

GlassPanacea:

A user-friendly free software tool for the formulation of glasses, glass-ceramics, and ceramics

A newly developed software tool eases the selection of chemicals and improves the accuracy of calculations for formulations of glasses, glass-ceramics, and ceramics.

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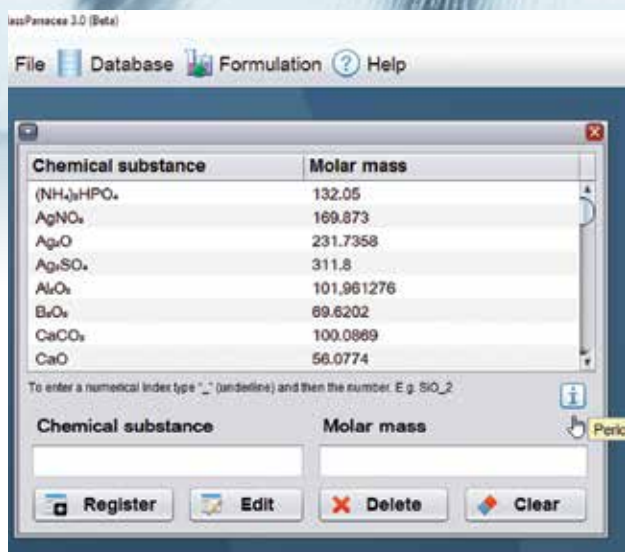


Figure 1. Database for query and registration of chemical substances

Glasses, glass-ceramics, and ceramics are extremely versatile materials with a wide range of applications in numerous segments of modern society. To synthesize existing and new materials of this class, immense chemical combinations are possible from all the 80 useful elements of the periodic table.¹ However, one must determine which chemicals and how much of each to use to prepare any formulation and batch.

Although this is a routine task, it can be time consuming to search for the molar mass of all necessary elements. In addition, the process easily is subject to errors when transforming units of the material composition, such as from moles to weight percent. During 40 years of teaching and research and 20 years as a journal editor, Edgar D. Zanotto has seen many students and researchers err in such calculations—unfortunately, these errors sometimes are never detected or are found only in later stages of research, when authors discover that some property of the material (e.g., density, viscosity, coefficient of thermal expansion, or glass transition temperature) falls far short of the expected value.

Therefore, to provide flexibility in the selection of suitable chemical formulations and to improve speed and accuracy of calculations of relative proportions of each chemical in a batch, we introduce a novel software tool called GlassPanacea. The software uses Java programming language and runs directly from an executable file with multiplatform support. Therefore, GlassPanacea can be used on various operating systems without installation. Its user-friendly and intuitive interface enables immediate application, even for users with little computer experience. This makes GlassPanacea a valuable tool for students, researchers, and engineers who develop ceramic materials using various synthesis techniques, including melting, solid-state reactions, sintering, and sol-gel processing.

Basic software options and additional features

GlassPanacea's workspace is simple and intuitive yet offers robust features. For instance, a "database" button in the menu command allows query and registration of new chemical substances for the purpose of a batch calculation (Figure 1). This is an open database that allows users to extend the default database or build their own. To assist this task, a periodic table is available through the "information" icon at the bottom right of the section. In addition, a "formulation" button opens a window for material batch calculations (Figure 2). This user-friendly section is divided into simple steps:

- **Step 1—Determination of amount of product.** We developed the program to simulate preparation of quantities ranging from a few grams to several tons of material. Therefore, the program can meet the requirements of laboratories, research centers, and the industrial sector.

- **Step 2—Indication of number of components per system (up to 10).** When a system composed of oxides, such as $\text{Li}_2\text{O}-\text{ZrO}_2-\text{SiO}_2$ (LZS) is considered, each individual oxide constitutes one component of the system. In this case, there are three components— Li_2O , ZrO_2 , and SiO_2 . Choosing the number of components enables only a corresponding number of data entry fields in additional steps.

- **Step 3—Selection of components to compose the intended system.** A selection filter is provided to facilitate this step. Therefore, it is possible to search for components of interest in the complete list of substances registered in the database or by grouping them into oxides, for example.

- **Step 4—Selection of composition based on mol%, wt%, or molar fraction.** To assist in filling out these fields, a percentage counter is displayed in yellow to show progress as the fields are filled. A value of 100% indicates that all fields are empty, and percentage decreases progressively as data are entered.

- **Step 5—Selection of chemicals that will provide components of the system.** Accessing the "select" tab for each component provides a list of preregistered chemical substances in the database. This provides flexibility in choices and enables simulation of various chemical combinations that may be more appro-

priate for experimental purposes.

- **Step 6—Setting parameters.** To meet the needs of many users, the software offers additional features available through "purity degree," "extra chemical," and "double chemical" tabs. Additional information about each feature can be accessed through the "information" icon at the top of the section.

- **Step 7—Formulation report.** After completing previous steps and pressing a "calculate" button, the software generates a report listing steps adopted by the user as well as the mass of all chemicals that should be weighed to obtain the desired amount of product. The software also provides optional buttons to reset calculations or save results. Partial reports are generated in this section to warn the user of possible errors that may have occurred in the preceding steps.

The "help" button in the standard menu command provides access to a user guide containing general information and step-by-step instructions for software features. Another available option is the "about" dialog box, which provides information about the software release, updates, and developer contacts. Because GlassPanacea is a beta version, the software may have some bugs and instability issues. Therefore, criticisms and suggestions are welcome and are valuable to enable improvement of the software and expansion of its functionalities.

GlassPanacea 3.0 (beta) is freely available in three languages—Portuguese,

Spanish, and English. An archive containing the software, initial information for use, and logo (~6 MB) can be downloaded for free at certev.ufscar.br.

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References

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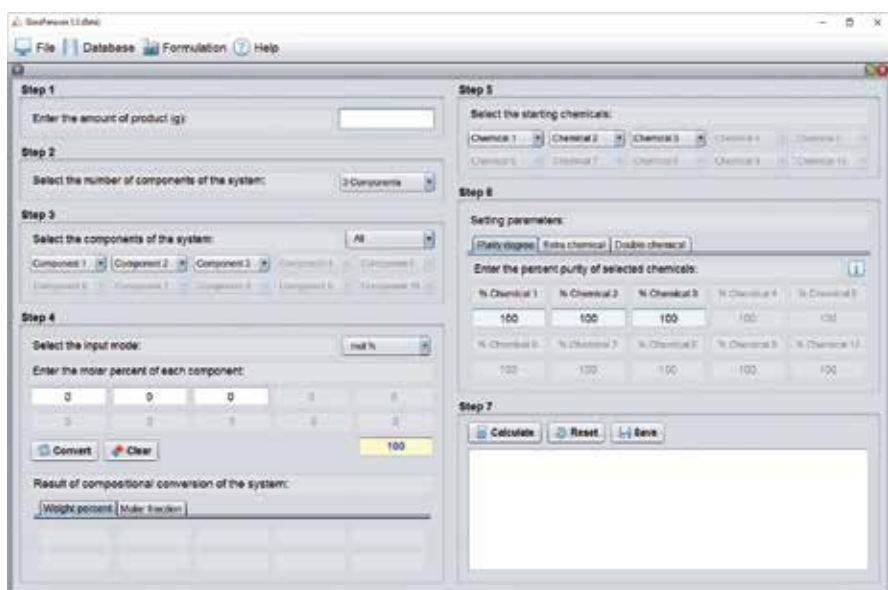


Figure 2. Overview of the formulation section.