Clemens HOLZER
Montanuniversitaet Leoben, Department of Polymer
Engineering and Science, Chair of Polymer Processing

The Future of Polymer Processing

UDK 001.18:678.7
Review Article / Pregledni rad
Received / Primljeno: 30. 5. 2011.
Accepted / Prihvaćeno: 10. 1. 2012.

Abstract

The 40th anniversary of the *Chair and Laboratory for Polymer Processing* at *FMENA* in Zagreb was a good opportunity not only to look back, but also to look into the future. What will the challenging topics be in science and research? What will be the demands from industry and customers? Modelling and simulation, although already at a high level, will become even more important, since the need will increase to understand and predict the processing of complex products with new materials. Since reliable material data are a key factor for good simulation results, a great deal of effort will be invested in this field. Simulation and good material data will then be the basis to develop polymer processes further beyond the now existing limits and thus enable new designs with new materials like special compounds, bio plastics or recycled material. Polymer processing will not only stay fascinating, but become even more exciting with the new possibilities and the new challenges that the future will bring.

KEY WORDS:
bio plastics
compounding
material data
polymer processing
simulation

KLJUČNE RIJEČI:
biopolimeri
podatci o materijalima
preradba polimera
simulacije
smješavanje

Budućnost preradbe polimera

Sažetak

Četrdeseta obljetnica Katedre i Laboratorija za obradu polimera na FSB-u u Zagrebu bila je prigoda ne samo za pogled unatrag nego i za pogled u budućnost. Koji će biti izazovi u znanosti i istraživanju? Koji će zahtjevi biti postavljeni industriji i kupcima? Modeliranje i simulacija, iako već na visokoj razini, još će više dobiti na važnosti, jer će se povećati potreba za razumijevanjem i predviđanjem obrade kompleksnih proizvoda s novim materijalima. Budući da su pouzdani podatci o materijalu ključan čimbenik dobrih rezultata simulacije, velik dio napora ulagat će se u to polje. Simulacija i kvalitetni podatci o materijalu bit će onda osnova za razvoj polimernih postupaka izvan sadašnjih granica i tako će omogućiti nove konstrukcije s novim materijalima kao što su posebni spojevi, bioplastike ili oporabljeni materijal. Obrada polimera neće samo ostati fascinantna nego će postati još uzbudljivija s novim mogućnostima i novim izazovima koje će donijeti budućnost.

Introduction

The *Chair and Laboratory for Polymer Processing* at the Faculty of *Mechanical Engineering and Naval Architecture University of Zagreb*, Croatia, is celebrating its 40th anniversary! This was, of course, a good reason to look back on a very successful history, but it is also an opportune time to look forward. What will the next 40 years bring? What will be the role of polymers and polymer engineering in the future? How can we get prepared for this future? What will be our focus in our teaching and in research and science?

The main challenges in the next decades will be the growing population, the concentration of people in expansive urban centres, and globalization, and the expected change of climate. Therefore, the big (technical) topics for mankind in the future will be energy & resources, food, health, mobility & infrastructure and communication. And there is no doubt that polymers will play a key role in finding successful ways in handling these challenges. Polymers will be the material of the new millennium and the production of polymeric parts – *green*, sustainable, energy-efficient, high quality, low-priced, etc. – will guarantee the availability of the best solutions all over the world.

Where can we see the advances: in insulating material for drastic saving of heating and cooling energy, new packaging solutions for the reduction of the loss of food along the supply chain, rapid analysis of diseases with lab on chip devices, and lightweight structural parts for vehicles and aircraft or power plants based on wind, sun or biomass. Polymers will be everywhere!

Simulation

The contribution of polymer processing to cope with future challenges starts with modelling and simulation. The research in polymer processing is driven by the strong will to understand what is going on in various processes and what the results will be. At present, the simulation is already very popular and used in many fields like 3-D flow simulation of the filling process in injection moulding, modelling of screws, mathematical models for understanding of the melt characteristics in the screw channels, calculation of heat transfer in moulds and so on.

In the future, the need for simulation will become even broader and deeper. Broader: not only the accurate simulation of the process itself will be in focus, but rather creating a whole virtual production starting from the molecule and finishing with the virtual testing of a virtual product will be the aim. With atomistic modelling, ideal compounds can be created using all kinds of polymers and fillers including inorganic or organic and all kinds of different shapes. Via multiscale modelling (from atomistic to nanometer to macroscopic scale) several length scales have to be bridged to predict the final properties of the part. There is already a great deal of existing know-how and even programs, but bringing it all together in a reliable virtual process will keep us busy for decades to come.

