Modern software developments: Stabilise glass quality and optimise batch costs

The calculation of the optimum proportions of raw materials for a given glass composition is a decisive factor in achieving quality and workability. Batch calculation software enables optimisation of glass batches and glass properties and is suitable for use in mass glass production and special glass applications. Henning Katte* reports.

The objective of batch calculation in glass production is compliance with a defined chemical glass composition which determines the physical and chemical properties of the final product but also has a decisive influence on melting and forming.

In view of constantly changing raw material and cullet compositions, the raw material weights have to be adjusted regularly based on the current raw material analyses and the desired chemical glass composition. In addition, economic aspects make it necessary to constantly look for alternatives (such as substituting raw materials with others in order to reduce batch and glass costs) but without changing the glass chemistry.

An early batch recipe can be found in a cuneiform inscription in the library of Assurbanipal, king of Assyria 668-631 BC: "Take 60 parts of sand, 180 parts of ashes of seaweed, 5 parts of chalkstone and you obtain glass".

For the following centuries, batch preparation was based solely on experience and lengthy experiments. In the 1930s, arithmetic approximation calculations were developed using simplified assumptions regarding raw material composition. Two decades later the use of multi-component raw materials and cullet in large-scale production made it necessary to use more sophisticated mathematical approaches. Since the 1980s, widely available personal computers have made it possible to use computer programmes for batch calculation.

Oxide	Sand	Feldspar	Dolomite	Limestone	Soda	Synthesis
SiO_2	99.5%	69.0%				72.0%
Al_2O_3	0.5%	18.0%				1.5%
CaO		2.0%	31.0%	50.0%		9.0%
MgO			21.0%	5.0%		3.0%
Na_2O		5.0%			58.5%	14.5%

SiO_2: $0.995\,x_1 + 0.690\,x_2 + 0.000\,x_3 + 0.000\,x_4 + 0.000\,x_5 = 72.0$

Al_2O_3: $0.005\,x_1 + 0.180\,x_2 + 0.000\,x_3 + 0.000\,x_4 + 0.000\,x_5 = 1.5$

CaO: $0.000\,x_1 + 0.020\,x_2 + 0.310\,x_3 + 0.500\,x_4 + 0.000\,x_5 = 9.0$

MgO: $0.000\,x_1 + 0.000\,x_2 + 0.210\,x_3 + 0.050\,x_4 + 0.000\,x_5 = 3.0$

Na_2O: $0.000\,x_1 + 0.050\,x_2 + 0.000\,x_3 + 0.000\,x_4 + 0.585\,x_5 = 14.5$

Fig 1. Basic method of batch calculation. The raw material analyses and the nominal glass composition can be expressed as a linear equation system.

0.995	0.690	0	0	0	72.0
0.005	0.180	0	0	0	1.5
0	0.020	0.310	0.500	0	9.0
0	0	0.210	0.050	0	3.0
0	0.050	0	0	0.585	14.5

1	0	0	0	0	67.890
0	1	0	0	0	6.458
0	0	1	0	0	11.820
0	0	0	1	0	10.413
0	0	0	0	1	24.235

Sand:	67.890	= 100 kg
Feldspar:	6.458	9.51 kg
Dolomite:	11.820	17.41 kg
Limestone:	10.413	15.34 kg
Soda:	24.235	35.70 kg

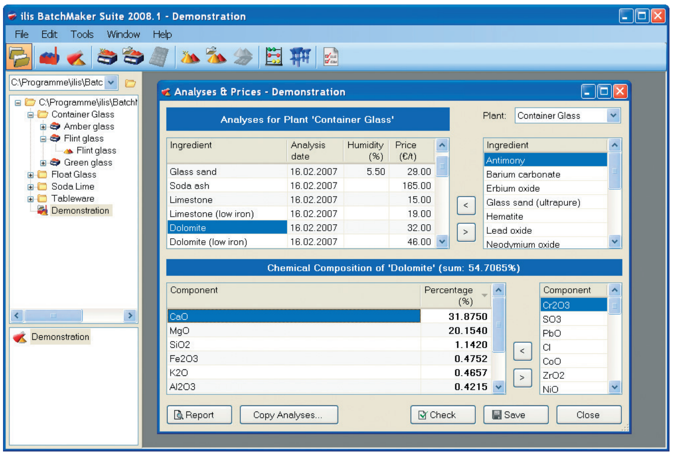
Fig 2. In matrix representation the linear equation system can be solved by using the Gaussian elimination method.

