Nanotechnology

Finishes with nanotechnology – get insight and optimize them

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Since ever, producers and formulators of finishes and paints have mastered special challenges to mix different components in a beneficial way. With nanotechnology, new additives and possible funtionalisations are added, which indeed enhance its applications, but make products also more complex to estimate their performance. What will work best? is the most important question, which nowadays can be answered well before extensive series of experiments.

Les inventeurs, ainsi que les producteurs de vernis et de couleurs ont relevé le défi de mélanger les composants à des fins utiles. La nanotechnologie amplifie ces possibilités, ce qui ajoute aux applications, mais qui, en même temps, en complique l'évaluation. La question pertinente est de savoir ce qui fonctionne le mieux. On essaye d'y répondre aujourd'hui déjà par des batteries d'essais.

The range for development and product innovation is limited by the pricing pressure, which is high for small and medium enterprises. Quick and efficient advancements in development as well as reliable and effective additives are requested. This assures a solid introduction onto the market and high acceptance by the customer.

Formulators usually believe the perfectioning of additives is assigned to the supplier. However, a raw-material supplier cannot foresee all possible applications, not to mention its conditions and limitations. Since nanotechnology occurs on smallest space, even minor constituents can achieve remarkable effects. This impact can also be too weak, too strong or just get completely wrong.

Only nanotechnology has enabled the analysis of thin films or nanoparticles. Besides AFM (Atomic Force Microscopy at atomic resolution), and analysis like XPS (X-ray Photoelectron Spectroscopy, an x-ray allows detecting elements on the surface), at TOF-SIMS (Time Of Flight Secondary Ion Mass Spectroscopy), an ion beam hits out ions of the surface, and detects them in a mass spectrometer to provide their chemical elements. All those experiments have in common, that they cover the composition at the time of analysis precisely and are located well at the spot, like in a unique snapshot.

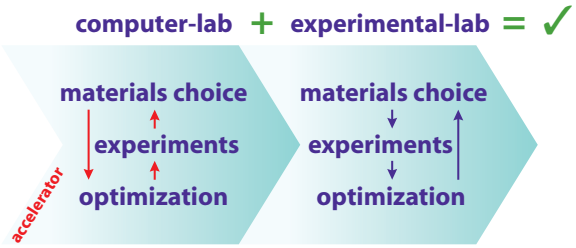

Figure 1: The cycle of optimization takes places in the computation lab separated from the wet lab and in advance in time: With the knowledge of the mixture one goes directly into the optimization process and derives recommendations for the wet lab. Successive research steps advance faster and competitive in pricing.

Most of these results are published in freeze frame illustrations, which means they are missing the awareness for a highly dynamic nanoscale world. At least in soft matters, such as polymers or finishes, the most important properties such as solubility, viscosity, permeability or elasticity are implied by molecular dynamics and interactions between those molecules.

Reproduction of the nanoworld

In the past decades with Molecular Dynamics simulations (MD) a method has been established at universities that provides a big chance for the necessary innovations. In the meantime the corresponding knowledge is available at fruitful partnerships for cooperation in development, contract research and consulting for industries.

In computers, the molecular building blocks of a system and the constitution of physical-chemical forces at thermodynamic motion are reproduced and calculated. This method is like an extreme slow-motion of the molecular dynamics, a sort of nano-imaging movie. It allows for insight in molecular instance and allows for the derivation of macroscopic material properties such as viscosity and elasticity. For this, only the constituent components (polymers, additives, solvents) have to be known. The physical properties are depending on the as well known models and environmental conditions such as temperature and pressure.

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Difference to other methods

The method is based on physical-chemical knowledge of the atoms, functional groups and molecules. Its working bottom-up, that is, the system is built from the basis, constituting the molecules atom by atom with its chemical bonds, and using the molecular building blocks for constitution of the systems. At this, plenty of experimental, theoretical and practical knowledge is involved.

A remarkable number of building blocks for biological, organic and inorganic chemistry exists so far as well as for most common solvents – and any time some additional are defined. The customer hasn't to become involved, the service provider takes care of this mind-splitting job with his experience, such that the customers developers can focus on their true challenges.

An advantage of the method is that it can be established well before the production of new materials. Therefore fresh ideas and new concepts can be checked and validated, insight and knowledge can be gained, and successive experiments will start on a higher level of knowledge and become more promising. This allows for a more efficient and less expensive development phase.

Success by early optimization

From the composition of intended components of a mixture and the environmental conditions the computational laboratory can predict the physical properties of the mixture and conclude on molecular insight. In several virtual experiments the best candidates for a certain application can be determined as well as the improper ones can be disapproved. In this way, the computational lab takes its share to avoid unnecessary experiments in the wet lab, keeps motivation of personal higher up and leads product development at faster pace (Figure 1).

The method is well suited for organic compounds, polymers and solvents in nearly any composition, for mixtures, composites and interfaces between solid, liquid or gaseous states. One can analyse structures as well as its dynamics, development and change, investigate the characteristics of

	structure	dynamics, development, change
		solubility, distribution
		interface
	cluster	interactions, aggregation
	adhesion	e.g. glue, finish
	structure	e.g. surface coatings
	forces	e.g. sensor
		e.g. wetting, reppellent
	diffusion permea-tion	solution, melt
		solids (e.g. membranes)
		mixed (e.g. Gel), release
		gas, ions, charges, fields

Figure 2: Schematic illustration of the calculable variety of physical phenomena.

