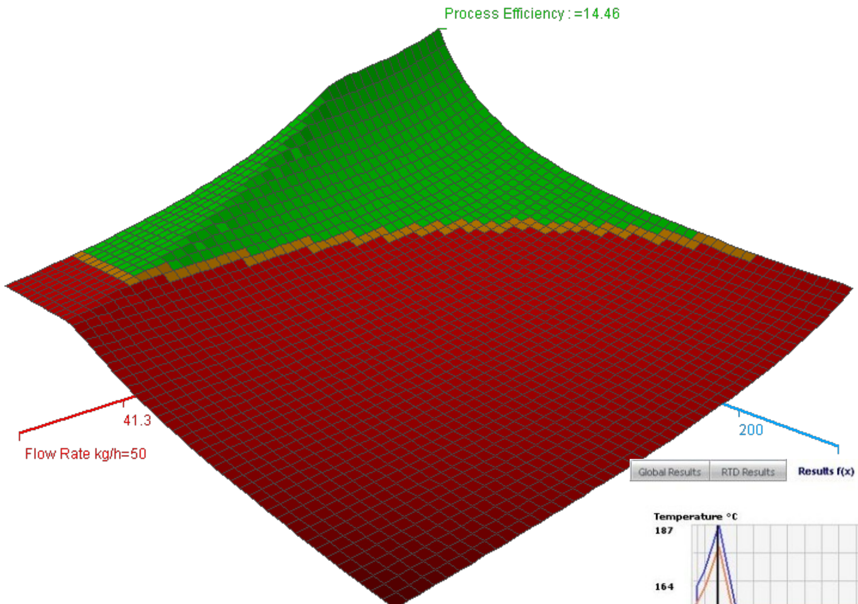
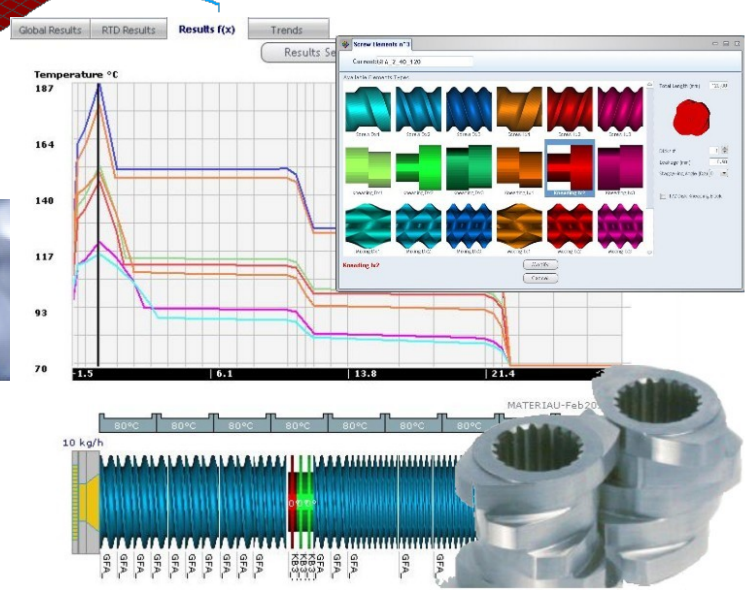
Simulation for Twin Screw Extruder

Control the Process to Control the Product

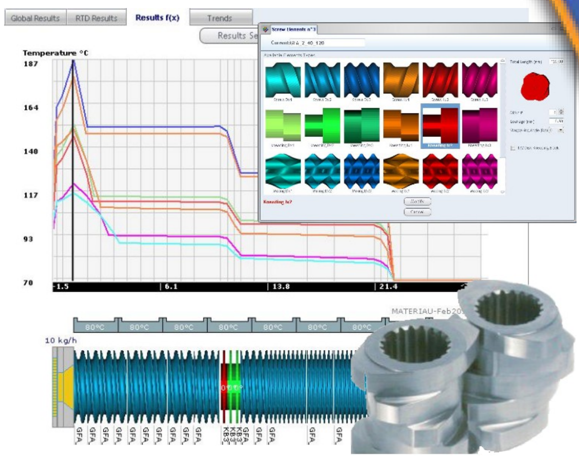




Ludovic® : performing virtual experiments

A virtual extrusion lab

As a simulation software, Ludovic® computes virtual extrusion configurations of corotating extruders. From a virtual setup, Ludovic® reproduces the components of the extrusion process (screw geometry, material, operating conditions) in a virtual lab. Ludovic® supports the **scheduling of experiments campaign** by performing an indeep **analysis of the material and process performance**.



