3. PHYSICOCHEMICAL CHARACTERISTICS

3.1 General

In Fig. 3.1.1, the part (tab) of the logical flowchart of EUCON® for the calculation of the chemical and volumetric composition of concrete is presented. The tab contains:

- a field that the user introduces the **input data** for cement composition and oxide analysis, and additions activity and oxide analysis.
- a **calculation button**, and
- a field of the **output results** including the reaction degree of supplementary cementing materials and the various additions, the calcium hydroxide content and the concrete porosity.

CHEMICAL AND VOLUMETRIC CHARACTERISTICS OF CONCRETE

INPUT

Tab "MIX DESIGN" data

Cement composition and oxide analysis (Oxide analysis of portland clinker, oxide analysis and activity of other main constituents of cement)

Oxide analysis and activity of additions (Oxide analysis and activity of silica fume and fly ash used)

▼

CALCULATION

(Reaction degree of other main constituents of cement and of concrete additions. Calcium hydroxide content, calcium-silicate-hydrate content, chemically-bound water content, concrete porosity)

Figure 3.1.1 Logical diagram for computer calculation of the main chemical and volumetric characteristics of concrete.

A general view of this tab is given as Fig. 3.1.2. The user has to fill in the “white boxes” or to accept the default values, and then to press the calculation button in order to calculate the chemical and volumetric characteristics of concrete. For the algebraic formulae used for these calculations and further questions, **please always advise the *Theoretical Background* [1], chapter 3**. In the sequence, each part of this tab is discussed in detail.

