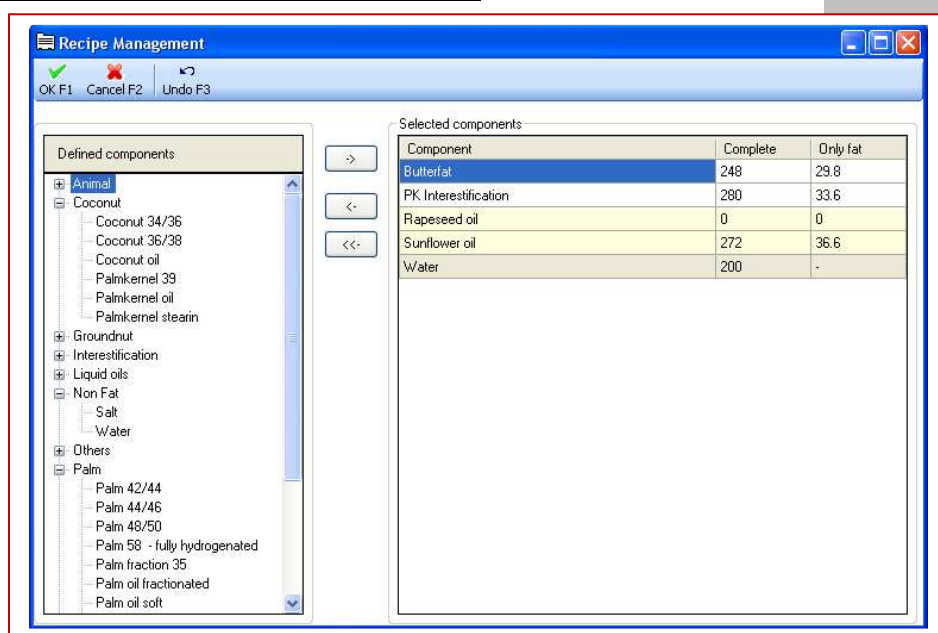
The software has a version control management, allowing always only one valid recipe for a defined period. Each change, even in the assemblies, triggers the creation of a new version. The status of the former recipe is automatically set to historic.

The recipe ingredients are normalized to 1000 kg, switchable to 100 kg. The fat recipe is always calculated in parallel to 100% total fat (see illustration). This is necessary for the calculation routines of *Oil-Expert.net*.

The recipes are presented as a linear list in the data sheet. For commercial purposes, the recipes can be outlined in more detail. For the commercial recipes assembled components, such as interesterifications, are split in their percentage shares.

The amount of the product in a recipe can also be "overloaded". This means, the total amount of a recipe can weigh more than 1000 kg. This is a common practice in refineries. The fatty components are normalized to 1000 kg, plus some additives in small quantities. Example:

Components	Amount [kg]	Amount %
Rapeseed oil	500,0	50
Palm oil	150,0	15
Transesterification	350,0	35
Sum Fat	1.000,0	100
Tocopherol-Acetate	0,1	-
Sum total	1.000,1	-



Oil-Expert.net

OIL-EXPERT.NET IN DETAILS – BASIS-MODULE: USER MANAGEMENT

Oil-Expert.net offers a sophisticated user management, which is multi-client capable and allows for the allocation of roles.

The role assignment is possible at various levels:

- Plant level
- Module level
- Functional level
Read only/modify/add//delete
- Dialog level
Fields and Buttons

The screenshots illustrate the user management interface. The top window, 'Master Data: Users', shows a list of defined users (admin, hcullman) and a form for editing a user. The middle window, 'Master Data: Rolls', shows a list of defined functions (Administration, Master Data, User) and a table for assigning roles to users. The bottom window, 'Master Data: Usergroups', shows a list of defined groups (Administrator, User, Test Group, Master data) and a table for assigning roles to usergroups.

Usergroups	Access
Administrator	<input checked="" type="checkbox"/>
User	<input checked="" type="checkbox"/>
Test Group	<input checked="" type="checkbox"/>

Dialog	Button	Access
Recipe Management	Cancel	<input checked="" type="checkbox"/>
Recipe Management	!! OK	<input checked="" type="checkbox"/>
Recipe Management	Undo	<input checked="" type="checkbox"/>
Recipe Management	Actual release: [1], valid si...	<input type="checkbox"/>
Recipe Management	Newest release: [1], valid s...	<input type="checkbox"/>
Recipe Management	Update selected component	<input type="checkbox"/>
Recipe Management	Update all components	<input type="checkbox"/>
Component Mixer	Cancel	<input checked="" type="checkbox"/>
Component Mixer	OK	<input checked="" type="checkbox"/>
Component Mixer	Print(Print graphic and valu...	<input type="checkbox"/>
Component Mixer	Undo	<input checked="" type="checkbox"/>
frmComponentRecipe	btnCancel	<input checked="" type="checkbox"/>
frmComponentRecipe	btnOK	<input checked="" type="checkbox"/>

Roles	Access
Administration	<input checked="" type="checkbox"/>
Master Data	<input type="checkbox"/>
User	<input type="checkbox"/>

OIL-EXPERT.NET IN DETAILS – SIMULATION AND OPTIMIZATION

Simulation

Simulation is the analysis of the systems too complicated to formulaic treatment. In order to obtain knowledge about the real model, experiments on a model are necessary.

