



SOLVAY

asking more from chemistry®

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
 - **CONDITONS** : 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 ?