Temperature evolution along the screw profile

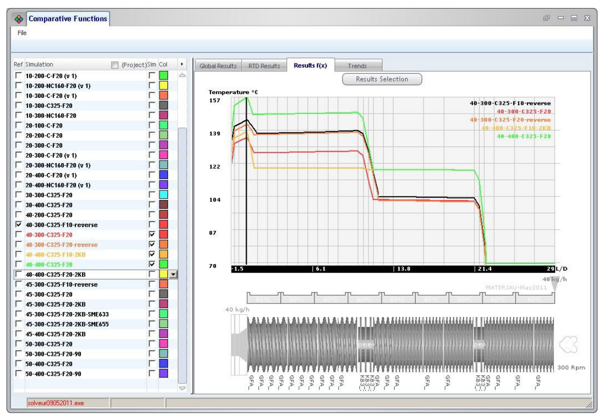
Cutting down real experiments

Using Ludovic® allows to reduce the number of real experiments. Ludovic® simulations support in figuring out the material behaviour during the extrusion process and the impact of the process conditions, by giving high added values data (temperature, pressure, shear viscosity history...).

A regular use of the Ludovic® software allows to save :

- **50% of trials on a formulation campaign**
- **50% on the material resources cost**
- **30% on the product time to market**

The virtual extrusion lab allows to compare hundred of configurations (screw profiles, process conditions and material evolutions) at a glance.



Comparison of the temperature evolution along the screw profile among a tenth of simulations

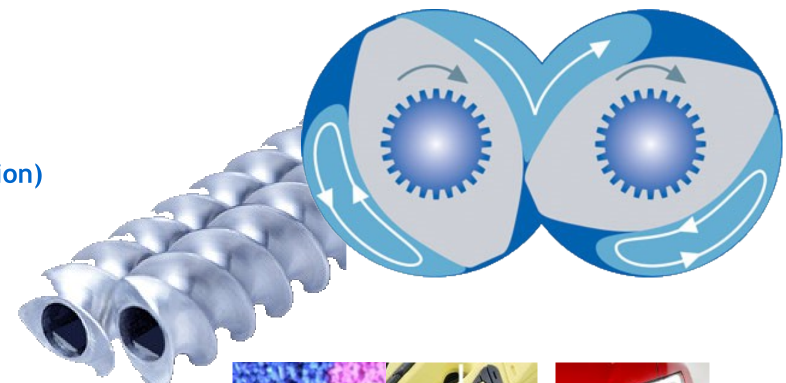
Ludovic® : principles of computation

Ludovic® is a simulation software dedicated to corotating twin screw extruders. The computation is based on the resolution of the physics equations (Navier-Stokes) inside the extruder channel. Screw elements are defined as self wipping elements. They are defined through customizable libraries.

Time tested model

Based on a robust 1D model, Ludovic® provides :

- **Fast results (average of 15s per computation)**
- **Reliable results**
- **Intuitive data setup**



Compatible with all TSE applications

Ludovic® allows to simulate all extruders and screw designs. Any kind of materials and complex blends can be analyzed (including **fillers and additives**) :

- **Polymers, masterbatches & composites**
- **Agro food**
- **Pharmaceutics and cosmetics**
- **Explosives and building materials**
- **...**

An asset in the product development

Supporting the development process

*"**Ludovic® is a valuable supplement** to experimental work that can provide insight into optimization, troubleshooting, and scale-up challenges of melt compounding and reactive extrusion processes.*
*The **accessibility** of the software to users without extensive simulation experience and rapid computation of results make Ludovic a **powerful alternative to more resource-intensive simulation approaches**.*
*Simulations can be tailored to different levels of detail and sophistication **providing valuable and rapid feedback** throughout the development process."*

Jane SPIKOWSKI,
process engineer

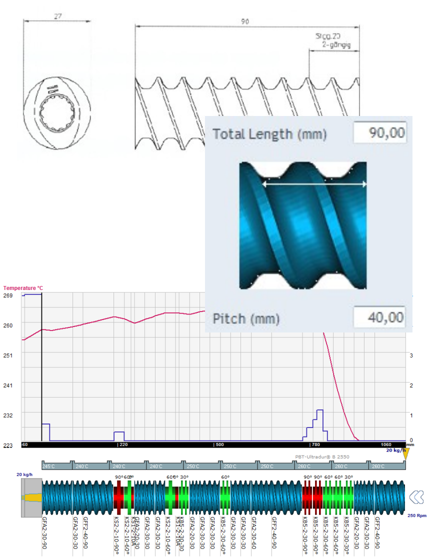
Exploring larger process conditions windows

Ludovic® includes different tools and wizards permitting in a very short timeframe, the exploration of very large processing conditions windows.

