# An overview of use of «  material informatics » in industry

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# My experience

**Short biography**

1999 : Diploma of Engineer : Ecole Centrale Marseille (promo 1999)

2002 : PhD on Mechanics, Université de la méditerranée

2002-2009 : Research Engineer at Centre de Mise en Forme des Matériaux (CEMEF), Sophia Antipolis, UMR Ecole des Mines de Paris, CNRS

Since 2010 Solvay R&I: Senior scientist. Expert in modeling of behavior and process of thermoplastic and thermoset polymers. In charge of activity in Finite Elements modeling and simulation, and mechanical characterisation laboratory,

**Research activity**

Process / Properties relationships of polymeric / composite materials

- 3D modeling of complex rheology of industrial polymers for injection/extrusion/foaming : process modeling
- Physical based modeling and coupling with phenomenological approaches
- Multiphysics modeling (thermo-chemio-mechanical, thermo-piezo-electricity…)

Material characterisation, data generation and use for design of materials / applications

- Finite element development and software implementation
- Multiscale modeling, coupling discrete and continuous models
- Data basis generation (from experiments and/or simulation) and optimisation

Is head of several collaborative projects (funded by French State) in automotive industry framework.

Is head of Solvay's R&I Mechanical Laboratory at Lyon.

# Commonly used vocabularies @ SOLVAY R&I

- **Taxonomy (non exhaustive)**
  - Generalities
    - NATURE : Mineral – Organic
    - CLASS : Reactive – non reactive
    - STRUCTURAL PROPERTIES : cristalline, amorphous, homopolymer, copolymer, monocristaline, polycristaline, … (which means different ways / parameters to describe material and characterize it to feed database)
  - Raw materials
    - Nature, STATE (liquid, solid, gas…), COMPOUND CONSTITUTION (Weight ratio, morphology, e.g. linked with dispersion / (un)miscibility …)
    - TYPOLOGY OF CHEMISTRY (radical, polyaddition, polycondensation, oxydoreduction…) Toxicology, etc…
    - THERMODYNAMICAL STABILITY (T° phase change, P stability, cristal stability….)
  - Manufacturing process
    - REACTIVE : With / without curing
    - CONDTIONS : Temperature / pressure cycles
    - CONSTITUTIVE BEHAVIOR AS A LIQUID: Behaviour during process : (non linear viscosity, tixotropy, existance of turbulence ? …), behavior curves (rheological database) which means different ways / parameters to describe material and characterize it (feed database)
    - CONSTITUTIVE BEHAVIOR AS A GAS: Solubility into solvants, Compressibility, Explosivity …
  - Application properties
    - CONSTITUTIVE BEHAVIOR AS A SOLID : Elastic properties, Behavior beyond elasticity (plasticity, creep, fatigue) which means different ways / parameters to describe material and characterize it (feed database), Physical properties (electric/electronic, optical, photovoltaic etc… ) which means different ways / parameters to describe material and characterize it (feed database)
    - ENVIRONMENTAL STABILITY : Ageing (T°, UV, chemical stability etc…)

- **Stored :**
  - Alpha-numeric data, curves, equations, images, texts, video
  - And be able to make them interact

# Example of bigdata @ SOLVAY R&I

- **Objective : accelerate innovation using modeling, database and optimisation for materials**

- **Need to accelerate translation of application requirements into material / chemistry specifications**
  - Process / Properties optimization
  - Polymer structure / processability optimization
  - Fast identification of OK / NOK existing components : justify why develop a new material if one existing on the shelf

- **Questionmarks who limit fast development of big data**

  - What has been to be stored
    - All ?
    - Order 1, order 2 parameters ? Make the database inclusive or exclusive ?

  - Data base generation :
    - Using experiments ?
    - Using models ?

  - Extraction of data from database
    - By statistics or A.I. ?
    - Using physical models ?