The questions that have to be solved are:

- What is the influence of the filler type (polymer, mineral, carbon), surface chemistry, size, shape and aspect ratio on the filler-matrix interfacial behaviour?
- How can the existing methods be adapted? Eventually, even new processing methods must be developed to optimize distribution, orientation, and interfacial properties of fillers (e.g., gradients in volume fraction or size, tailored textures, etc.). Can these methods be up-scaled to the necessary mass production scale?
- How can multifunctional, often contradicting, properties be realized (e.g., high stiffness requires strong covalent bonds, while biodegradability would need rather weak bonding)? What can we learn from natural nanocomposites in this respect?

Another aspect of the broader use of simulation is the use of expert systems in the development process. Using both expert knowledge and internal know-how from companies and combining this content management system with injection moulding simulation and precise measurement of the parts (Figure 1) will lead to a significant reduction of the development times and the correction loops.

With the help of modern camera systems, the troubleshooting e.g., in injection moulding, will also be developed further by expert systems or neutral networks. In the future, it should be possible that the faults will be recognized automatically by a camera system. By converting the pictures and processing the data in expert systems, the machine parameters will be adjusted immediately to ensure a defect-free production (Figure 2).

Deeper: although the simulation of the injection moulding process has already reached a very high level, there are limitations in the simulation of polymer processes like the weakness to take into account the pressure dependency of material data, which leads to a bad shrinkage and warpage prediction. Since many research groups are working eagerly on these topics and the progress in mathematics and computer technology will help us strongly, the future will bring new knowledge and better solutions for simulation.

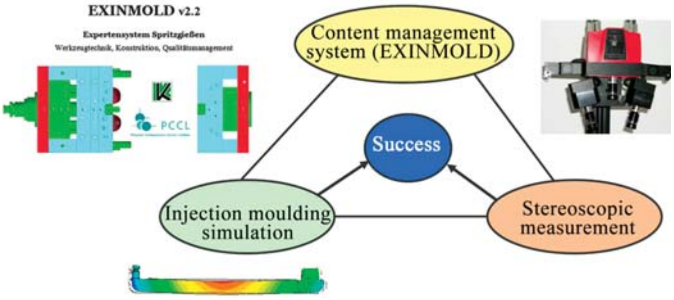

FIGURE 1 – Software supported expert system for injection moulding[1]