The 4 tabs technology

The GUI organized in 4 tabs allows to build in a few minutes a **simulation scenario** with all the required inputs

- **Extruder/screw geometry**
- **Material/fillers characteristics**
- **Processing conditions**
- **Computation parameters**

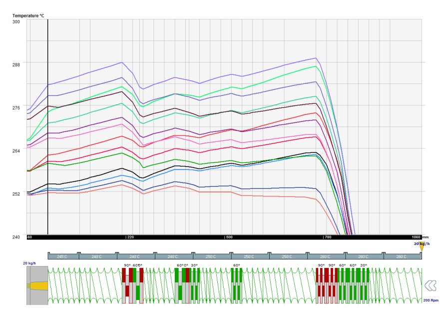


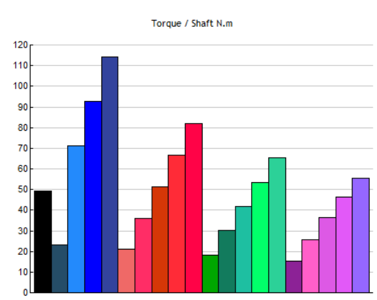
Average time for performing a complete simulation data set up : 10 minutes
Average time for a computation : 20 seconds

As a reminder, on the extruder, a complete data set-up (with screw design) means at least 4 hours.

Advanced comparison

Simulations are analyzed in real-time in the comparison mode.
The visual analysis really **highlights the potential** of each simulation. This helps in **defining the best configuration** for the product/process development.

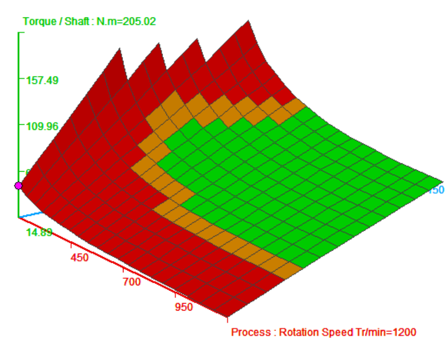




As a reminder, in the lab, it takes a few days for testing different screw designs, changing processing parameters and anaylising the results. With numerical simulation, it takes a few hours.

Design Of Experiments

Performing a Design Of Experiments (DOE) allows to study the **impact of the input parameters variation (defined by the user) on the material/process outputs**.
In Ludovic®, performing a DOE means **a hundreds of simulations** which provide **trends** on the material reaction to hundreds of potential configurations.



Above picture : *the DOE highlights the functioning domain taking into account the product and extruder characteristics.*

Average time for performing a DOE : ~1hour

As a reminder, exploring a complete functioning domain on a machine means a few weeks/months.

A regular use of the Ludovic® software affords a fast learning curve. It also proposes to capitalize on the process knowledge. The **observed ROI** on the first year is **~90%**.

Industrial applications

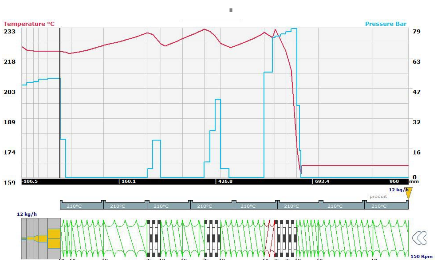
Polymer compounding : a case of Polypropylene extrusion
Quantification of the main key areas of the process by Ludovic®

Polypropylene behaviour

As a classic thermoplastic, the polypropylene (PP) material presents a well known behaviour during the extrusion process. Its behaviour can be easily controlled during extrusion.

Challenge

The use of the Ludovic® software allows to quickly identify the **key zones** of the polypropylene (PP) extrusion process.