Examples: crash test, flight simulator, weather forecast

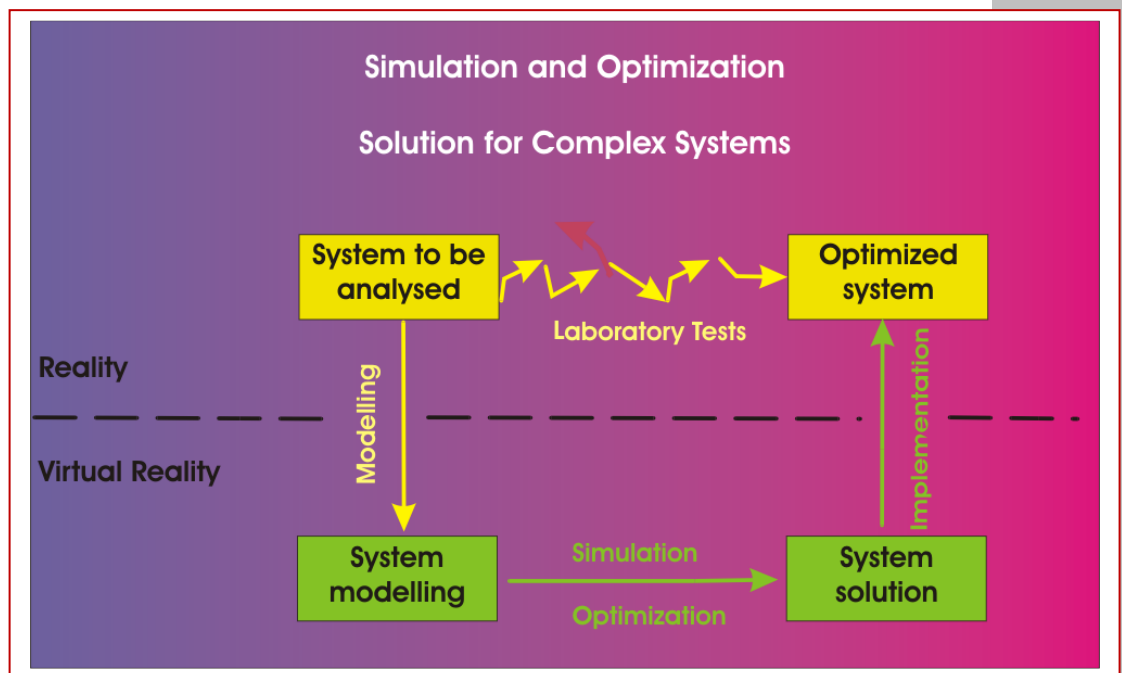
Optimization

Optimization of linear objective functions (linear equations)

Examples: production planning, mixing problems, simplex method

Advantages

- Using simulation it is possible to calculate non-linear systems (Solid fat Content for example). We have developed a corresponding simulation model.
- Instead of extensive laboratory tests, a satisfactory result is reached in a short time on the PC. This leads to an enormous saving of time and money.
- Optimization allows you to determine quickly and easily the lowest price of a fat blend, e.g. by changes in price of raw materials. The optimization process considers all default specifications..



Calculation – Product development - Specifications

With the help of this module **any analytical value of fat blends** can be calculated quickly and easily. You can enter up to 10 components. By pressing a button the following values are calculated:

- Fatty acid spectrum
- Triglycerides
- Tocopherol content
- Sterol content
- Solid Fat Content considering eutectic effects
- Refractive index, iodine value, saponification value
- Miscellaneous analyses
- Price

After entering the components their proportion can be changed using sliders. The result of the changed blend is immediately available as a value, along with the corresponding graphic.

Fatty acids, triglycerides, tocopherols and sterols to be calculated are determined automatically by changing the components. Only the analytical values actually available in the selected components are calculated and displayed. For example tocotrienols can be calculated only for palm products and corn oil.

