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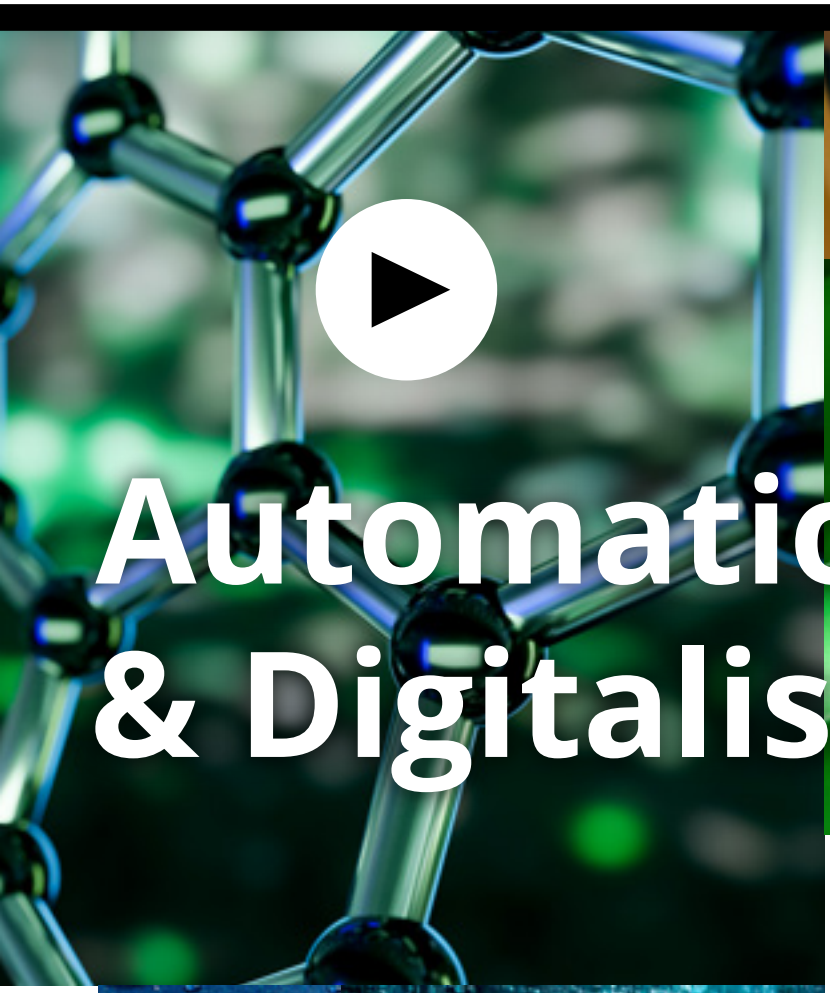

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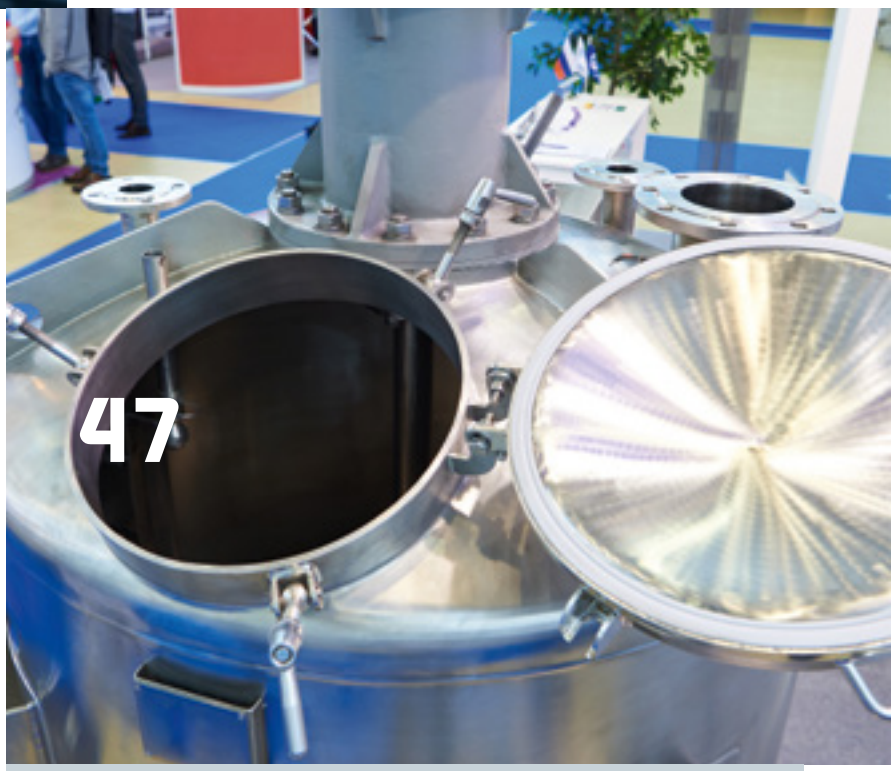