Evolution of temperature and pressure along the screw profile (from a Ludovic® computation)

Inside Ludovic®

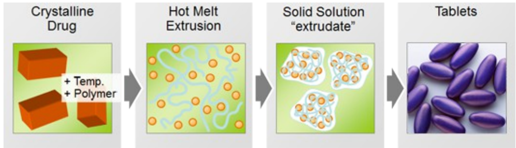
The simulations consist in the computation of the material flow inside the screw channel, in order to predict the mechanical behaviour of the PP. In this way, the pressure and temperature increase zones are readable on the results display.

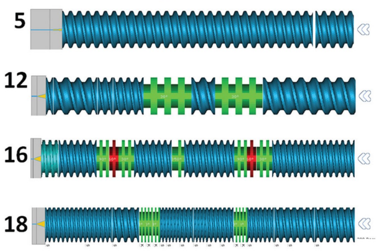
The numerical approach allows a quick quantification of the main key areas of the process: how much degrees does the temperature increase with a 45° staggering angle? How much the pressure increase with a reverse screw elements with a narrow pitch?

All those questions are answered by Ludovic® and helps in figuring out the right adaptation of the process configuration for respecting the material characteristics.

From "Experimental and theoretical study of twin screw extrusion of polypropylene", by O.S. Carneiro, J.A. Covas, B. Vergnes

Pharmacy applications : Hot Melt Extrusion
From lab scale to pilot scale





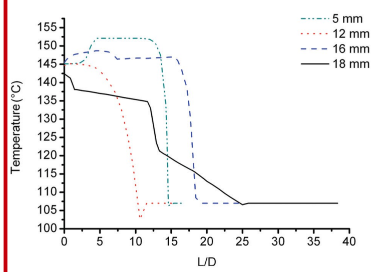
4 screw profiles designed in Ludovic®

Early drug product development

The main concern of pharmaceutical product development is the available amount of API (Active Pharmaceutical Ingredient), used for manufacturing tablets and medicines. It is hence necessary to define a strategy to successfully develop a melt-extruded product, with the optimization of the crystalline drug in early product development.

Challenge

The sensitivity of the API to the high temperature is the key of the process success. As the scale up strongly impacts the temperature in the extruder, using Ludovic for screening the API reaction on different machines diameter (see middle left) is benefitful for preserving API characteristics and cutting down trials and experimental work.



Temperature vs. Screw diameter

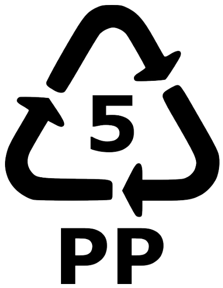
Inside Ludovic®

Ludovic® is used for the scale-up of a solid dispersion extrusion with emphasis on energy distribution, mean residence time and temperature profile along the screw. Simulation shows a high potential to identify high-energy intake spots. Thus, efficient screw designs for scale-up can be identified and highlighted, and product quality can be optimized and scale up feasibility can be estimated.

In this way, the extrusion black box becomes a transparent and well-designed process.

From "Modeling of the Impact of Extruder Configuration on the HME Procss and Product Characteristics during Scale Up" 2013 - AAPS San Antonio, by K.G. Wagner, D.E. Zecevic

Reactive extrusion: PP Peroxyde-induced degradation
Ludovic® : predicting a complex viscosity evolution



PP degradation

Polypropylene (PP) when polymerized exhibits a high molecular weight (MW) which involves high viscosity, which might be tricky for its processability. To improve this latter, MW can be tailored by reactive extrusion (e.g degradation of PP induced by peroxide).

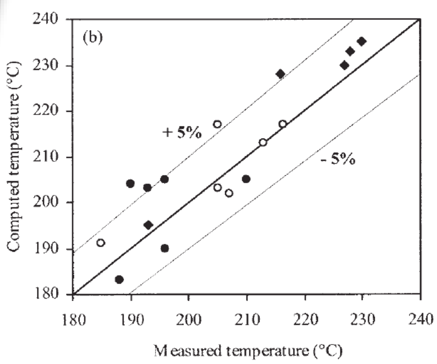
Challenge

The stake is to couple the thermo-mechanical behaviour and the reaction along the extruder in order to accurately predict the molecular weight evolution. As a first insight, the temperature evolution is analyzed for determining the simulations accuracy (see the picture down left).

Inside Ludovic®

First, Ludovic® simulations are performed to analyse the temperature evolution. Computed results are in agreement with the experimental measurements (see lower left). This step is a first answer for getting the trends of the reaction. In a second time, coupled computations are performed to take into account the evolution of ther material viscosity regarding to the reaction rate.

