Simulating High-Pressure Polymerization Processes

- Acquisition of Thermophysical Properties and their Impact -

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Despite that the high-pressure polymerization of ethene and is co-monomers is a well-known and well-established process it is still and very interesting and challenging object of investigation. This originates from the facts that with a very limited number of co-monomers an extreme large variety of products are accessible. The majority being known may be attributed to the class of commodities. However, among such materials there are also highly specialized ones from areas of advanced technology such as parts of human implants, encapsulation material for photo-voltaic elements, medical packaging or insulation material for ultra-high-voltage cables that are an indispensable element for transport of electrical power enabling the energy transformation of our society. Moreover, such materials are the classical example of product by process as process conditions and reactive environment control the microscopic structures of the formed polymeric material. These further-on determine the application properties. Understanding this coupling helps formulating design principles of new polymeric materials.

During the lifetime of this process the volume of production and the demand on plant size continuously grew. Nowadays, the typical production scale of a single line is about 400 kt / á. In combination with the fact that operation pressure ranges up to 3500 bar and ethene tends to deflagration at such conditions at high temperatures it means that running such plants one has to consider certain risk prevention measures. All this holds back from the traditional trial & error approach in developing new variants and opens the door for simulations as a design tool.

The very fundamental base for such simulations are well defined thermophysical properties. The quality of such data determines in an ultimate manner the soundness of simulation models at all. For the sake of compensating the lack of such data being directly measured often extrapolation methods are used, assuming a sound predictive potential of the applied theories. In that respect it is highly desirable to test for the feasibility of direct measurements at pressure and temperatures close to process conditions such as 3000 bar and 300 °C.

The contribution will illuminate the capabilities of such simulation models for process and product design, their needs for qualified input and the impact of the uncertainty of input parameters. In the focus of interest there is a calorimetric device, a high-pressure high-temperature transitiometer and it‘s capabilities. If time permits the scope will be widened towards investigation of safety related data on the deflagration of ethene at high-pressure conditions up to 3000 bar.