CLAIMS

1. A volatile liquid chemical compound physical parameter database construction method (100), characterized in that it comprises:

- a step (105) of controlled deposition of a chemical compound in an inert container, a predetermined quantity of the chemical compound spreading over a predetermined surface of the container,
- a step (110) of airflow generation, the airflow being directed in the direction of the deposited chemical compound,
- a step (115) of measurement of a quantity of evaporated chemical compound at different measurement times,
- a step of measurement of relative gas phase concentrations for several initial ingredient concentration in the liquid chemical compound at preset experimental pseudo-equilibrium conditions corresponding to equilibrium conditions,
- a step (120) of evaporation rate calculation depending on the measured evaporated chemical compound quantities measured at pseudo-equilibrium conditions,
- a step (125) of volatility calculation depending on the evaporation rate calculated, a first linear regression function linking evaporation rate to concentration at equilibrium conditions and a second linear regression function that converts pseudo-equilibrium evaporation rates into volatility and
- a step (130) of storing, in a database, the calculated evaporation rate and the volatility calculated.

2. A construction method (100) according to claim 1, which further comprises:

- a step (135) of computing at least one gas phase concentration of the chemical compound for a given volatility of chemical compound,
- a step (140) of measurement of the psychophysical intensity of the chemical compound for at least one said gas phase concentration,
- a step (145) of modeling of a mathematical formula of psychophysical intensity of the chemical compound as a function of gas phase concentration based on at least two of the measured gas phase concentration values named “dose-response curve” and

- a step (150) of recording, in a database, the psychophysical intensity formula modeled parameters of the chemical compound.

3. A construction method (100) according to claim 1 or 2, which comprises a plurality of steps (105) of controlled deposition of a chemical compound at different temperature, the evaporation rate being calculated for each said temperature and stored during the step of storing.

4. Database constructed according to the database construction method of any one of claims 1 to 3.

5. A fragrance physical composition evolution prediction method (200) to provide predictive, real-time, fragrance performance metrics, characterized in that it comprises:

- a step (205) of selecting at least one chemical compound identifier in a computerized interface,
- a step (210) of inputting, for each selected chemical compound, a quantity of said chemical compound,
- a step (215) of modeling a deposition of the quantity of each selected chemical compound on a virtual surface by setting at least one parameter of the model,
- a step (220) of simulating, by a computing system, for each modeled deposited chemical compound, the stripped quantity of said chemical compound in an airflow for at least two different times as a function of:
    - the quantity of each said chemical compound,
    - a first value representative of a virtual surface size of the deposited chemical compound,
    - a second value representative of a virtual airflow directed at the deposited chemical compound configured to virtually strip the chemical compound from the surface,
    - a third value representative of an activity coefficient of each said chemical compound and
    - a volatility associated to said chemical compound stored in a database according to claim 4 and
- a step (225) of displaying, for each chemical compound, of an indicator representative of the computed evaporated mass of said compound over time.

6. A prediction method (200) according to claim 5, further comprising a step (230) of computing a gas phase concentration of the virtually stripped chemical compound as a function of the stripped quantity computed, the step (225) of displaying being configured to display the gas phase concentration computed.

7. A prediction method (200) according to claim 6 when claim 5 depends on claim 2, further comprising a step (235) of computing a psychophysical intensity of each selected chemical compound as a function of the gas phase concentration computed, the step (225) of displaying being configured to display the psychophysical intensity computed over time.

8. A prediction method (200) according to claim 7, in which at least two chemical compounds are selected, the method further comprising a step (240) of computing a global psychophysical intensity comprising:

- a first step (241) of matching a value for concentration for each compound against a corresponding dose-response curve to provide a psychophysical intensity value for that compound,
- a second step (242) of matching each said psychophysical intensity value against a dummy dose-response curve to provide an artificial compound concentration value,
- a step (243) of addition of each artificial compound concentration value to form a virtual concentration value and
- a third step (244) of matching the virtual concentration value against the dummy dose-response curve to provide a global psychophysical intensity value for the composition.

the step of displaying being configured to display the global psychophysical intensity computed over time.

9. A prediction method (200) according to either claim 7 or 8, in which at least two chemical compounds are selected, the method further comprising a step (245) of computing a psychophysical intensity linearity of the composition of said at least two compounds based on the computed psychophysical intensity of each selected chemical compound over time, the step (225) of displaying being configured to display

the psychophysical intensity linearity of the composition of said at least two compounds.

10. A prediction method (200) according to any one of claims 7 to 9, which further comprises a step (250) of chemical compound identifier selection, said chemical compound identifier being selected if the psychophysical intensity at a given time is below a determined value and a step (255) of display of said chemical compound identifier.

11. A prediction method (200) according to any one of claims 5 to 10, in which at least two chemical compounds are selected to form a composition, the method further comprising a step (260) of computing of the composition evolution over time as a function of the stripped quantity calculated over time.

12. A prediction method (200) according to any one of claims 5 to 10, which further comprises a step of construction of the liquid chemical compound physical parameter database storing the volatility associated to said chemical compound by carrying out the method of claims 1 to 3.

13. A liquid chemical compound physical parameter database construction system (300), characterized in that it comprises:

- a means (305) of controlled deposition of a chemical compound in an inert container (306),
- a means (310) of airflow generation, the airflow being directed in the direction of the deposited chemical compound,
- a means (315) of measurement of a quantity of evaporated chemical compound at different measurement times,
- a means of measurement of relative gas phase concentrations for several initial ingredient concentration in the liquid chemical compound at preset experimental pseudo-equilibrium conditions corresponding to equilibrium conditions,
- a means (320) of evaporation rate calculation depending on the measured evaporated chemical compound quantities measured at pseudo-equilibrium conditions,

- a means (325) of volatility calculation depending on the evaporation rate calculated, a first linear regression function linking evaporation rate to concentration at equilibrium conditions and a second linear regression function that converts pseudo-equilibrium evaporation rates into volatility and
- a means (330) of storing, in a database, the calculated evaporation rate and the volatility calculated.

14. A fragrance physical parameter evolution prediction system (400) to provide predictive, real-time, fragrance performance metrics, characterized in that it comprises:

- a means (405) of selecting at least one chemical compound identifier in a computerized interface,
- a means (410) of inputting, for each selected chemical compound, a quantity of said chemical compound,
- a means (415) of modeling a deposition of the quantity of each selected chemical compound on a virtual surface by setting at least one parameter of the model,
- a means (420) of simulating, by a computing system, for each modeled deposited chemical compound, the stripped quantity of said chemical compound in an airflow for at least two different times as a function of:
    - the quantity of each said chemical compound,
    - a first value representative of a virtual surface size of the deposited chemical compound,
    - a second value representative of a virtual airflow directed at the deposited chemical compound configured to virtually strip the chemical compound from the surface,
    - a third value representative of an activity coefficient of each said chemical compound and
    - a volatility associated to said chemical compound stored in a database according to claim 4 and
- a means (425) of displaying, for each chemical compound, of an indicator representative of the computed evaporated mass of said compound over time.