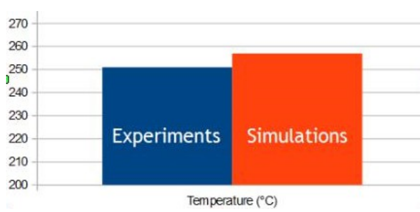
As a result, Ludovic® predicts the average MW as well as the complex viscosity of the PP along the screw profile. This coupled computation helps in figuring out the final viscosity of the PP taking into account both thermo-mechanical phenomena and chemical reaction.



Correlation between measured and computed temperatures

From "Evolution of the Peroxide-Induced Degradation of Polypropylene along a Twin Screw Extruder : Experimental Data and Theoretical Predictions" by F. Berzin, B. Vergnes, S.V. Canevarolo, A.V. Machado, J.A. Covas

Saturated Polyester material Extrusion
Showing the hidden behaviour of a PBT



Ludovic shows a strong agreement between simulations results and experiement measurements

Hidden evolution of the material

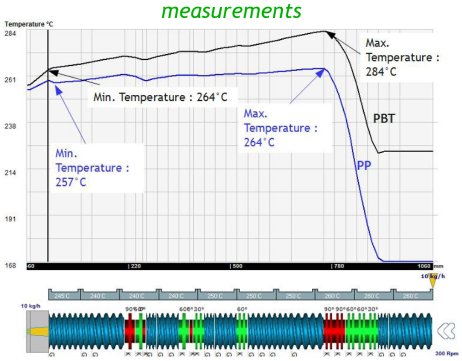
During the extrusion process, materials are seen as locked inside a black box. Measurements on pressure, temperature, shear and also viscosity are not so convenient to perform. That's the reason why some measures are done at the die exit. But those values are sometimes not relevant of the real material behaviour during the whole process. The PBT (Polybutylene Terephtalate) is one of those sensitive material.

Challenge

In the PBT extrusion, performed measurements are not always relevant of the **whole material history**. Indeed, very often temperature measurements are realized at the die/screw exit. But they neglect the **maximum temperature of the PBT**, reached at the melt. This can lead to wrong asumptions regarding to the product properties. The PBT as to keep high performance capabilites, especially in the heat resistance (used for lighting relays and connectors).

Inside Ludovic®

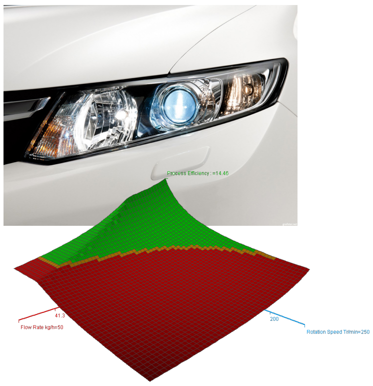
Ludovic® is used as a witness of the whole thermo-mechanical history of the material. It shows that the output temperature (264°C) is much lower than its maximum temperature at melt (284°C). As a comparison, the PP shows a more regular temperature curve. That is the reason why it is important to focus not only on the measured temperature at the die, but also on the **temperature all along the process**. In this context, Ludovic® helps in analyzing the invisible impact of the process conditions on the PBT, to **keep a full functional material**.



Comparison of PP and PBT temperature evolution

From an application performed in collaboration with Proplast - Italia

Nanoclays composites :
Ludovic® as a tool to achieve the best end-user mechanical properties

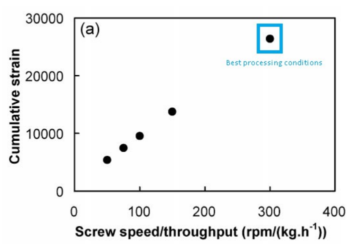


Performances reinforcement

Nanoclays are compounded by twin-screw extrusion with thermoplastic resins for mechanical performance reinforcement. As they allow to reinforce materials while making them lighter, nanoclays composites are especially used in **automotive** and **aeronautic** industries. Since decades the scientific literature strongly links the level of dispersion of these nanofillers in the thermoplastic matrix for this end-user enhancement.

Challenge

The ultimate goal is to use Ludovic® as a tool to determine how the extruder setup can be changed to generate a better dispersion of the nanoclays into the composite. This is the path for making nanocomposites with superior mechanical properties.