The screenshot shows a software interface for calculating fat blends. It features a section titled 'Components' with five rows, each representing a different oil component. Each row includes a checkbox, a percentage value, the component name, and a slider control. The components and their current values are:

Component	Percentage (%)
Coconut oil	18.7
Palm oil standard	41.7
PK Interestification	16.6
Rapeseed oil	0.0
Sunflower oil	23.0

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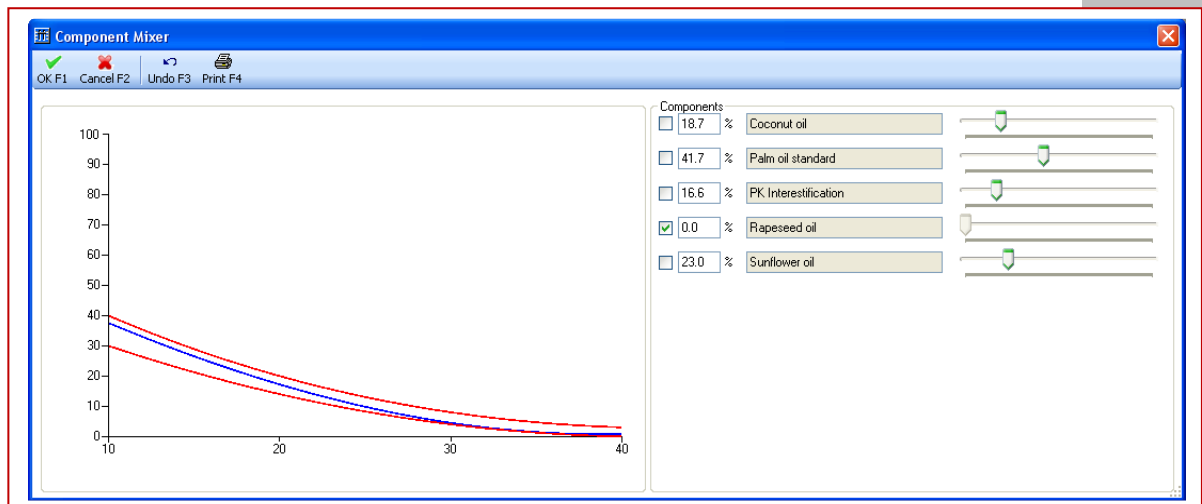
OIL-EXPERT.NET IN DETAILS – MODULE: CALCULATION / SIMULATION

Oil-Expert.net allows for a simple and rapid prototype developing of new fat blends with special properties on your PC.

After specifying a recipe once all selected parameters are calculated. Using the slider the percentage of each component may be changed quickly. The effects of changes on the parameters are immediately visible on the screen.

The advantage of this method is a huge time saving. Instead of series of tests and the corresponding analysis, in most cases it is sufficient to perform a control analysis only with the end result of the simulation.

Another useful effect is the possibility to check specifications for fats or fat blends or those coming from customers as regards their plausibility and feasibility on the PC.



OIL-EXPERT.NET IN DETAILS – MODULE OPTIMIZATION

This module allows the **optimization of the fat blend** in terms of specifications and the **price optimization** in accordance with predetermined criteria.

Besides the optimization, it also allows for product development on a PC: After entering the predefined specifications the program looks for the best solution for the composition.

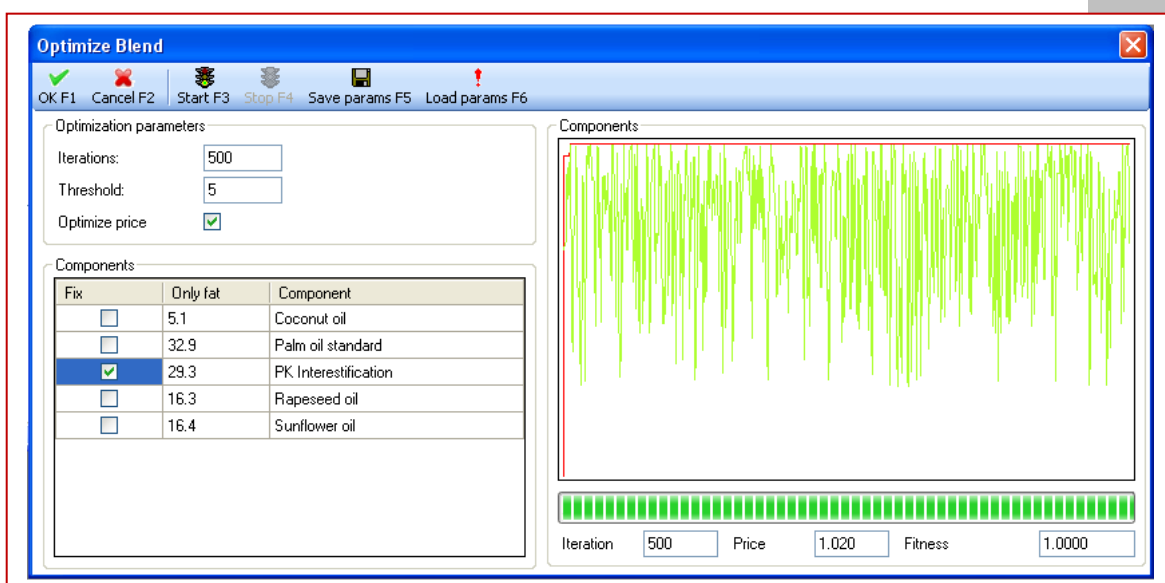
You can define a list that can contain any number of components. The optimization algorithm will automatically select the right components. If there are several options available to meet the required specifications all possible solutions will be stored and displayed.

