ON A SOFTWARE DEVELOPMENT THAT ASPIRES TO MAKE RESIDUE VALORISATION EASIER

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Introduction

Driven by environmental legislation and awareness, associated with increased processing and landfill costs, but also valorisation opportunities, an increasing interest exists for the valorisation of metallurgical slags, tailings, ashes and sludges. Efforts are certainly happening at bilateral projects and regional ones (*e.g.* European projects like MetGrow+[1]), supported by policy and action plans[2] yet, a collective effort to streamline work on residues' valorisation seems absent for the time being. A bottom up movement based on voluntary involvement, might be able to contribute to this direction. Having this in mind, we try to develop an open access, free-to-use software. If successful, we believe the use of residues will become easier, and results ultimately predictable.

Software architecture

The structure of the software is around modules. These units can be stand-alone, or can interact and feed each other with data. The first module is that of the database. Conceptually, the database looks like the RRUFF database for minerals[3]. Instead of pure minerals, residues and treated residues can be found by searching based on *e.g.* chemical composition or industry of origin. For each residue, the following information can be retrieved and downloaded: location, bulk chemistry and microchemistry of amorphous and/or crystalline phases, particle size distribution, X-ray powder diffraction, infrared and Raman spectra, with the option to include additional information, like data from nuclear magnetic resonance and Mössbauer spectroscopy. The database has been built by users, and the proper acknowledgment is given. Samples can be sent however also to the administrators, *i.e.* KU Leuven, and measurements are performed again, at no cost, in order to verify the information listed. This creates a smaller database, the critically assessed one, within the bigger pool of data.

At a second stage, these residues (now raw materials) are introduced in existing or upcoming processes, and there are two separate modules for this task, *i.e.* that of high temperature and that of low temperature. The applications targeted can potentially incorporate substantial volumes in both cases, that is, cementitious and inorganic polymer binders for mortar and concrete development. The high temperature module

is the first after the database module. From a processing perspective, there is a roasting process, a clinkering process and a melting process. The common denominator in all these processes is the high temperature and the formation of liquid phase, to small (roasting) or greater extent. Depending on the specifics, thermodynamic calculations can be incorporated by 3rd party software to predict the final outcome. The clinkering processes are well established when it comes to ordinary Portland cement (OPC), but emphasis is also placed in other clinkers, *e.g.* calcium-sulfoaluminate and calcium-sulfoferroaluminate cements. In the OPC case, the clinker is designed based on the silica ratio, alumina-iron ratio, lime saturation factor[4] and the results are qualitatively predicted by the well-established Boque equations (and the modified ones[5]). For the new clinkers, work is on-going, both for the raw materials' design of the clinker as well as for the prediction of the final mineralogical assemblage, for instance[6]. Apart from information on the quality of the clinker, data regarding the process itself are also generated, *e.g.* CO_2 emissions. The roasting and melting process coexist, and are treated (for now) as a mass balance exercise, where the final chemistry is calculated. The roasting process targets applications that require materials that require thermal activation in order to, for instance, enhance their pozzolanic performance and deliver blended cements or make them more suitable for the synthesis of inorganic polymers and geopolymers. A classic example for the latter would be the thermal treatment of kaolin to give metakaolin but other process also emerge[7]. The melting process, in combination with other software and calculation tools, can lead from predictions of surface tension, density, viscosity (…) to solidification trajectories, where the crystal phases to precipitate are predicted.

The low temperature module follows, where raw materials in the database, either as produced or after high temperature processing (see paragraph above) are used to synthesise inorganic polymer binders, mortars and concrete. The work herein is borrowing ideas from a range of mix design software for concrete, *e.g.* the HIPERPAV® III software developed by the U.S. Federal Highway Administration (FHWA). The module "Process assessment" conducts calculations to support the choice of processing option. Economic calculations can be performed with a fixed or variable price of the residue and accessory raw materials, while environmental calculations can be added for inorganic polymers and blended cements based on equations proposed elsewhere[8]. The performance with respect to radioactivity or leaching can also possibly be modelled and become an addition in future updates.