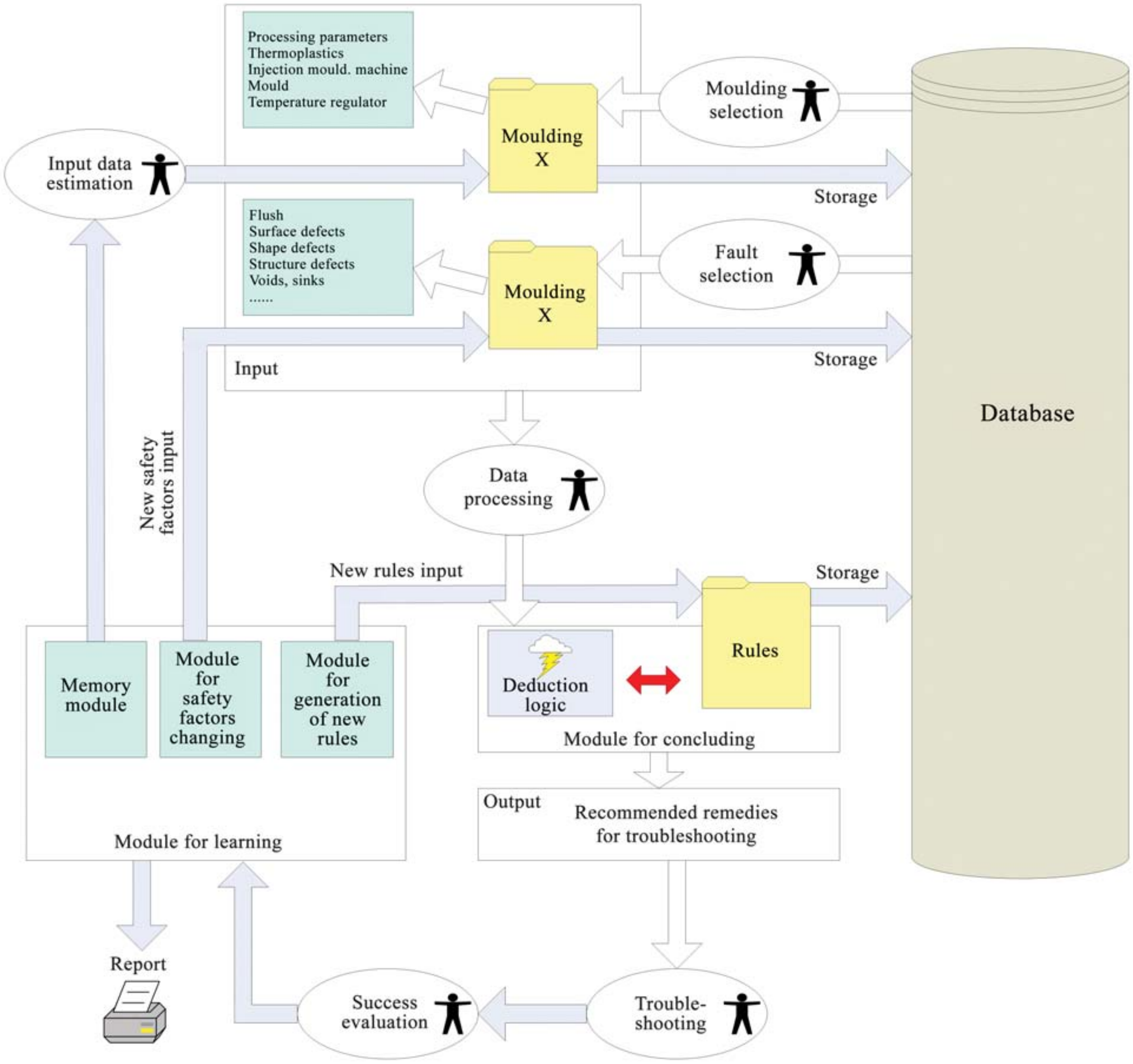

FIGURE 2 – Example for an operating strategy for a troubleshooting system in injection moulding[2]

In extrusion technology, similar technological characteristics to those in injection moulding are of considerable importance and there is the same large demand in modelling and simulating. Screws and dies can already be calculated, but the basic processes like the melting process in the solid conveying zone, the conversion process from granules or powder to melt has not been yet understood well enough. Simulations are becoming very complex and difficult, especially when it comes to twin-screw systems with various screw elements (e.g., used in compounders) or to multilayer films for packaging industry. In these fields, much work needs to be done in the next years to come closer to virtual processing of the extrusion.

The existing models tend to only work well with amorphous thermoplastics. The crystallization kinetics for the cooling of semi-crystalline thermoplastics is still a major issue to be solved; not to mention high filled thermoplastics, polymers with long fillers or thermosets and elastomers.

Nevertheless, simulation is a tool that will help us extensively to create fast, reliable and economical processes in a very short time and with almost no development cycles, thus reducing the time-to-market, the costs and the resources needed for the design of new products or new processes.

One final word on simulation; at the end there is always the comparison of the calculated values and the measured data from experiments on the machines. In the research lab it is usual to use the equipment with many sensors to gain ideal and most of all reliable data right from the place where the quality of the product is determined – from the tool itself. But in industry the use of sensors is for a lot of reasons not very common, so the tool remains an uncontrolled black box.

Currently, in polymer processes, a widely developed processing machine is often used and equipped with many sensors adjusted to control circuits. Contrary to this fact, in the mould where the product quality is formed, just a few sensors are installed. Actually, the range of different in-mould sensor types is small, most common are temperature and pressure sensors.[3]

The aim in the future must be to develop new sensors to build more intelligent moulds. The sensors should be easy-to-install in the mould, should have long lifetime cycles and should have fast exchangeability times (for best maintenance). Another aspect is to develop in-mould actors to control more effectively the product quality. Recent research in injection moulding has shown that, e.g., especially the hot runner system (Figure 3) is a minimally explored section of the mould with a high potential of influencing product quality. New sensors in combination with advanced control systems should lead to new control strategies in the polymer processes to increase efficiency of the production.