Calculated values enclosed by the given will be shown in green elsewise in red.

The program also determines the degree of compliance (Full conformity = 1, no match = 0).

You usually need 100 iterations per calculation. But even 1000 calculations are usually through within a few seconds.

As another option, it is possible to fix the percentage for one or more components. It could be useful in case of expensive components for cost reasons. In the subsequent optimization only the percentages of the remaining components have to be changed.



OIL-EXPERT.NET IN DETAILS – MODULE OPTIMIZATION

This optimization problem is solved using genetic algorithms. The basis for the genetic algorithms consists of biological processes, such as the population of living organisms (in our case the fat blends), the competition between organisms and their reproduction. This way a selection of "higher stages" (i.e. better match) can be made.

Genetic algorithms are particularly used in calculations with very complex and high-dimensional algorithms, as in the present optimization. They are characterized by short processing times and optimal results.

Predetermined parameters for the optimization:

Threshold value	Value for the minimum share (percentage) of a component (eg 2%). This way the selection of many components with very small amounts can be prevented, because such blends are not produced in reality.
Matching	Solutions achieving at least the preset value (eg 95%) will be saved.
Iterations	Number of cycles necessary to calculate an optimal blend ratio for a certain number of components. Usually 100 cycles are sufficient.
Number of components	Maximum number of components used to obtain a result (adjustable).
Populations	Number of blends in one generation (see below). The components of the blends are statistically defined after a preliminary selection of usable components. Reasonable values for the populations, i.e. blends vary between ten and fifty. After optimization of their percentage the populations are "mutated", "crossbred" and "selected for the next generation."
Generations	Number of mutation cycles. Useful optimization results can be achieved in most cases after 10-20 generations.

A brief introduction to the technique of genetic optimization is presented in the Appendix.

OIL-EXPERT.NET IN DETAILS – MODULE: REVERSE CALCULATION

Oil-Expert.net – Investigation of unknown fat blends

In order to investigate the components and composition of an unknown fat blend (eg investigation of competitive products), a complete analysis is required (fatty acid spectrum and Solid Fat Content, in cases of doubt also tocopherols and sterols).

After input of the determined values, the same analysis possibilities as already mentioned under point optimization, including optimization are available. The difference is that here the measured values are compared with the calculated values (100% conformity = 1).

The reverse calculation shows the advantages of genetic search algorithms. Without presetting certain components you can search with all available components. It is also possible to select the components in a template.

The screenshot displays two windows from the Oil-Expert.net software. The top window, 'Hits of Simulation', shows a table of simulation results and a table of components. The bottom window, 'Simulation of Mixtures', shows simulation parameters and a graph of the simulation progress.

Hits of Simulation

No.	Fitness	Price
1	0.9915	2.046
2	0.9896	2.074
3	0.9888	1.900
4	0.9885	2.013
5	0.9865	1.894
6	0.9847	1.755
7	0.9836	2.062
8	0.9830	1.843
9	0.9797	2.025
10	0.9778	2.055

Component	Whole part	Fat part
Butterfat	0	31.5
PK Interestification	0	32.3
Sunflower oil	0	36.2

Simulation of Mixtures

Simulation parameters:

- Iterations: 100
- Threshold: 5
- Fitness: 0.9500
- No. of comp.: 5
- Populations: 50
- Generations: 30
- Max hits: 10

Aktuell beste Übereinstimmung: 0.9868

Name	Unit	Min	Req	Max	Calc
Solids					
10°C	%	30	35	40	34.3
20°C	%	14	17	20	19.5
				8	6.7
				3	1.3
					1.3
					0.6
					0.9
					1.3
				9	4.9

Simulation graph showing Best fitness vs Generation. Generation: 1, Population: 36, Best fitness: 0.9868.

