Federal Ministry
Republic of Austria
Digital and
Economic Affairs

Christian Doppler
Forschungsgesellschaft

Mathematics for efficiency and control

Mathematical models make it possible to calculate the behaviour of tiny particles in large facilities. The results can be used to increase the efficiency and quality of the production of polyolefins.

The topic

Polyethylene and polypropylene are among the most frequently used synthetic materials, particularly in the packaging industry, as insulating material for cables and capacitors, in the automobile industry, as raw materials and as coatings for pipelines. Borealis has its own technology to produce these high-quality materials on a large industrial scale. With its motto of "creating added value through innovation", the company is very keen on increasing the efficiency of its technology for making synthetic materials.

The research question: how can the production of synthetic materials be further optimized?

Polyethylene and polypropylene are produced in fluidized bed reactors from their monomers, which are supplied in the form of pellets about 2 mm in size. The fluidized bed reactors are industrial-scale facilities about the size of a church tower. The raw materials (monomers) are introduced in a gaseous form and converted to solid polymer chains with the help of a catalyst in a process that releases heat. In the ideal case, all of the resulting polymer pellets would have identical sizes and properties but this only happens if the

CD Laboratory for Particulate Flow Modeling

Head
Assoc.Univ.Prof. Dr Stefan Pirker; University of Linz

Operation
01.01.2009 – 31.12.2015

Commercial partners
Borealis AG, PLANSEE SE, Primetals Technologies Austria GmbH, RHI Feuerfest GmbH, ThyssenKrupp Resource Technologies GmbH, voestalpine Stahl Donawitz GmbH, voestalpine Stahl GmbH

Three questions to ...

Dr Norbert Reichelt
Senior Group Expert Polyolefin Technology, Borealis AG

Why is basic research so important for innovation?
Innovation comes about from the combination of knowledge from various branches of science and the private sector. Although basic research is costly and time-consuming, it paves the way for new knowledge that can one day be applied in the private sector.

What are the biggest challenges in collaborating with universities?
For the collaboration to work well, all partners should agree on the problem to be addressed, the state-of-the-art and the necessary approaches. Agreement of this kind needs time and a continuity of collaboration.

What do you like most about the CD Laboratory funding scheme?
The CD Laboratory funding scheme tackles precisely these challenges. The seven-year duration of the laboratories provides the framework for a successful collaboration with basic research that benefits the universities and the industry.

reactors are precisely controlled down to the level of the individual particles. It is important to control and predict the behaviour of all particles as accurately as possible, as each tiny irregularity increases the use of energy and raw materials, produces more rejects and can lead to costly production stops. The technical challenges can be studied empirically on the laboratory scale but the results cannot be simply transferred to the production facilities because of the disparity in scale between the tower-sized reactors and the laboratory equipment. There is a need for new, complex mathematical models and elaborate numerical simulations.

Collaboration in the CD Laboratory

Borealis can only undertake the fundamental research at the necessary level of complexity in collaboration with an external partner with appropriate expertise, which is why the company chose to work with scientists at a university. Prof. Pirker and his team in the CD Laboratory for Particulate Flow Modeling have longstanding experience with mathematical modelling, as well as the necessary resources and computer power. The CD Laboratory has developed and validated a mathematical model based on a description of the problem and using appropriate data sets from Borealis.

Results

The mathematical model developed in the CD Laboratory, the Subgrid Model, can model all key parameters and thereby enables optimization of the process technology. The retention time of the monomers in the reactor, the temperature profile of the reactor and the precise gas flows in the fluidized bed can all be calculated. The results have already been implemented, based on the modelling and on an experimental validation on the laboratory scale – which was also performed in the CD Laboratory. The scientists have used their model to investigate the available facilities in detail and to optimize them, whether they were pilot-scale or production facilities. Borealis has secured patent rights to all relevant technological advances but the model's methodology has been published and made available to the scientific community via the freely accessible open-source simulation platform CFDEM (www.cfdem.com) for further optimization. The CD Laboratory for Particulate Flow Modeling has also enabled a staff member to qualify as an Associated Professor. The success encouraged Borealis to establish a new CD Laboratory in 2016 to continue its research, again with the University of Linz.

Scientific challenge

The numerical description of interactions between particles or between particles and a liquid or gas on an industrial scale is highly complex and requires fundamental research in fluid mechanics. The results are widely applicable: to tiny particles in the fluidized bed reactor, to coarse-grained bulk solids in a charging process, to powder-metallurgical forming, in which metal powder is pressed into the desired form, and to many other instances. The CD Laboratory's most notable success is that NASA used the mathematical models developed in the CD Laboratory for the blast furnace to simulate the interaction between the wheels of the Mars probe "Curiosity" and the rocks on Mars.

Added value for the company

The results from the CD Laboratory are improving the efficiency of the facilities, which now use less energy, require less material and produce fewer rejects; furthermore, production stops are significantly less frequent. The optimized Borstar technology is being sold and licensed on the global market.