Material Data

The reliability of flow simulation results in polymer processing depends mainly on the input material data, process parameters and numerical model. In particular, the rheological data of the polymers have the biggest influence on the accuracy of the flow analysis. For the analysis of the flow behaviour and measurement of high quality material data for the process optimisation and improved simulation of extrusion or/and injection moulding, the slit die system with flush mounted pressure transducers along the flow channel has proved to be the most suitable (Figure 4). This system also offers the possibility to use an injection moulding unit or an extruder for the melt processing (measuring the viscosity at high shear rate under practical conditions directly on the processing machine). This enables the history of the melt to be taken into account and more congruent data can be measured. Moreover, highly filled and new materials with few or non-existing material data (e.g., powder injection moulding (PIM) feedstocks or wood-plastics composites (WPC)) can be measured. In the future, the need for individual and very accurate measured material data will increase enormously due to the growing use of compounds.

Additionally, the pressure and temperature dependency of other material data like the thermal conductivity is an important material property for the injection moulding simulation of polymer parts. Up to now the pressure dependency of the thermal conductivity has not been taken into account in simulations. However, the research results indicate that this influence is not negligible. Figure 5 shows that an increase of the pressure from 0 to 80 MPa leads to a rise of the thermal conductivity up to 25% for semi-crystalline polymers.[6]

The Edges of Polymer Processing

The importance and therefore the market for micro- and nanostructured polymer parts increased strongly within the last years.[7] While the market volume only for microfluidic devices in 2006 was 600 million USD, it is predicted to reach 1.9 billion USD in 2012.[8] This also applies to the whole production of micro- and nanostructured polymeric parts.[7] A reason for this large increase is the wide range of applications which span from micro optics (e.g., microdisplays) or microelectromechanical

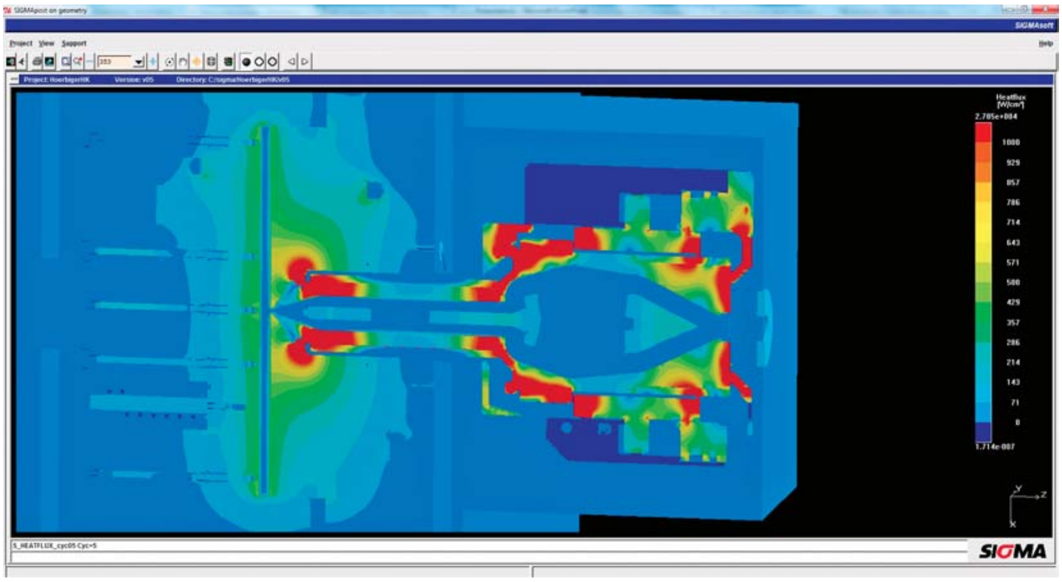

FIGURE 3 – Simulation of the heat flux in a hot runner system[4]

