Machine means for design, control and economic optimisation of polyolefine production processes and their products

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Abstract
The polymer industry and especially the producers of polyolefines move towards producing polyolefines with increased strength. This gives polyolefine applications with thinner container walls, thinner films and pipes. This again leads to a reduction in weight, transport cost and material usage, making the use of plastics more attractive and enhancing its environment advantages over other materials even further. To obtain this advantage more tailoring of the molecules is required. For a cost-effective way of to do this computer modelling tools are used. Examples of this will be discussed.
The converters being the customers of the producers needs to run their machinery closer to the limits so as to utilise their assets better and better. This sets more stringent requirements for more even product quality with smaller and smaller variations. The producer’s hence needs to control the product quality and production process better and better. This is achieved with increasing utilisation of model based control.
The lowering of the cost of transport and the abundance of raw material as Naphtha and petroleum gasses in the eastern countries constrains European economical operation more and more. Plastics pellets are raw materials and its demand varies with the faith people have in the economy of the area and the world in general. These variations show to be difficult to predict and they are bumpy. The most economical way of producing the plastic pellets depends on the price to be obtained for prime products and the transition product and the costs of the raw materials. Tools to do economic optimisation depending on the marked conditions will be discussed.

Discussion
The polymer industry has seen a sustained growth during the last decades, with a substantial marked world wide. The growth in the West European marked is from 1 to 8 % depending on the type of polymer. The world wide marked is estimated to be 10^{12} Euro per annum. The main use of polymer materials is for packaging and distribution. Here one experience large savings in the weight and volume of packaging material. This especially compared to older type of packing materials as cardboards, glass and wood. Modern cars have seen a marked reduction in weight and thereby also fuel consumption. It is estimated that introduction of plastic materials in cars reduces the fuel consumption in the European Union by 12 million tons per annum.

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Polymers are monomer molecules joined together to form long molecules containing thousands of repeat monomer units. There are basically three types of polymers: Thermoplastics, Elastomers and Duroplastics. The Thermoplastics can be reversibly melted and harden, examples are polyethylene and polypropylene.

The other types have a certain degree of cross linking of the molecules so that they are permanently set when harden. Borealis produces polyethylene and propylene with different processes. Depending on the process used the polymer formed can vary markedly, examples are the production of Low Density polyethylene that is formed under 1200-3200 bar high pressure using radicals as the starting point for the polymerisation, while High density polyethylene is produced in 20-50 bar pressure processes using catalyst as the starting point for the polymerisation.

The design of the product needed for the market and the process to produce this product needs to be designed. The tools used are computer simulations together with experience from bench scale and pilot scale reactors. To define the process variables the thermodynamic behaviour of the fluids in the processes needs to be described together with the reaction kinetic steps. Joining these descriptions together and including the mass and heat transfer balances also the mass transfer on a micro and meso scale will give a description of the polymer molecules. The description of the molecules will often be in the form of a distribution of polymer chain lengths, having a very broad distribution. Simplifying the description of the polymer length distribution giving the number average molecular weight, Mn, and the weight average molecular weight, Mw, is quite normal. The width of the distribution is often expressed as the polydispersity index which is the ratio of the Mw/Mn.

Examples of such simulation tools are HighSiM, Aspen/Polymer Plus and Predici.

Material to produce pipe requires strength, however only making the material strong makes processing of it difficult and requiring a lot of processing energy. The trick is to make the material strong, but on the same time add a component of “lubricating” material so that processing the pipe material to pipes becomes “easy”. The material is made bi-model one strong part and one “lubricating” part. To have the freedom of tailor-making each part of the bimodal distribution each mode is made in a separate reactor. Changing the operating conditions of each of the reactor will change each of the modes.

The requirements by the customer are getting more and more stringent. The product shall be delivered on time and to the required quality. This requires the introduction of advanced process control where the control scheme applied contains knowledge of complexity of the process and how it is operated. Borealis has applied APC to their production plants for quite a long time and seen marked improvements in the operability and the steadfastness of the quality of the produced product.