Basic principles

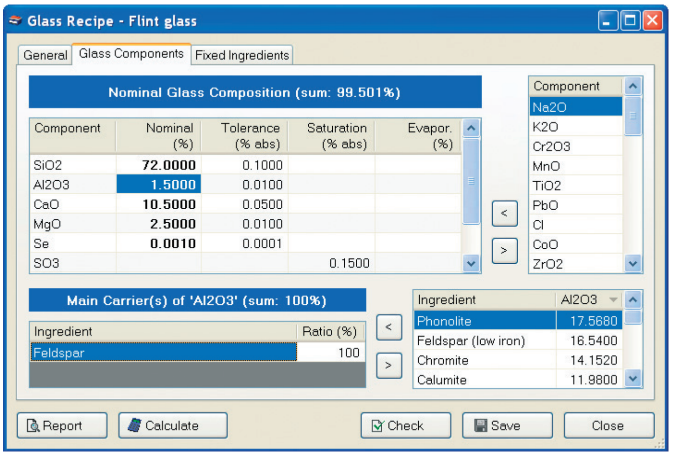
The first prerequisites are knowledge of the chemical composition of the raw materials used and of the desired glass composition. The chemical compositions can be obtained by wet chemical analysis and/or automated methods such as AAS (Atomic Absorption Spectroscopy) or XRF (X-ray Fluorescence Spectroscopy).

Fig 1 shows the calculation principle for a simple glass composition consisting of five oxides. The first five columns in the upper table show the chemical compositions of the raw material used (each one as a primary source for one of the oxides in the glass, i.e. sand for SiO_2, soda for Na_2O, limestone for CaO, dolomite for MgO and feldspar for Al_2O_3).

The column on the far right lists the desired glass composition, also called theoretical glass composition or glass synthesis. The table is converted into a linear equation system, one line for each oxide, and using variables x_1 to x_5 as placeholders for the wanted raw material proportions. The target composition can be found on the right side of the equations. The equations can be described by an extended coefficient matrix, as shown in ***fig 2***, and after transforming this into an identity matrix (1 on the principle diagonal, otherwise 0), e.g. using the Gaussian elimination method, the matrix column



▲ Fig 3. The chemical analyses and prices of all raw materials and cullet used are administered in clearly arranged tables.



▲ Fig 4. Glass recipe for a typical bottle flint glass in BatchMaker.

on the far right shows the raw material amounts. At the end, these values are normalised by rule of proportions.

To verify the calculation result, the determined values and the raw material compositions can be used to calculate back the theoretical glass composition, which of course has to be equal to the desired glass composition.

Of course, the equation system is only solvable if there are exactly as many linear independent equations (i.e. raw materials) as variables (i.e. chemical components). If, for instance, one raw material is used as a primary source for two oxides, no unique solution exists and thus the above calculation scheme will fail. Moreover, natural raw materials and cullet contain many more components than needed and these have to be taken into consideration. Therefore, in industrial practice, more sophisticated mathematical algorithms have to be used to find the optimum batch composition.

Modern batch calculation

BatchMaker software has been developed to simplify the process of batch optimisation and glass formula development by combining batch calculation with a reliable prediction of resulting glass properties such as viscosity, thermal expansion, hydrolytic resistance etc. The software features a convenient graphical user interface and the extensive application of state-of-the-art software technologies such as .NET and XML simplifies data exchange with laboratory information management systems and batch plant control systems. ***Fig 3*** shows the analyses for a typical container glass plant.

The glass recipe (see ***fig 4***) contains the nominal glass composition with tolerances as well as additional information such as fixed additives (e.g. refining and reducing agents) and cullet percentages. By clicking the 'Calculate' button in the glass recipe window, the raw material weights are automatically computed and displayed as a batch recipe (see ***fig 5***). Besides the raw material weights, the batch recipe window offers much more helpful information. If, for instance, the iron percentage exceeds the limit, the BatchMaker software shows which raw material introduces which amount of Fe_2O_3.