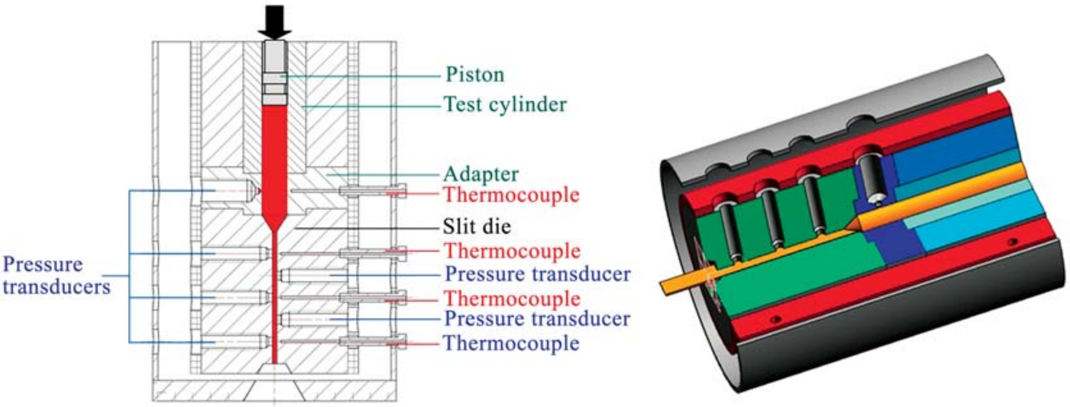

FIGURE 4 – Slit die system for analysing the flow properties of high filled polymers directly on the processing machine or high pressure capillary rheometer[5]

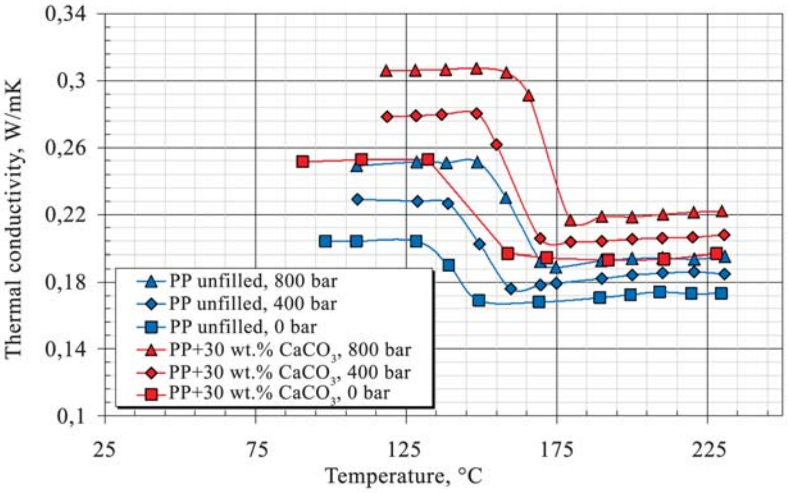

FIGURE 5 – Thermal conductivity as function of temperature and pressure for unfilled PP and PP filled with 30 wt.% $CaCO_3$[6]

systems (e.g., inkjet heads) to microfluidic components,[7,8] (e.g., medical devices for blood analysis).[8,9] Finding these methods which allow mass production of these applications at low costs would open up many opportunities, especially for the medical health care.[8] Thermoplastic polymers are cheaper than the normally used silicon[9] and have unique thermal, mechanical and electrical characteristics which allow them to be used in many applications.[7] Moreover, several less sophisticated methods for low-cost replication of microstructures exist and would permit smaller clean room production lines. This is an important factor for small companies that want to enter this business.[9]

The first step for the future success of these methods is to determine the limits of polymer processing now. Some hints of these limits can be found in the research work performed at the *Institute of Polymer Nanotechnology* (*INKA*) in Windisch, Switzerland.[10] To reach the limits, a tool with 18 nm wide structures has been produced on silicon and has been replicated via injection moulding using a *variotherm* cooling / heating system (Figure 6).

We are only at the beginning in the basic research field of the production of micro- and nanostructured polymeric parts; we have to become familiar with the main influences of the process on the structured parts as a starting point. This is important because there are key parameters in the production of microstructures which are of less significance in the manufacturing of standard polymer parts, e.g., the importance of the ejection forces or the different methods of cooling / heating the tool to gain the best results.