OIL-EXPERT.NET IN DETAILS – CRYSTALLIZATION PROPERTIES

Oil-Expert.net – Estimation of crystallization properties

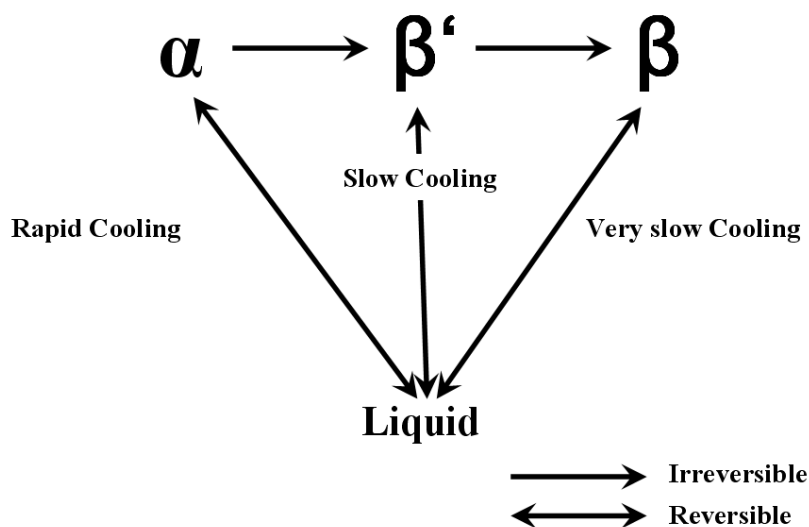
Fats crystallize polymorphously. There are three crystal structures: α , β and β' whereby the β -phase is the most stable one in the given order.

In order to achieve specific properties, e.g. certain plasticity, it is important to have the knowledge of the crystal modification of triglycerides. These properties are dependent on the triglyceride composition. The relationships are very complex and it requires the analysis of triglycerides.

Oil-Expert.net delivery includes triglyceride compositions of all major components and can perform an assessment of fat blend post-crystallization after solidification. This is important for example when assessing the "sandiness" of margarine blends.

Further calculations with the help of triglycerides will be available in upcoming updates.

Fat Crystallization



OIL-EXPERT.NET IN DETAILS – MODULE: INTERESTIFICATION

Calculation of the SFC values of interesterifications

Oil-Expert.net calculates the Solid Fat Content of interesterified fat blends from the fatty acid composition of a mixture. The base for the calculation is the statistical distribution of fatty acids on triglycerides after the chemical interesterification.

For statistical work you need to have a sufficient number of known interesterifications – about 100 records. Based on the input of the fatty acids and the Solid Fat Content an algorithm determines the factors to calculate the Solid Fat Content at various temperatures. Since the interesterification is never completed up to 100% in normal operation, you can set a correction factor for each temperature. Enzymatic interesterifications can also be calculated by adjusting the correction factors.

If sufficient experimental material is available, the Solid Fat Content is calculated automatically from the fatty acid spectrum of a given fat blend.

Fatty Acid	Amount %	SFC	%
C 4	0	10°C	60
C 6	0	20°C	37
C 8	0	25°C	0
C 10	0	30°C	18
C 12	0.4	35°C	11
C14	1.1	40°C	5
C 16	42.9		
C 18	4.3		
C 18:1	40.5		
C 18:1 trans	0.2		
C 18:2	9.5		
C 18:2 trans	0.1		
C 18:3	0.4		
C 18:3 trans	0		
C 20	0.2		
C 20:1	0.2		
C 22	0		
C 22:1	0		
C 24	0		

Name	Calc.	Last mod. on
Palm oil 3	<input checked="" type="checkbox"/>	09.11.2012
Palm oil 2	<input checked="" type="checkbox"/>	09.11.2012
Palm oil 1	<input checked="" type="checkbox"/>	09.11.2012
Sunflower 5	<input checked="" type="checkbox"/>	09.11.2012
Sunflower 4	<input checked="" type="checkbox"/>	09.11.2012
Sunflower 3	<input checked="" type="checkbox"/>	09.11.2012
Sunflower 2	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Rape 8	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Rape 7	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Rape 6	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Rape 5	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Rape 4	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Rape 3	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Rape 2	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Rape 1	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Coconut 6	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Coconut 5	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Coconut 4	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Coconut 3	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Coconut 2	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Coconut 1	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Olein 4	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Olein 3	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Olein 2	<input checked="" type="checkbox"/>	09.11.2012
Palm stearin/Olein 1	<input checked="" type="checkbox"/>	09.11.2012
PK/Stearin 5	<input checked="" type="checkbox"/>	09.11.2012
PK/Stearin 4	<input checked="" type="checkbox"/>	09.11.2012
PK/Stearin 3	<input checked="" type="checkbox"/>	09.11.2012

OIL-EXPERT.NET IN DETAILS – CASE STUDY

A recurring job for a fat chemist is the development of a recipe based on given analytical parameters – usually solid fat content and fatty acids – with which the analytical parameters can be realized and which covers the available commodity portfolio.

In order to find an appropriate recipe, many blends and analytical investigations in the laboratory are needed. If using *Oil-Expert.net* the time required is reduced to one or two hours – from analysis to final specification.

The time savings is due to the consistent use of simulation and optimization. The development cycle begins with the creation of a new project and the input of the measured analytical values (Please see the flow-diagram on the next page).