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AUTOMATION IN COATINGS RESEARCH

In the field of science, combinatorial and high-throughput technologies have revolutionised research and development processes. The key to success lies in appropriate experimental design, efficient data processing and advanced data mining software as well as automation. This development is demonstrated here for polyurethane coatings.

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9 From combinatorial chemistry to lab automation and data sciences

9.1 Introduction and history

Combinatorial and high throughput technologies have been established and implemented during the last two decades of the past century and mainly applied in the area of drug discovery. Design of experiments techniques, highly automated and parallelized seamless handling/testing of small-scale samples and the use of high-performance data-mining software were essential to the success realized in pharmaceutical research and development.[1]

Even though first ideas were reported much earlier[2], the transfer of concepts for combinatorial and high throughput technologies into material sciences started to become successful in the middle of the 1990s.[3] Due to the complex requirements of material sciences, combinatorial and high throughput approaches are consisting of even more different and complex stages than in drug discovery. Adequate design of experiments at the beginning, appropriate data handling and finally efficient data mining and assessment are the critical backbone of potentially successful experimental workflows. The broad range of formulations, application and curing procedures of miniaturized samples turned out to be of most importance and hence, very critical for coatings, adhesives and sealants related preparation workflows (see Figure 9.1).

In the first decade of combinatorial and high-throughput approaches, the combinatorial (small scale) syntheses of components also required miniaturization creating significant challenges in designing equipment that could blend formulations, apply them to a substrate, and test them. Moreover, these miniaturized technologies required extended validations especially in coatings workflows to assure that the results are comparable with conventional testing procedures.

In the early phases of combinatorial and high throughput developments, two different approaches were used: On the one side, material-science based companies, such as Bayer MaterialScience, now Covestro, BASF[4], Dow[5], GE, DuPont[6] started building their own facilities internally to address company specific developments. On the other

U. Meier-Westhues, K. Danielmeier, P. Kruppa, E. P. Squiller: Polyurethanes

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hand, technology providers, including start-up companies, such as Symyx Technologies Inc. (its hardware business evolved into Unchained Labs Ltd.), hte GmbH (Heidelberg, Germany) and Bosch (Waiblingen, Germany) started developing flexible workflows that incorporated powerful software tools, automatized (and often miniaturized) building blocks for synthesis, formulation, and physical-analytical testing (cf. first patents of Symyx Technologies Inc.[7]). In many cases technology-oriented companies and big innovative material science companies started co-operating to further accelerate and optimize specific developments.[8]

Figure 9.1: Dosing unit for high viscous liquids

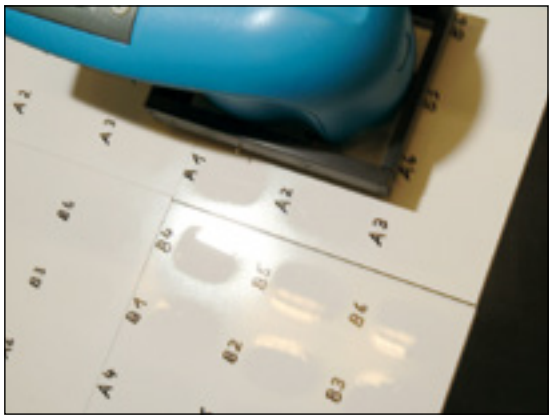

Figure 9.2: Miniaturized spray applied coatings ready for optical analysis

Applications of combinatorial and high-throughput techniques during the past decades revealed – especially in coatings workflows – several limitations in the initial approach.

In many cases the parallelized combinatorial small-scale synthesis of components turned out to be less important for coatings and adhesives and could be omitted (see Figure 9.2).

This led the providers of high-throughput equipment (such as Chemspeed Technologies, Bosch, Labman, and others) to build platforms that forgo miniaturization. Their equipment now provides, besides a comprehensive software solution, automated preparation and handling of formulation, application and preparation of samples, and flexible testing procedures all at normal full scale[9] (see Figure 9.3). Materials manufacturers[5, 10] as well as small and medium-sized enterprises (SME's)[8] have adopted their use in their R&D and quality insurance processes[11].