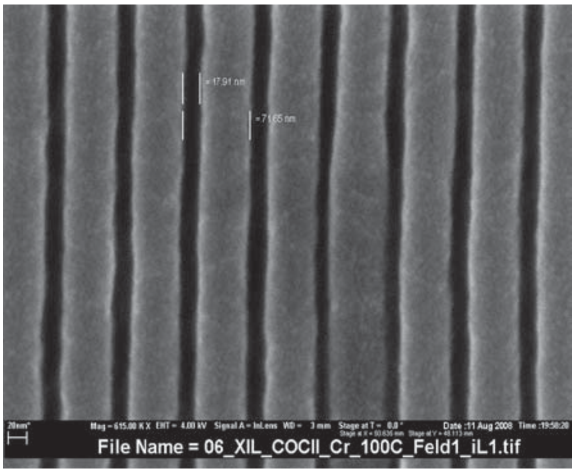

FIGURE 6 – 18 nm channels injection moulded in cycloolefinic copolymer (COC)[10]

Another critical issue at the limits of polymer processing is the production of thin walled parts, e.g., for medical applications or the electronic industry. Since the melt quickly solidifies when getting into contact with the colder surface of the mould cavity, very high injection speeds are needed to produce thin walled parts. The limits of common injection speeds can be overcome by the very promising method of expansion injection moulding (developed by *Engel*, Austria). By closing the nozzle before injection, a pressure of up to 250 MPa can be produced, which after opening the nozzle practically explodes the melt into the cavity (Figure 7).[11] Extreme high shear rates are reached – up to 1 mio s^{-1}! The fundamentals of this process have to be studied by using simulation under these extreme conditions, measuring the material data and understanding the material degradation. Thus, future parts with exceptionally thin walls (down to less than 0.3 mm and flow length / wall thickness ratios up to 450:1) can be designed and produced.[11]

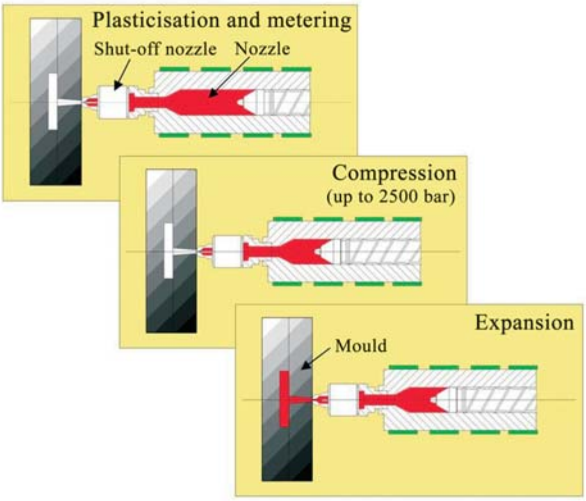

FIGURE 7 – Processing steps for the expansion injection moulding[11]

Processes for Special Materials

Compounding has always played an important part in polymer processing. Nevertheless, over the last years it developed from just material converting (e.g., extending a polymer matrix with mineral fillers) to its own field with high industrial and scientific interest. Many new research projects have been launched during the last few years and it is to be expected that this trend will continue even more distinctively. One of the largest topics in compounding is nanotechnology or more precisely, the use of nano-scaled fillers which can be found in many of the current and future research topics. In this connection, the correct (chemical and physical) preprocessing of fillers and matrix is essential to achieve the needed properties following the *from-pit-to-part* strategy for tailor-structured fillers. Very promising topics in the future will be:

- Recycling: the research will focus on the reinforcement of recycled polymers, since there is a great demand from industry (and society!). By using mainly mineral fillers the material properties of recycled polymers will be improved and thus it will be possible to use the recycled material for high quality applications. Furthermore, organic fillers like algae (Figure 8) or organic waste will be used to transform petrochemical polymers into biodegradable polymers. A completely new technology for the processing of recycled materials has been introduced lately – the conical co-rotating twin screw extruder by *MAS Maschinen und Anlagenbau Schulz* GmbH. Large input volumes resulting in excellent feeding characteristic, high melt pressure build-up, excellent homogenization characteristics and low specific energy consumption make this system very appropriate especially for the recycling of flakes.
- Multifunctional materials: a very important field of research in compounding with a very high impact are multifunctional materials. This group of materials is of great import to both industry and science and includes the following: active fillers, intelligent packaging, metal substitutes (in terms of mechanical and temperature properties), lightweight or self-X materials (self-cleaning, -healing, -assembling, etc.).
- Industry needs: in the production, often small material quantities with special properties are needed which are not available commercially. For the development of such compounds, but also for high mass production, a new technology is coming on the market: the injection moulding compounder. This new machinery is a combination of a commercial twin-screw extruder and an injection moulding machine, with many advantages like processing in the same heat, gentle treatment of sensitive polymers and fibres or the possibility of fast material development.