The easiest and fastest way to find a suitable recipe is to use the search engine. Using the recipe library all records with the same parameters as the input data are found quickly.

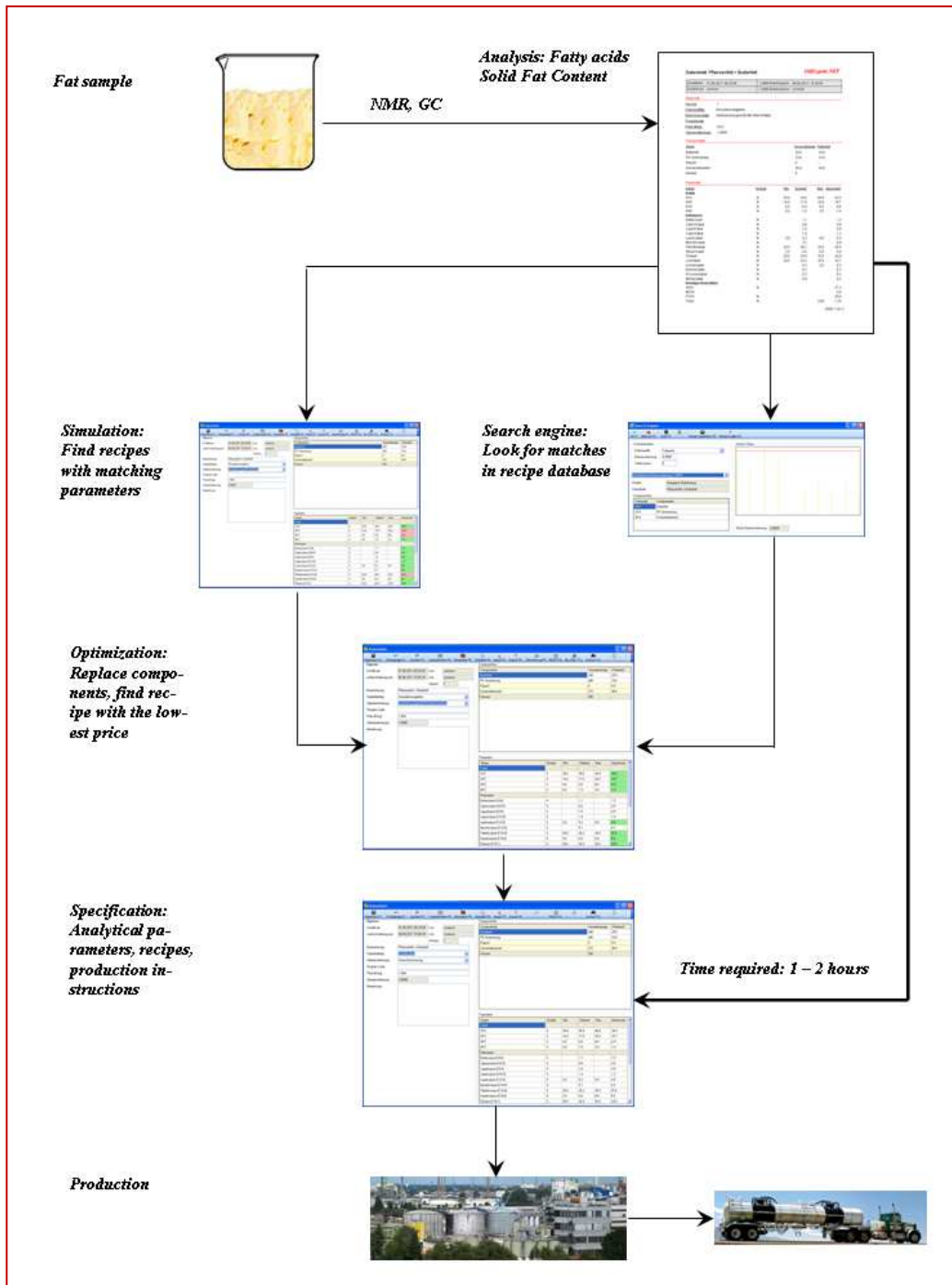
If no match is found in the recipe library, one or more possible recipe can be generated using the simulation mode of *Oil-Expert.net*. The raw materials to use can be defined before starting the simulation.

Once you've found a recipe the price optimization can follow. For this procedure other raw materials can be added, such as liquid oils, palm fractions, etc. The result of the price optimization is the recipe with the lowest commodity price in compliance with all existing specifications.

Finally the specifications can be extended, e.g. by additional analytical parameters and production instructions.

OIL-EXPERT.NET IN DETAILS – CASE STUDY

From Fat Sample to Production



OIL-EXPERT.NET IN DETAILS – MODULE: DATA IMPORT/-EXPORT

Oil-Expert.net has cConnect, a comfortable interface for data import, updating and export.