The last module is trying to propose options from the back-end, that is the application. Instead of selecting raw materials for certain processing and end-product requirements, in the "Target" module the user is provided with three options for a specific high temperature or low temperature product (see respective modules to see what these are). The options are compressive strength, cost or environmental impact. Per criterion, a second level of options is given, that of "optimise", "aim to max/min" (depending on the case) or "ignore". The operation of this module is still suggestive,

as the database with compressive strength, cost and environmental impact is under development.

Apart from the database and above mentioned calculations, the software also provides a toolbox with support calculations per module. These can involve complex calculations on the slag properties, *e.g.* the slag properties as calculated by K. Mills[9], or consider more simple calculations, *e.g.* the transformation of molar ratios to mass, or oxides to elements, and vice versa. Calculations on the activating solution used for inorganic polymers are also included herein.

Software structure

The running home page of the software is presented in Figure 1 (left), followed by an overview of the content of two modules, Figure 1 (right).

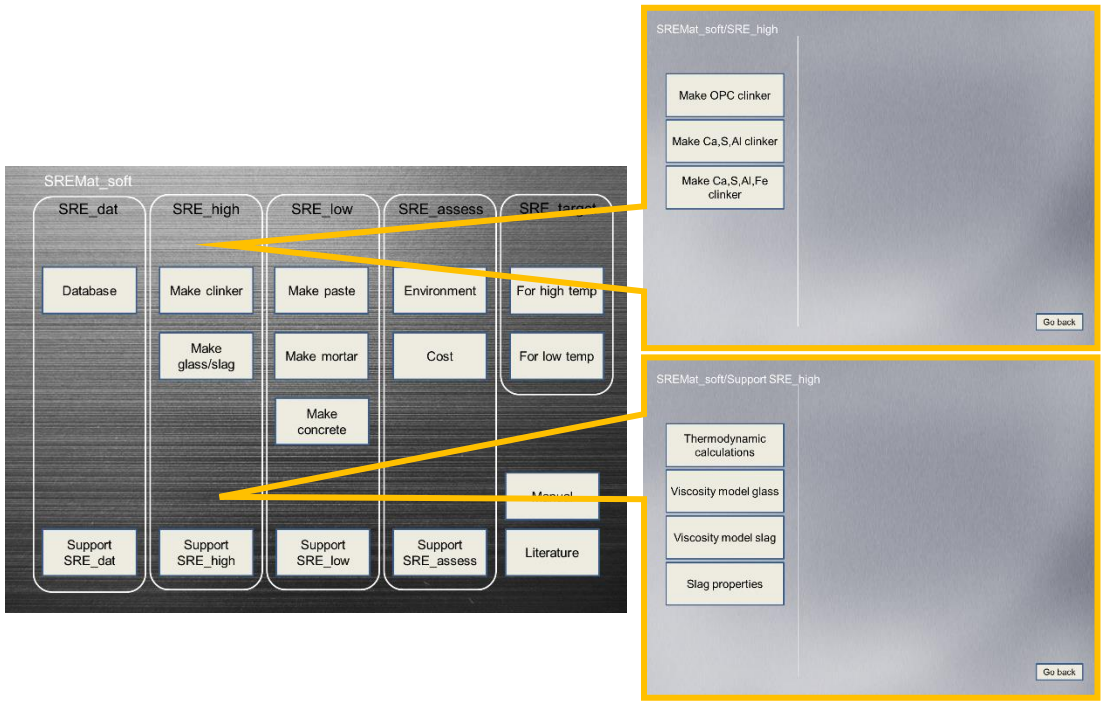

Figure 1: Overview of the software and its modules

Instead of conclusions

The software presented herein will be available to the public on a beta version before September 2017. A number of modules are also envisaged for the future, where *e.g.* the reactivity of raw materials is assessed and linked to properties of final binder, or where the output of the work is feeding machine learning algorithms or statistical analysis toolboxes, generating realistic predictions on performance.

As already presented, the intention is to gather available information into one cohesive platform, pieces of one narrative: residues can be used to deliver high quality

binders. It is expected that the initial versions will be incomplete, with bugs and a plethora of items that will ask attention and development. This is not intimidating; we see this initiative as the starting point of a tool for the whole community and it eventually comes down to us, and our personal involvement, to transform it into a fully-fledged software for all.

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