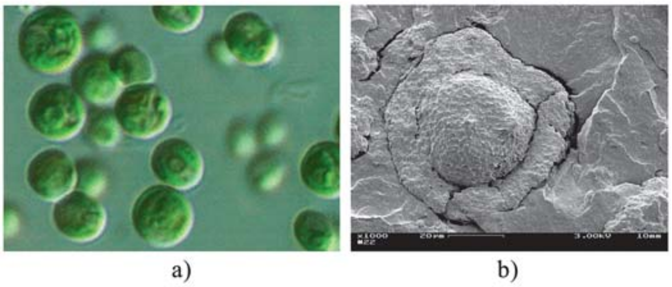
a) b)

FIGURE 8 – Chlorella algae (A)[12] processed with polyethylene (B) for achieving biodegradability[4]

At the high end of compounding there are compounds based on high temperature exceptional properties, for instance, as material replacement of metal parts. Likewise, the aircraft industry, in their effort to reduce weight at reasonable costs, and the machine industry, in their search for high-tech polymers for precise machine elements under harsh environmental conditions (Figure 9), look to high-end compounding for solutions. The base polymers used are high temperature polymers like PI, PPS, PSU or PEEK which can be difficult to process. By blending, compounding and filling with glass or carbon fibres – even long fibres – the processing sometimes seems impossible. Nevertheless, there is a strong interest to use these *high-tech* compounds and the polymer processing research institutes and industry will invest considerable resources to understand these processes and to advance their development. The process and material optimisation will have to go hand in hand and of course, we come back once more to the question of reliable data for simulation.

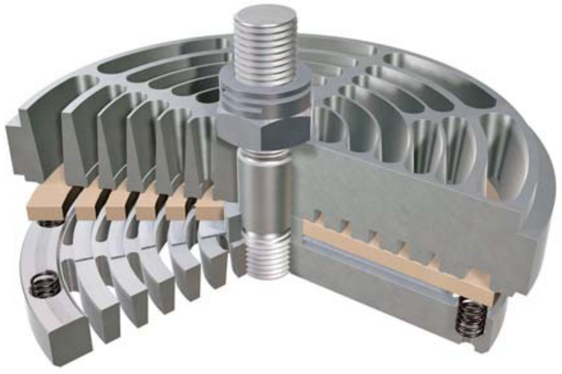

FIGURE 9 – High-tech valve with parts made out of PPS / carbon fibre via injection compression moulding[13]

Bioplastics

Another type of polymeric-based material that is becoming more and more important are bioplastics. In general, there are two types of bioplastics: (1) materials based on renewable resources, and (2) those which are biodegradable. Bioplastics offer a vast potential in future applications in the field of plastic commodities because of their sustainability.[14] Nevertheless, the basic scientific investigation of these materials with regard to the influence of process parameters on the achievable properties, such as temperature stability, mechanical properties at room and higher temperatures, barrier properties and optical or haptic properties is less than sufficient.[15] In the last few years, biodegradable polymers have become increasingly important, especially for packaging applications. High-tech films like highly mineral-filled multilayer film made of polylactide (PLA) with a foamed core have been already developed (Figure 10),[16] but the products and the technology are in the formative stage and will continue to grow in the next few years. The blending of PLA with a second polymer using tailor-made compatibilizers in order to tune the mechanical properties is an important field of research that will be dealt with in the next few decades.

Boeing has been developing a sensational new airplane – the *Dreamliner 787* – with about 50 weight % of carbon fibre composites. One reason for the delivery delays are the problems with processing the polymer composites – which brings us to another field of polymer processing - the processing of thermosets. Since this is a completely another topic, it may be addressed in a future article.

Conclusion

Polymer processing is a wide field and an extremely fascinating one for science, research and industry. In the last decades a giant step has been made bringing the polymer processing technologies to the high level where they are now: Modelling and simulation made a deep look into the processes possible, the necessary material data are achievable at a high and praxis-relevant level and new materials and technologies have been developed. Yet, the new technologies are still waiting to be developed further and the new materials always demand more innovative processing strategies. As it always goes, the more questions are answered the more new questions have to be asked. In the coming decades, we will face many challenges that will be solved with the close cooperation between mechanical engineering, material science, electronics, control technique, chemistry, etc., in short, polymer engineering and science!