For example, you can update daily prices of raw materials by pushing a button. The same applies to product specifications. cConnect also imports and updates new components, recipes and specifications.

Step sequence to get a template:

- Select a database format for the import (eg Text, Access, Excel, Oracle)
- Select tables
- Select the fields to be linked
- Select a search criterion (unique, preferably product code number)
- Run import, update or export
- Save template

The import export module can update data from a variety of databases (Access, Excel, Oracle, SQL Server, etc.), but can also import them or export from/to text files.

Interfaces are developed as customized solutions for a client for a fixed price.

BENEFITES AND ADVANTAGES

The investment in the purchase of *Oil-Expert.net* pays off if the monthly benefit is higher than the monthly charges for using the program. The inversion of the argument reads: "*Oil-Expert.net* costs success and profit every month during which the program is not used!"

The benefits of **Oil-Expert.net** result from

- a) competitive advantages and
- b) cost reduction.

Competitive advantages

Oil-Expert.net accelerates lab processes. This allows you to react quickly and effectively on

- trends in raw material markets,
- customer requests and
- disorders in the production

In addition

- analysis,
- simulation to develop new products and
- results from different scenarios

are quickly available, or may be feasible in the first. This results in additional competitive advantages.

Cost cutting

Oil-Expert.net reduces

- costs for product development
- costs for the laboratory and
- costs for raw materials

COMMODITY COST-REDUCTION BY OPTIMIZATION OF FAT BLENDS

Oil-Expert.net allows to respond quickly and easily to fluctuating raw material prices by identifying alternative fat blends developed and calculating them, taking raw material prices into account, with the aim to get the recipe with the lowest price.

Cost savings can be calculated easily from the individual production and capacity data. The following example shows that *Oil-Expert.net* amortizes within a short time.

		[EUR/kg]	[EUR]			
			1 to	10 to	100 to	1000 to
Standard-recipe	22% Palmoil 30% Interestification 48% Rapeseed oil	0,683	683	6.830	68.300	683.000
With OilExpert optimized regarding to all specifications	24% Palmoil 30% Interestification 46% Soybeen oil	0,673	673	6.730	67.300	673.000
	Cost saving:	0,100	10	100	1.000	10.000

Example: Vegetable margarine

COST-SAVINGS THROUGH SIMULATION

The reduction of analysis and test series makes room for more important work, e.g. for high-quality analysis and professional documentation of results.

In the overloaded environment of today's laboratories, *Oil-Expert.net* gives sale and production departments the possibility to offer a fast support service.

Experiment and Analysis	Time expense [min]	Costs [EUR]	Count/Year	Cost/Year [EUR/Year]
Blending	50	62,50 €	500	31.250,00 €
Interesterification	120	150,00 €	50	7.500,00 €
				38.750,00 €

MINIMIZATION OF COST ANALYSIS

Oil-Expert.net gives the possibility to avoid long test series by simulation of fat blends on the screen. The simulation reduces significantly the number of analysis. In most cases only the analysis of the final result is necessary.

Example:

Annual cost savings in the case of analysis reduction by 2%, 5% or 10% at 75 EUR laboratory costs per hour.

Analysis	Time expense [min]	Costs [EUR]	Count/Year	Costs/Year [EUR/Year]	Cost saving through calculation		
					2%	5%	10%
SFC-Values	10	12,50 €	25.000	312.500,00 €	6.250,00 €	15.625,00 €	31.250,00 €
Fatty acids	30	37,50 €	3.000	112.500,00 €	2.250,00 €	5.625,00 €	12.250,00 €
Sterols	60	75,00 €	100	7.500,00 €	375,00 €	375,00 €	750,00 €
Tocopherols	60	75,00 €	100	7.500,00 €	150,00 €	375,00 €	750,00 €
				440.000,00 €	9.025,00 €	22.000,00 €	45.000,00 €

ANALYSIS OF COMPETITIVE PRODUCTS

By analyzing samples of competitors – Solid Fat Content and fatty acids are usually enough - *Oil-Expert.net* can automatically calculate a recipe reflecting the entered values of the analysis.

SYSTEM REQUIREMENTS

In order to perform the iterations in the optimization rather quickly, we recommend a PC with the minimum equipment as follows:

- 4.048 MB main memory
- 21 inch screen (1920 x 1080 resolution)
- 2.000 MB free disk space
- Operating system: Windows 7, Windows 10

Due to the extensive data material you need at least a 21 inch monitor with the given resolution, even better a 24 inch monitor. On a smaller monitor screen some windows are not displayed in full and must be laboriously scrolled.

INSTALLATION AND TRAINING

Installation of *Oil-Expert.net* corresponds to the usual standard of programs and requires no special skills.