The price of the polyolefin does vary more and more prices cycles are squeezed into a shorter time span. The need for adapting the operation of the production plants to these fast changes is hence growing. Typically the price of the product is strongly related to the quality of the product. The good price is only obtained inside small variations in the end product properties. The optimisation of the change from one grade to the next is challenging as the function of the price premium has abrupt changes going from one grade to the sub standard product and again over to a new grade. The economic optimiser will also want to change the same set points as the quality controls so a
A hierarchical system handling the optimisation is needed. The economic optimiser, e.g. the Pathfinder from IPCOS, works on simplified process models so as to be able to do the calculations fast enough. To ensure that the simplified process model represents the process well enough an estimator for example in the form of an extended Kalman filter will be applied. Adjusting the allowed speed change for the manipulated variables and introducing the cost and price for the raw materials and the price of the product enables a notable savings in the cost for the grade change.
**Monomer:**
- R1R2C=O
- Methylmaleic (R = CH3)
- Maleic anhydride (R = O)
- Acrylonitrile (R = C≡N)

**Polymer:**
- Poly(methyl methacrylate) (PMMA)
- Polymethylacrylamide (PMA)
- Polyacrylamide (PAM)

**n:** Degree of polymerization

**Thermodynamic**

- Improved methods in describing polymers are SAFT (Statistical Associating Fluid Theory) and PC-SAFT (Polarizable Continuum Model).
- Other methods: Non-Continuum Spectroscopy

**Reaction Kinetics:**
- Site activation
- Site deactivation
- Site inhibition
- Chain propagation
- Chain transfer

**Production conditions affects the physical properties of the product**

- **Polymerization**
  - Radical
  - Coordination
  - Cationic
  - Anionic

**The distribution of polymer chains with different lengths**

**High-conversion simulator**
- Molecular: Simulate the dynamic simulation of polymerization
- Predictive: Simulate the structure and chemical dynamics of polymerization
- Molecular: Molecular weight distribution

**A tool for Tracker, Talker, Sniffer, Seller...**
**Borealis**

Distribution of long-chain branches

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**Borealis PE Technology**

- **Polymer reactor**
  - Develop particle morphology
  - Polymerization in parallel
  - $T = 65^\circ C$, $P = 30$ Torr

- **Loop reactor**
  - To produce linear PE
  - From $T = 65^\circ C$, $p = 30$ Torr
  - $T = 115^\circ C$, $p = 2$ atm, $20$ hrs

- **Gas Phase reactor**
  - To produce high molecular PE
  - Gas phase polymerization
  - $T = 85^\circ C$, $p = 25$ atm, $21$ hrs
  - $T = 130^\circ C$, $p = 2$ atm, $3.5$ hrs

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**Binnodical concept - Benefit for customers**

**Material saving in pipe**

- Higher pressure rating for gas pipes
  - 7 bar
  - 6 bar

- Material saving for water pipes
  - 87% reduction

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**Borealis**

Borstar tailor makes the polymer

- Output of the reactor

- 5% of reactor capacity

- 10% of reactor capacity

- 5% of reactor capacity

- 5% of reactor capacity

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**Example from LDPE Rieningen, No. of production steps**

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**Borealis**

Borstar PE HIP process

- The Borstar PE process consists of two reactors in series

- Borstar: New PE polymers

- Borstar PE HIP: New PE polymers

- Borstar PE HIP: New PE polymers

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**Substandard quality, LDPE Reningen**

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Economically Optimal Dynamic Grade Transitions

Objective: Maximise Added Value during a transition

\[ TVT(T) = \sum price_i \times (\text{yield}_i - \text{cost}_i) \times \frac{dv}{dt} \]

- **REV** = **COST**

Price of product to be obtained depends on grade.

Less loss of revenue with the optimised trajectory.