Evolution of cumulative strain regarding to the screw speed/throughput

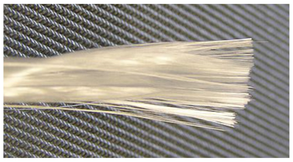
Inside Ludovic®

Ludovic® highlights the correlation between cumulative strain and the end-user mechanical performance. It also make a connections between the process output and the processing parameters (here, the screw speed - see lower left).

Hence, the best mechanical properties are achieved at the **highest cumulative** strain which is performed at high screw speeds and low throughputs.

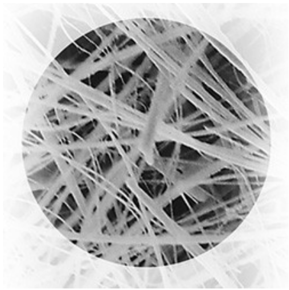
From "Optimization of Extrusion Parameters for Preparing PCL-Layered Silicate Nanocomposites supported by Modelling of Twin-Screw Extrusion", by N. Watzeels, H.E. Miltner, C. Block, G. Van Assche, B. Van Mele, H. Rahier, K. Van Durme, B.Bogdanov

Model integration in Ludovic® :
Glass fibers length prediction along the screw profile



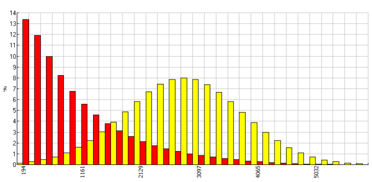
Mechanical performance reinforcement

Glass fibers are compounded with polymers to enhance their mechanical performance since the 1960's. This performance improvement is linked to the fibers length. Indeed, the longer the fiber is, the more resistant the composite will be. As they are processed by twin screw extrusion, the key point of the process is to save the fibers length.



Challenge

The stake is to monitor and control the glass fiber breakage in a corotating twin-screw extruder by the integration of a theoretical model in Ludovic®.



Evolution the fibers length in a screw element

Inside Ludovic®

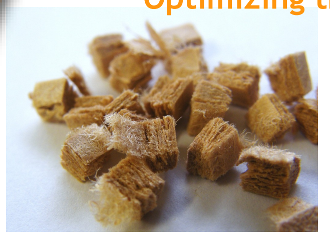
Ludovic® integrates a unique model of **glass fibers evolution computation**. It allows to evaluate the fibers size evolution in each screw element. This length evolution is computed from an initial fiber size distribution (see lower left).

This Glass Fibers model allows to control the size of the fibers along the process and then adjust the process parameters/screw design for getting the best composite with the optimized mechanical final properties.

The beside picture illustrates the fibers evolution. In yellow is represented the initial fibers size distribution. In red is represented the final fibers size distribution.

From an internal SCC application, coming from the FONLIMICS FP7 project

Wood Fibers Composites (WFC): Optimizing the mixing efficiency while preserving the fibers characteristics



Wood fibers extrusion targets

Wood fibers are more and more used in composites as they promote the renewable natural resources and offer a broad range of advantages : they are lighter than glass or glass fibers and allows to reach high resistance levels.

Processing wood fibres in a twin-screw extruder is challenging because the objective is to obtain a good dispersion of the fibres into the matrix while avoiding burnt wood fibres (caused by high temperatures).

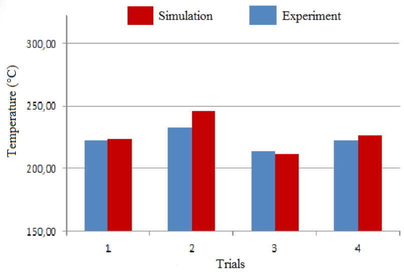
Challenge

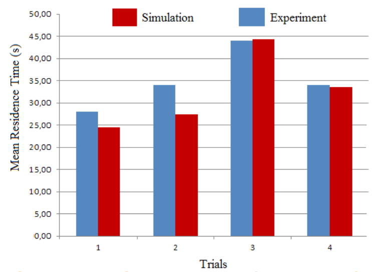
The Ludovic® software is used to catch the compromised processing conditions : the wood fibers are mixed enough (to be well dispersed) and the material temperature does not exceed the threshold of the fibers thermal resistance.

Ludovic® is used in a trial campaign for comparing those computed values to the measured ones in order to validate the adapted processing conditions, matching to the composite requirements. Then, optimized conditions are extrapolated.

Inside Ludovic®

Temperature and residence time are compared (numerical results vs. Experiments) for a final validation. The Ludovic® results are always very closed from the measurements (see middle and lower left). This virtual trial campaign helps in cutting down costs generated by the tests and trials method **(about 50%)**.