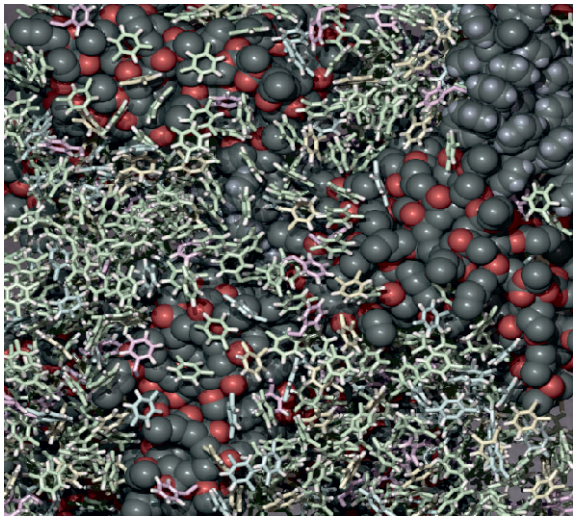

Figure 3: The solvent (technical xylene) is forming the pores in polyacrylester and polystyrene. One recognices, that the solvent (hexagons) is not distributed equally, but tends to form layers or channels.

aggregates and agglomerates, adhesion, diffusion, adsorption, permeability or wetability. With its typical composition, paints and finishes are a good example (Figure 2).

Properties of mixtures

Knowledge of the influence of components on viscosity, adhesion and diffusion is helpful for the control of the processing, the adherence and the dispersion. For the properties of mixtures a special offer exists: xirrus.ch/matters, where you can directly request your target values online. Besides the actual properties available, density, viscosity, heat capacity, thermal conductivity, diffusion coefficient, and elasticity, further properties are possibly predictable on individual request.

Procedures at hardening

To estimate and control the time of processing and the development of film layers, the evaporation of solvents, the chemical structures that establish at polymerisation and the drying process can be investigated further.

Product performance in the finish

To estimate the quality of the final product, one can look closely at the surface, such as it will be enough water- or oil-repellent, or how the permeability of vapor, of air or oil would be. The calculation of the stiffness or hardness can serve the optimization of layer properties.

Examples of applications

The trend off organic solvents towards aqueous systems is of no return. This is necessary from aspects of environmental sustainability, but implies technical difficulties, since the solvent properties of water and organic solvents are totally different. The comparison illustrated in Figure 3 and 4 shows how the same polymeric chains will conform different.

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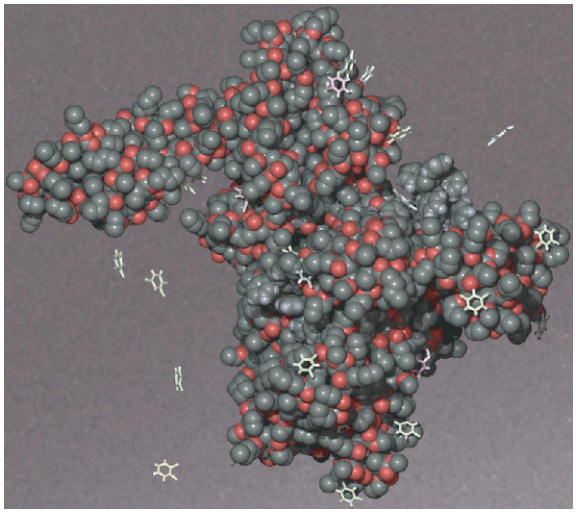

Figure 4: The same polymers in aqueous solution containing 2 volume-% of technical xylene provide a completely different image. The polymer aggregates nearly total, there are no pores to detect and the few organic solvent molecules mostly stay close to the polymeric surface. The water is not shown, since the view onto the structure becomes more clear.

The example of such a mixture shows the molecular, nanoscale reasoning for the experimentally observed disapproval of the film formation. It suggests which additives may be good candidates to counteract this phenomenon. And the named considerations can be checked upon their applicability. Afterwards, one only has to obtain or produce the most-promising candidates and follow the approach further. The method is suited for any thinkable, never ever tested, nor even ever synthetised mixture, to obtain first hints about the expected properties or interesting key values. This is the strength of the molecular quality of the models and the included dynamics, which would be very expensive to observe experimentally on these scales.

Conclusion

The developers claim, the meaningful exertion of Molecular Dynamics simulations (MD) for surface technology currently consists of individual services and consulting for technological and product development in the early stage — or for unexpected challenges in manufacturing processes, at the point of material choice and in molecular design. They identify answers on key questions: whether coated nanoparticles adhere, how additives influence the viscosity at 250 °C or how a surface would soak oil.

The method enables investigations of the application of nanotechnology, whether in paint or finish or elsewhere. Likewise, the complexity of the problem can be understood well, and nanotechnological applications can be accompanied successfully. Hereby, for the customer it is not necessary to think into the numerous models, their compatibility, the academical sources or the stumbling blocks in practice during its application. The problems and challenges can be treated directly and focussed, and feasible solutions can be shown. So far, the satisfaction of the advised speaks for itself. ■