Acknowledgements

Special thanks to Dipl.-Ing. Ivica Đuretek who is always the strong link between Zagreb and Leoben. I would also like to thank him and Dipl.-Ing. Martin Burgsteiner, Dipl.-Ing. Thomas Kisslinger, Prof. Dr. Stephan Laske and Dipl.-Ing. Florian Müller for contributing to this paper.

REFERENCES

1. Chair of Polymer Processing and Polymer Competence Center Leoben
2. Chair and Laboratory for Polymer Processing, Zagreb
3. Kazmer, D. et al.: *Feasibility Analysis of an In-mold Multivariate Sensor*, Intern. Polymer Processing, XXVI(2011), Carl Hanser Verlag, Munich.
4. Chair of Polymer Processing, Leoben
5. Đuretek, I., Friesenbichler, W., Holzer, C.: *New Insights into Characterization of Flow Properties of PP Based Wood Plastic Composites*, 26th annual meeting of the Polymer Processing Society, Conference Proceedings, Banff, July 4th – 8th 2010.
6. Đuretek, I., Friesenbichler, W., Kucher, C.: *Thermal Conductivity of Talc Filled Polypropylene Measured at High Pressures*, 25th annual meeting of the Polymer Processing Society, Conference Proceedings, Goa, March 1st – 5th 2009.
7. Giboz, J., Copponnex, T., Mélé, P.: *Microinjection molding of thermoplastic polymers: a review*, J. Micromech. Microeng., 17(2007), IOP Publishing, R96-R109.
8. Attia, U. M., Marson, S., Alcock, J. R.: *Micro-injection moulding of polymer microfluidic devices*, Microfluid Nanofluid, 7(2009), Springer-Verlag, 1-28.
9. Zengerle, R.: *Vorlesungsunterlagen zu* Mikrosystemtechnik Technologien & Prozesse, Abschnitt 12 *Heißprägen & Spritzgießen*, 15. 2. 2006.
10. Holzer, C. et al.: *Replication of Micro- and Nanostructures on Polymer Surfaces*, Macromolecular Symposia, Special Issue: Modern Trends in Polymer Science EPF'09 96(2010)1, 316–323.
11. Steinbichler, G.: Präzisionsspritzgießen- Maschinen und prozesstechnische Besonderheiten, 17. Leobener Kunststoff-Kolloguium, 2003.
12. www.danziger138.de/chlorella/chlorella.htm, 27.04.2011
13. Fa. HOERBIGER Kompressortechnik Holding, Vienna
14. Lim, L.-T., Auras, R., Rubino, M.: *Processing technologies for Poly(lactic acide)*, Progress in Polymer Science, 33(2008), 820-852.
15. Mitomo, H. et al.: Improvement of heat stability of poly(L-lactic acid) by radiation-induced crosslinking, Polymer, 46(2005), 4695.
16. Laske, S. et al.: *Biopolymer Paper for Laser Printing Applications,* PPS-25 - Program & Abstracts, 2009, 78–79.

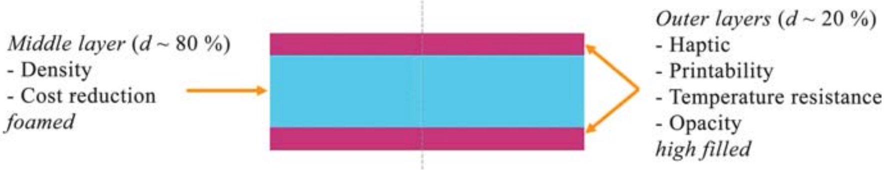

FIGURE 10 – PLA multilayer film with foamed core[4]

CONTACT
Clemens HOLZER
Montanuniversitaet Leoben, Department of Polymer Engineering and Science
Chair of Polymer Processing
Otto Gloeckel-Str. 2, 8700 Leoben, Austria
E-mail: clemens.holzer@unileoben.ac.at

Obavijest čitateljima

U prošlom je broju *Polimera* došlo do pogrješke pri obrojčavanju stranica, te je broj umjesto sa stranicom 61 započeo sa stranicom 49, a završio sa stranicom 96 umjesto 108. Ispravno obrojčane stranice su u našem e-izdanju.

Uredništvo