Oil-Expert.net is modular:

- Basic modules
 - Master data management
 - Workflow management
 - Project management
 - Search engine
 - Recipe management
 - User management
- Calculation and simulation of fat blends
- Price optimization
- Reverse calculation – calculation of the recipe based on analytical values
- Calculation of SFC values for interesterifications

Oil-Expert.net

Training

To take advantage of the benefits of *Oil-Expert.net* effectively, we recommend a four-day training seminar we arrange locally. In this case Dr. Cullmann Consulting also takes care of the software installation. Alternatively the instruction can be performed in Hamburg at the Dr. Cullmann Consulting office.

AMORTIZATION

Amortization

The payback occurs when the monthly benefit exceeds approximately 1,200 EUR (cost savings + other benefits). These values are based on a leasing-financing. After the leasing term has expired the amortization is naturally extremely low.

Leasing

It is possible to make a leasing contract together with our financing partner. This requires the fulfillment of usual conditions regarding leasing transactions.

MISCELLANEOUS

Maintenance / Licenses

The license for *Oil-Expert.net* is purchased and granted on a permanent basis. Additional regular license fees are not charged.

Maintenance costs are calculated only when specific actions apply. Customers doesn't need a service contract.

Agreements with other software manufacturers such as database software, programming environment or other standard software programs such as Word or Excel are not affected herewith.

Updates

The software requires no regular updates but they are offered.

Integration into other programs or systems

Oil-Expert.net can be integrated into complex systems on demand, e.g. ERP systems, LIMS QM modules, etc.

CONTACT

We would be glad to provide you with further information. Please feel free to contact us.

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Demo Version

From now on a demo version is available with full functionality. This version is six months runnable and can be extended if necessary. If interested, please contact any of the above contacts.

Subject to changes in design and scope of delivery as well as further technical development! © Dr. Cullmann Consulting

APPENDIX: GENETIC ALGORITHMS

Genetic algorithms are used when a mathematical problem analytically can't be solved or is hard to solve. Genetic algorithms combine and change solutions until one of these solutions meets the requirements.

The basic idea of genetic algorithms is to randomly generate a number of solution candidates (individuals) and to select those which best match a particular quality criterion. This allows to change their properties (parameter values) and to combine them with one another in order to generate new solution candidates (new generation). This technology is particularly suitable for cases where you have no idea where the global minimum could be.

Genetic algorithms are also used in several programs, eg.:

- **Oil-Expert.net**
Optimization of fat blends with non-linear parameters (Solid fat Content).
Recalculation to get one or more possible recipes starting with analytical values (Solid Fat Content, fatty acids).
- **Peak-O-Mat (Now distributed by LAIX Technologies)**
Peak indexing of gas chromatograms (Fatty acids and Triglycerides) with automatic compensation of column aging. No known mathematical algorithm can be used in this case.

To illustrate this, here is a real life example with **Oil-Expert.net**:

In the recalculation of analytical values to a fat mixture, eg made on the basis of a competitor product, it is important to enter as many analytical values as possible, because that limits the number of possible fat blends.

Generation

A generation consists of individuals or populations. In this example (figure on the next page), 30 generations are allowed, each consisting of 50 populations.

Population

Here, populations or individuals represent the fat recipes and are limited to five components.

Number of components

Maximum number of components in a population (recipe).

Threshold value

The minimum proportion of a component can be set using a threshold value. In the example, the value is set at 2%. All proportions under 2% of a component are deleted, and those of other components are supplemented in the appropriate ratio to 100%.

Iterations

Maximum number of change cycles for each population. Recipes are changed statistically in small steps calculating the fitness. The recipe with the best fitness is stored.

Fitness

Also called match. Fitness is the sum of the least squares of calculated and measured values of the analysis. In our example the value is set to 95% or 0.95. The algorithm has reached the value of 0.9868 already in the first generation after 31 populations have been processed.

Max Hits

Specifies the number of the recipes found to be used for further processing. In this example, a maximum of five hits with the best match are taken. Under certain circumstances there can be a great number of fat blend possibilities you can realize with predetermined parameters.

Below is a brief process description of a genetic algorithm:

1. Generate the initial population for the first generation. Fifty recipes are generated statistically in this case. Not only the number of components listed can be limited, but also the components themselves, to save unnecessary computation time (for example by raw materials hardly occurring in practice, like grapeseed oil or palm kernel stearin).
2. Calculation of compliance for each population (recipe). In this step, the recipes are simultaneously statistically changed (100 iterations).
3. Selection of the 10 best recipes with the best match. The other 40 recipes "die".
4. Generate the population for the next generation. Ten selected populations are taken. Forty new recipes are created statistically.
5. Continue with Step 2, until 30 generations are created. The algorithm can be terminated at any time if needed, e.g. after achieving a sufficient grade of fitness.