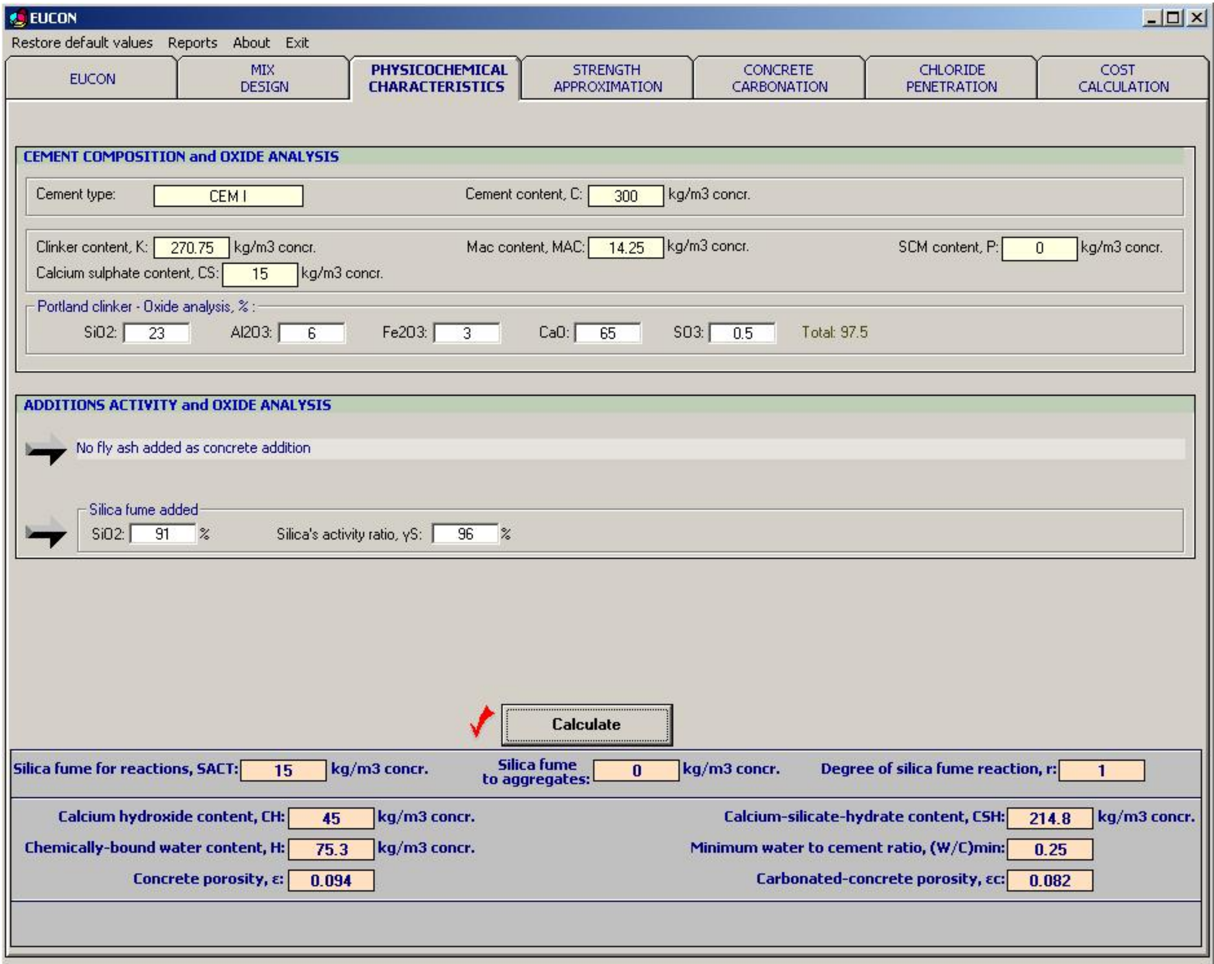

Figure 3.1.2 General view of the tab “PHYSICOCHEMICAL CHARACTERISTICS” of the EUCON® program.

3.2 Cement composition and oxide analysis

Cement composition

Cement type:	It is a reminder for the cement type used (see tab "MIX DESIGN").
Cement content, C:	It is a reminder for the total cement content in the concrete volume, kg/m^3 (see tab "MIX DESIGN").
Clinker content, K:	The absolute clinker content (including the various additives) in the concrete volume. It is calculated as [(PK/100) C (100-PCS)/100]. UNITS: kg/m^3 concrete
Minor additional constituents content, MAC:	The absolute content of minor additional constituents (mac) in the concrete volume. It is calculated as [(PMAC/100) C (100-PCS)/100]. UNITS: kg/m^3 concrete
Other main constituents (SCM) content, P:	The absolute content of the other main constituents (supplementary cementing materials- SCM) in the concrete volume. It is calculated as [(PSCM/100) C (100-PCS)/100]. In the case of cement type CEM V, these composite cements contain, apart the clinker, certain amounts of both slag and other pozzolanic materials, and then the SCM is separated in **SL** =[(PSL/100) C (100-PCS)/100], referring to slag content in the concrete, and **P** =[(PPO/100) C (100-PCS)/100], referring to the other pozzolanic materials content in the concrete. UNITS: kg/m^3 concrete
Calcium sulphate content, CS:	The absolute content of the calcium sulphate in the concrete volume. It is calculated as [(PCS/100) C]. UNITS: kg/m^3 concrete

Oxide analysis and activity

Portland clinker – Oxide analysis, %:	Introduce here the chemical analysis of portland clinker in terms of oxides: SiO_2, Al_2O_3, Fe_2O_3, CaO, and SO_3. Use the default values, if you do not have a more accurate oxide analysis. UNITS: % by mass LIMITS: the total sum of the oxides ≤ 100 DEFAULT VALUES: These in Table 3.2.1

Other main constituents in cement (SCM) – Oxide analysis, %:	It gives first the name of the other main constituent used in cement production. Introduce here its chemical analysis in terms of oxides: SiO_2, Al_2O_3, Fe_2O_3, CaO, and SO_3. Use the default values, if you do not have a more accurate oxide analysis. UNITS: % by mass LIMITS: the total sum of the oxides ≤ 100 DEFAULT VALUES: These in Table 3.2.1
Silica's activity ratio, γS: Alumina's activity ratio, γA:	Introduce here the percentage of the oxide SiO_2 or Al_2O_3 in the SCM, which contributes to the pozzolanic reactions (the glass or amorphous phase). Use the default values, if you do not have a more accurate result. UNITS: % by mass LIMITS: $0 \leq \gamma \leq 100$ DEFAULT VALUE: These in Table 3.2.1

Table 3.2.1 Typical oxide analysis (%) and activity ratios, γ (%), of portland clinker, silica fume, siliceous and calcareous fly ashes, and various SCM used in EN 197 (data from [1]).

	Cementitious/pozzolanic materials	SiO_2	Al_2O_3	Fe_2O_3	CaO	SO_3	γS/γA
1	Portland clinker	23	6	3	65	0.5	-
2	Blast furnace slag	36	9	1	40	0.5	90
3	Silica fume	91	1	1.5	0.7	0.4	96
4	Pozzolana (natural)	58	15	5	6	1	50
5	Pozzolana (natural, calcined)	53	42	1	0.1	0	80
6	Siliceous fly ash	53	20	9	4	0.6	82
7	Calcareous fly ash	39	16	6	24	4.3	71
8	Burnt shale	38	10	6	35	5	90
9	Limestone	2	1	0.2	2	0.1	50
10	Various SCM for CEM II	50	16	7	12	1.5	65
11	Various SCM for CEM IV	50	20	7	10	1	65

12	Various SCM for CEM V	50	20	7	10	1	65

3.3 Additions activity and oxide analysis

This field of data appears in the case of the use of additions such as fly ash (siliceous or calcareous) and/or silica fume. Otherwise, an indication of non-use of these materials appears.

