Introduction to the numerical Simulation of Twin Screw extruders

Ludovic® : 2D Twin-Screw numerical Simulation
XimeX® : 3D General Purpose Numerical Simulation
Numerical Simulation: Why?

Simulate the Equipment to Understand the Process

Understand the Process to Control the process

Control the Process to control the Product

Production
New product time to market Optimisation
Scale-Up
Stability vs process parameters
Re-Engineering of existing Production (REACH)
Optimisation of the « Test & Trial » process
Variability of raw products (recycling ..)

Research & Development
Indeep analysis
New products (bio based, Nano ...)

Universities
A good alternative of real cases
Provide understanding of the physics
pedagogical
2 different approaches for different objectives

<table>
<thead>
<tr>
<th></th>
<th>Ludovic®</th>
<th>Ximex®</th>
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</thead>
<tbody>
<tr>
<td><strong>Model</strong></td>
<td>The equations of the flow are hard coded for standard screws elements</td>
<td>The Navier &amp; Stockes are computed on a FEM domain.</td>
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<tr>
<td><strong>audience</strong></td>
<td>Engineering &amp; production</td>
<td>Research &amp; development</td>
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<tr>
<td><strong>Target</strong></td>
<td>Dedicated TSE</td>
<td>TSE, Single Screw, BUSS, Batch Mixers ...</td>
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<tr>
<td><strong>Computing Time</strong></td>
<td>500 simulations / h</td>
<td>&lt;4 h to 4 Days&gt;</td>
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<tr>
<td><strong>Principle</strong></td>
<td>Stationary</td>
<td>Transient</td>
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Ludovic® XimeX®: Applications fields

Many Products...
- Food Processing
- Polymers
- Bio-polymers
- Pharmacy
- Cosmetics
- Energy
...

Many Applications...
- Croquettes, cereals...
- Compounds, plastics sheets
- Compounds with fibers
- Tablets
- Lipsticks, rimmel
- Propergol
...

« control the process to control the product »
Preparation: a 5 steps process ...

Your Process

RPM  T°C  Kg/h

with Ludovic

RPM  T°C  Kg/h

Slipping Effect, User's Results, melt computation, Expansion, Reactive Extrusion

Local Execution or .Net Execution

« control the process to control the product »
Features

- **Setting**
  - Opened to all TSE
  - 5 Tabs technology

- **Physics**
  - Simple melt model vs Advanced Melt zone computation
  - Power, Carreau, “set of points” rheology definition
  - Reactive Extrusion (uncoupled vs coupled)

- **Execution**
  - “One Shot” execution
  - “Sequence” execution
  - Comparative & statistical analysis
  - Optimisation Module (on going)
  - Ready for Neural Meta-Model

« control the process to control the product »
Mean residence time: 39.96 s
Dissipated energy (viscous dissipation - screw): 137.95 kWh/t, equivalent to 47.00%
Specific energy (solid transport - screw): 65.38 kWh/t, equivalent to 22.27%
Melting Energy (screw): 27.75 kWh/t, equivalent to 9.45%
Dissipated energy (viscous dissipation - die): 4.76 kWh/t, equivalent to 1.62%
Total conduction energy (screw + die): 57.70 kWh/t, equivalent to 19.66%
Total material energy: 178.15 kWh/t
Total material energy (abs. value of conduction): 293.54 kWh/t
Power engine: 35.38 kW
Torque / shaft: 1049.14 N.m
Conduction power:
Barrel 1: 0.0000 kW
Barrel 2: 0.0000 kW
Barrel 3: 0.3511 kW
Barrel 4: -0.3053 kW
Barrel 5: -0.7251 kW
Barrel 6: -1.2504 kW
Barrel 7: -2.5920 kW
Barrel 8: -1.7303 kW
Barrel 9: -2.3297 kW
Reactive Extrusion

Definition of a "chemical reactor":
This is the Evolution law of reaction rate : $X$ as a function of temperature and residence time.

In the coupled mode, Ludovic® links the product viscosity evolution (as a function of de $X$) with the transformation rate.

Exemple of Applications
Radical polymerization of Styrene
Controlled degradation of Polypropylene
Dynamic Vulcanization of thermoplastic elastomers
Caprolactone Polymerization

...
Comparative & Statistical analysis

Compare wide number of simulations
Trends Identification
Process key parameters tracking
Process Parameters / results correlation
Automated experiment
Control of the plan parameters
Unlimited results recording
Display of Results (2D, 3D)
Results export to Excel

1681 « One Shot » Simulations: Preparation 5 mn – Execution: 53 mn

Exemple of Applications
Prediction of the Kneading elements weariness on the mixing efficiency
Torque evolution as a function of the flow rate
Optimisation of the Flow Rate / rotation Speed
25 kg/h

24% diminution sur le couple
12% diminution sur temps de séjour moyen

« control the process to control the product »
The Optimiser (on going)

Based on a genetic algorithm methodology
Unlimited degree of freedom in the parameters choice
Multiple objectives:
- Min, Max, Reference Curve
Constraints:
Ex: Max power of the engine, Torque, Max beared temperature

Ludovic provides the 5 best « candidates »
on a population of 3000 « One Shot » Simulations

Example of Applications
Scale-Up
Optimisation of the Screw performance (Mixing ...)

Ready for Neural Meta-Models
Neural models produce real time optimisation
models (forward & backward propagation) for
operating domain analysis (in situ)
Applications

Global Macroscopic Analysis
Degradation temperature Limit
shaft pressure
Temperature, Pressure, stress over the global process

Global Macroscopic Analysis
Twin Screw inter mixing area
Wear phenomenon analysis
Coupling with « Strength of materials software »
Maximum shear Rates computation
Support for blade/screw design
Die equilibrium

Microscopic Analysis
Distributive Mixing
Dispersive Mixing

« control the process to control the product »
Exemple : Pressure as a function of the staggering Angle
Microscopic analysis

- Macroscopic
  - Mechanical
  - Computation
- Numerical
  - Particles
  - Computation
- Physical model
  for particle behavior

Quantification of the Mixing Efficiency
- Local Elongation
- Entropy (Shannon, Reyni)
- Intensity of Segregation

Physical Phenomena
- Fibers Breaking
- Agglomerate erosion

« control the process to control the product »
Carbon agglomerate Diameter Evolution
Define the Initial position of the particles...
Animations ...