Nanoscopic approach of a chemical reaction

Concept of chemical entity

A chemical entity corresponds to any stable arrangement of elements (ion, molecule, individual atom, …).

A few or a lot?

A chemical entity is TINY small in size: a glass of water contains around 1024 molecules of water. Therefore, a chemical reaction involves a HUGE number of entities. A statistical and probabilistic approach can thus be used when studying a chemical reaction.

Alone or in group?

1. *Solide state.*

Compact and ordered medium. The chemical entities making up the solid vibrate around their equilibrium position, but come into very little contact with each other.

2. *Gaseous state.*

Dispersed and highly disordered environment. The chemical entities making up the gas circulate freely in a "vast" space. They can travel "great" distances before encountering another entity.

Note: This characteristic is at the origin of the perfect gas approximation. When studying such a gas, it is assumed that the gaseous entities do not interact with each other. They act as if they were alone in the medium under study.
However, at high pressures, we can no longer neglect the interaction between entities making up the gas.

3. *Liquid state.*

A compact, but disordered medium. The chemical entities making up the liquid move freely in a "reduced space", and therefore have many opportunities to cross paths.
This is why so much chemistry takes place in the liquid state.

Collision

The encounter between two entities is rather brutal.
Depending on the speed (and therefore energy) of each entity, this collision can have 2 consequences:

- Low-energy collision: entities merely deviate from their trajectory.
- Collision with **sufficient energy** to break one or more covalent bonds. This is known as an **effective collision.**

Returning to stability

The entities resulting from the shock are generally not stable.
They will therefore seek to combine with each other to form new, stable chemical species.
To do this, they can:

- Reform the same entities as before the shock.
  It's as if nothing had happened.
- Form new, stable entities.
  In this case, a **chemical transformation** has taken place.

Chemical reaction

A chemical transformation is **modelled** by a reaction equation.
This equation indicates the **evolution of the system from the initial state to the most stable, and therefore most likely, final state**.
Through the use of stoichiometric coefficients, it translates the **principle of conservation of matter**: Nothing is lost! Nothing is created!
Stoichiometric coefficients also indicate the proportions in which a transformation takes place: Everything is transformed!
The construction of a progress chart enables you to theoretically follow the evolution of a system over time, from the initial state to the final state.

Note: The final state, EF, corresponds to the state showing no further macroscopic evolution: the quantities of reactants and products no longer change. Experimental, it can be reached by measuring a characteristic quantity of the system (conductivity or conductance, pH, absorbance, etc.).