Fly ash added

Oxide analysis, %:	It gives first the name of the fly ash (siliceous or calcareous) added as addition in concrete production. Introduce here the fly ash chemical analysis in terms of oxides: SiO_2, Al_2O_3, Fe_2O_3, CaO, and SO_3. Use the default values, if you do not have a more accurate oxide analysis. UNITS: % by mass LIMITS: the total sum of the oxides ≤ 100 DEFAULT VALUES: These in Table 3.2.1
Silica's activity ratio, γS: **Alumina's activity ratio, γA:**	Introduce here the percentage of the oxide SiO_2 or Al_2O_3 in the SCM, which contributes to the pozzolanic reactions (the glass or amorphous phase). Use the default values, if you do not have a more accurate result. UNITS: % by mass LIMITS: $0 \leq \gamma \leq 100$ DEFAULT VALUE: These in Table 3.2.1

Silica fume added

Oxide analysis, %:	Introduce here the total SiO_2 content in the silica fume. Use the default value, if you do not have a more accurate result. UNITS: % by mass LIMITS: $0 \leq SiO_2 \leq 100$ DEFAULT VALUE: This in Table 3.2.1
Silica's activity ratio, γS:	Introduce here the percentage of the oxide SiO_2 in the silica fume, which contributes to the pozzolanic reactions (the glass or amorphous phase). Use the default value, if you do not have a more accurate result. UNITS: % by mass

	LIMITS: $0 \leq \gamma S \leq 100$ DEFAULT VALUE: This in Table 3.2.1

3.4 Calculations

For the algebraic formulae used for these calculations and the theory that they based on and for further questions, **please advise the *Theoretical Background* [1], chapter 3**. Click on the "**Calculate**" button to estimate:

the reaction degree of SCM and additions:

SCM for reactions:	The amount of SCM (other main constituents of cement, fly ash or silica fume as additions) that can participate in the pozzolanic reactions (active part). UNITS: kg / m^3 of concrete
SCM to aggregates:	The amount of SCM (other main constituents of cement, fly ash or silica fume as additions) that cannot participate in the pozzolanic reactions and thus may be included to the aggregates (inert part). UNITS: kg / m^3 of concrete
Degree of SCM reaction, r:	The ratio of SCM (other main constituents of cement, fly ash or silica fume as additions) for reactions to the total SCM content. UNITS: dimensionless LIMITS: $0 \leq r \leq 1$

the main chemical composition of concrete (final):

Calcium hydroxide content, CH:	The final calcium hydroxide content in the concrete volume (100% cement hydration and pozzolanic action). It has a significant effect on concrete carbonation. UNITS: kg / m^3 of concrete
Calcium-silicate-hydrate content, CSH:	The final calcium-silicate-hydrate content in the concrete volume (100% cement hydration and pozzolanic action). It has a significant effect on concrete strength and concrete carbonation. UNITS: kg / m^3 of concrete

Chemically-bound water content, H:	The final chemically-bound water content in the concrete volume (100% cement hydration and pozzolanic action). UNITS: kg / m^3 of concrete
Minimum water to cement ratio, (W/C)min:	The minimum water/cement ratio required for the completion of clinker hydration and pozzolanic reactions. UNITS: dimensionless (by mass)

and the main volumetric composition of concrete (final):

Concrete porosity, ε:	The ratio of pore volume (final) to the total volume of concrete (100% cement hydration and pozzolanic action). It has a significant effect on concrete strength and concrete durability. UNITS: dimensionless (by volume)
Carbonated-concrete porosity, εc:	The ratio of pore volume (final) to the total volume of the carbonated concrete (100% cement hydration and pozzolanic action- 100% carbonation). It has a significant effect on concrete strength and concrete durability. UNITS: dimensionless (by volume)

By obtaining the above estimation on concrete's chemical and volumetric composition you may:

- **accept these results** and continue in the next tabs to estimate strength, service life and cost.
- Otherwise, **you may change any input data from the present tab and/or tab "MIX DESIGN"** in order to correct the output results of this tab, **until final acceptance.**