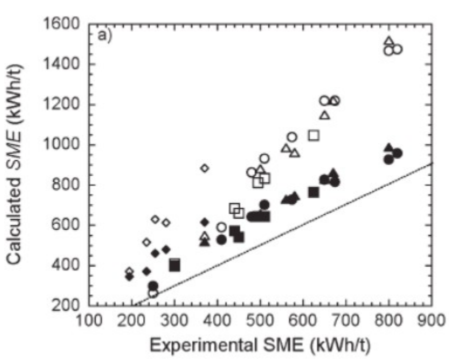


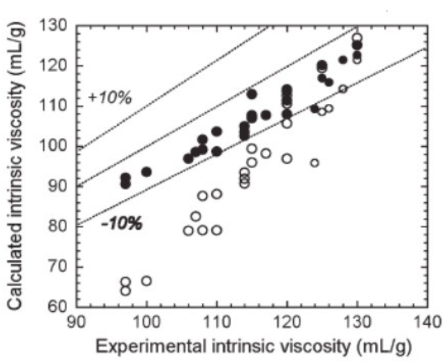


Opposite : Comparison of measured and computed results : temperature and mean residence time

From a collaborative work performed with ICMA SG, Woodforce and Scion Research

Agro-Food extrusion: Prediction of starchy product degradation during extrusion





Starchy product degradation

The extrusion of starchy products is a tricky process as it modifies the basic structure of the material (loss of the grain structure, degradation of amylose and amylopectin chains…).

Challenge

The ultimate objective is to predict with Ludovic® the starch transformation considering the influence of the Specific Mechanical Energy (SME) on the intrinsic viscosity. Indeed, those two values are considered as a reliable whitnesses of the the starch reaction.

Inside Ludovic®

Computations of SME and intrinsic viscosity are performed with and without coupling and are compared to the experiments.

The advantage to take into account the specific effect of SME on starch viscosity is clearly shown in these graphs.

Whatever the processing conditions, the starch transformation is estimated by simulation with an error lower than 10% (when it could reach more than 30% without coupling).

Opposite : Correlation of measured and computed values SME on the upper left, intrinsic viscosity on lower left

From "Importance of coupling between Specific Energy and Viscosity in the Modelling of Twin Screw Extrusion of Starchy Products" by F. Berzin, A. Tara, L. Tighzert and B. Vergnes

Ludovic® : a full packaged solution

The Ludovic® package includes the Associated Services, aimed at providing a continuous support to the users :

Advanced Training

An initial training is included for getting the basics of the Ludovic® principles. Two days are planned :

- **1st day : how to use the Ludovic® software**
- **2nd day : getting into customer applications**

Ludovic® Club & Academy

These meetings organized by SCC (once a year) gather industrials, researchers and developers to pinpoint the next priorities of the Ludovic® developments (new physical models, new options...).

Consulting*

Twin screw process can b analyzed by SCC within a consulting background performed for the customer. Specifications are drawn on demand.

Hot Line

A hot line is available to support the customer in the use of the Ludovic® software.

Specific developments*

Development of models regarding to specific customer needs, integration of new functions...
On demand

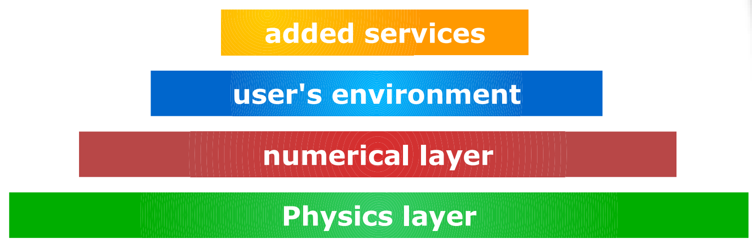
Customer engineering*

SCC provides engineering resources together with software as an on-site support.

**Provisions of services performed on demand and submitted to a specifications drawing*

Ludovic® : as a summary

Ludovic® is a 1D/2D software based on the **physics basics**. It is included in an **intuitive user's environment** for speeding up the process analysis and supported by Associated Services for a fast ROI.
Ludovic® is provided as permanent or temporary license. It is commercialized since 1998.
Consult SCC for more details.



With the support of top level laboratories

Ludovic® has been developed by the CEMEF (from Mines ParisTech) with the support of the INRA (French NationalInstitute for Agricultural Research), two renowned french laboratories.

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