Of course, the calculated batch recipe is only as good as the underlying glass recipe. Therefore, the following should be considered as best practices to achieve the best possible matching of nominal and calculated glass composition:

- Register the complete chemical analysis for all used raw materials, since missing minor oxides or impurities will be considered as evaporation losses during the calculation.
- Define nominal values only for oxides and elements that are really desired in the glass, i.e. components that have a wanted effect on the physical and chemical properties.
- Reserve some space in the nominal glass composition for minor oxides and impurities and enable the automatic SiO_2 adjustment. The SiO_2 value will then vary slightly from calculation to calculation but the important oxides (Na_2O, CaO, MgO, A_2O_3) will meet their nominal values.
- Use each raw material only for one particular oxide in the nominal composition. Consider introducing an additional raw material if you have fewer raw materials than oxides to control. If this is not possible, assign the raw material to the oxide which is more important. This is probably better than spreading the error to both oxides in equal measure.
- Consider evaporation losses (especially SO_3) by empirically comparing the calculated glass composition with the actual glass composition (measured with XRF or similar) and entering the determined percentage in the glass recipe.

Prediction of glass properties

During the development of new glass formulas, great importance is attached to reliable prediction of glass properties as this can drastically reduce the number of trial melts and thus the expense of time and costs.

Even during normal production, it is important to be able to predict how changes in the glass chemistry, whether intentional or not, effect the processing ability and the product properties promised to the customer. The calculation of the relevant glass properties on the basis of the current glass analysis is therefore an important building block in the sense of process stability.

There is a large number of simple mathematical models for calculating glass properties based on chemical composition. Each model is only valid for certain glasses. Unfortunately, in many literature models, the application limits are not clearly defined and an error consideration is frequently not possible. For this reason, BatchMaker

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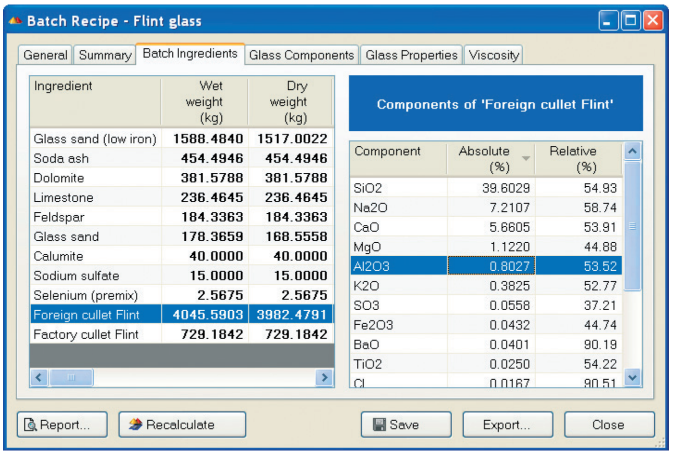
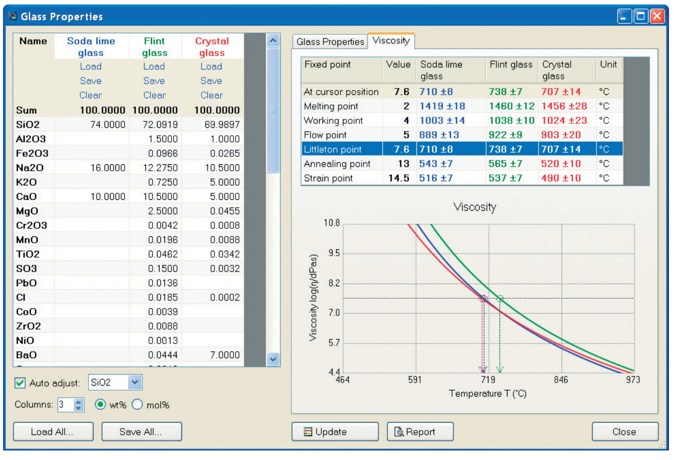


▲ Fig 5. Calculated batch recipe showing the raw material weights to meet the specifications of the glass recipe from fig 4.



▲ Fig 6. Viscosity curves for three different glass compositions.

uses modern calculation models based on the statistical analysis of hundreds of single analyses, which allows a clear statement about application limits and confidence intervals. ***Fig 6*** shows as an example the temperature dependent viscosity curve, as well as important viscosity fixed points for three different glasses. The confidence interval is stated in each case after the calculated temperature.

Data transfer to batch plant

Instead of manually entering the calculated raw material weights into the batch plant control system, it is of course beneficial to transfer the data automatically. This prevents typing errors as well as missing or redundant raw materials. Since BatchMaker stores all its data in machine-readable XML format, it is a simple matter to integrate a corresponding import function into modern batch plant control software.

Where it is not feasible to extend the control software accordingly, a special tool, BatchLink, allows batch recipes to be read and directly transferred to the PLC, either using RS485-style communication or OPC-based. ■

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