Control the process to control the Product

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Ludovic®

Introduction to Twin screw process simulation how does it work …

Control the process to control the Product

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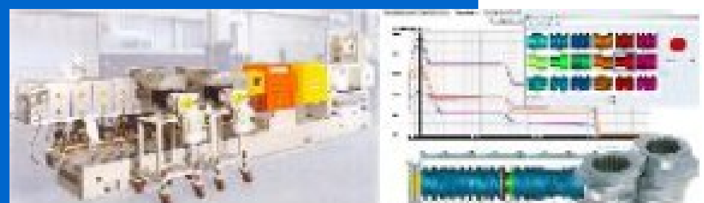
SC-Consultants : industrial processes simulation

- 3 main activities
  - Software development
  - Consulting
  - Strategic Initiatives (R&D)
- Strong R&D partnership
  - Bonn University
  - CEMEF
  - Fraunhofer ICT

SC-Consultants background

- Mechanics impact on the process

Extrusion



Extrusion range

1D/2D quick calculation software for twin-screw and single-screw extrusion processes

Mixing

Mixing range

3D software especialy applied to your own industrial cases about extrusion and mixing processes

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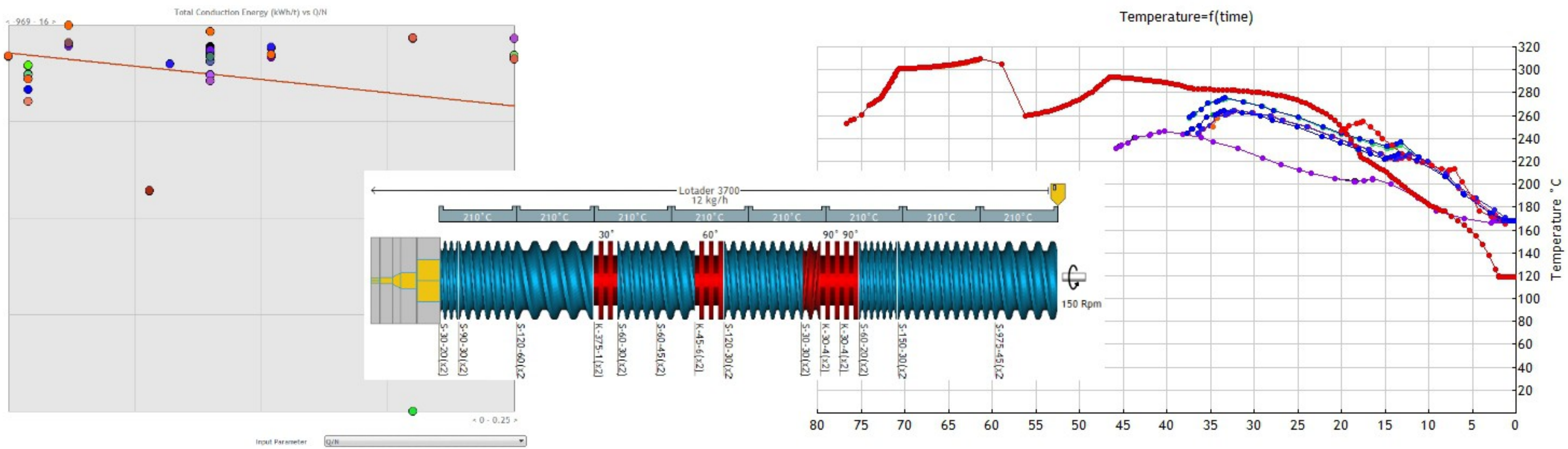
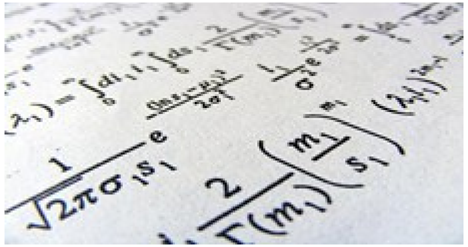
Ludovic® software

- Corotating twin screw extruder simulation
  - Generic application
  - All packaged
  - Process-driven results
  - Fast overview



What is modeling ?

- Reproducing a physical phenomena by a model



What is simulation ?

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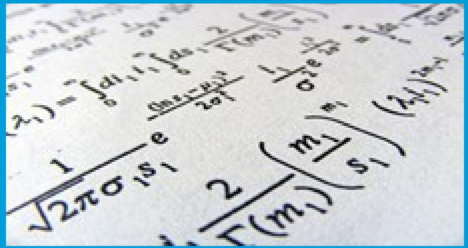

Software environment

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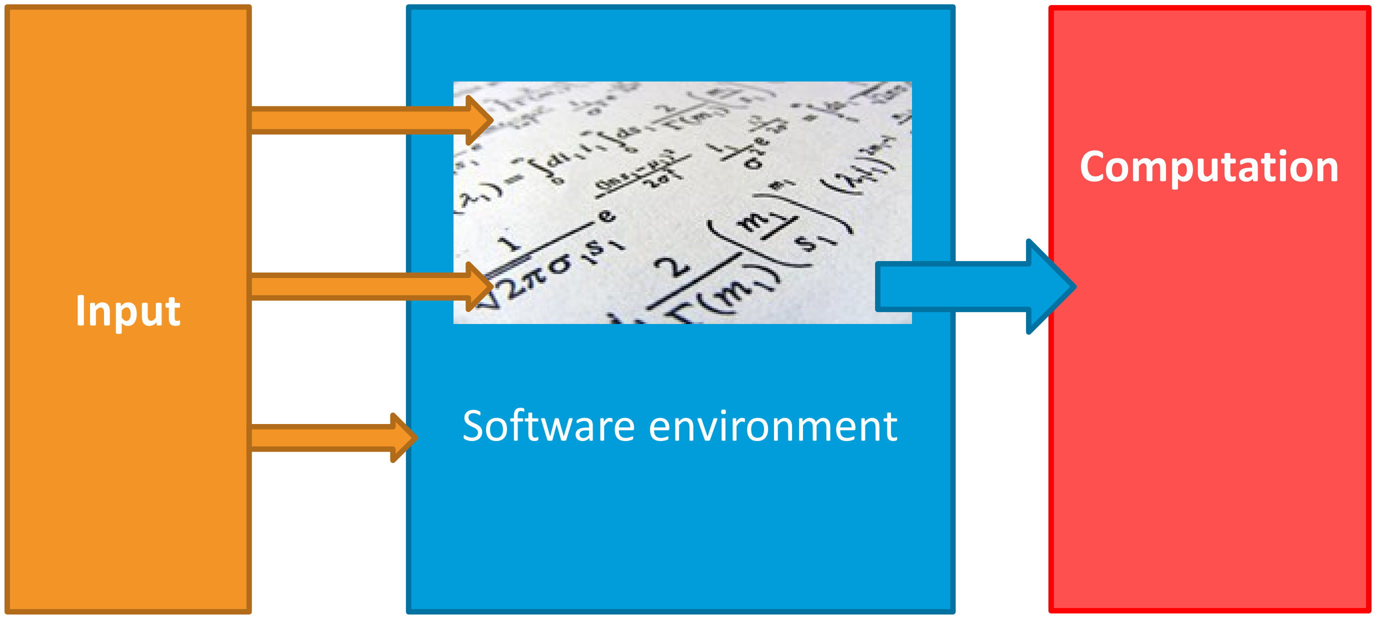
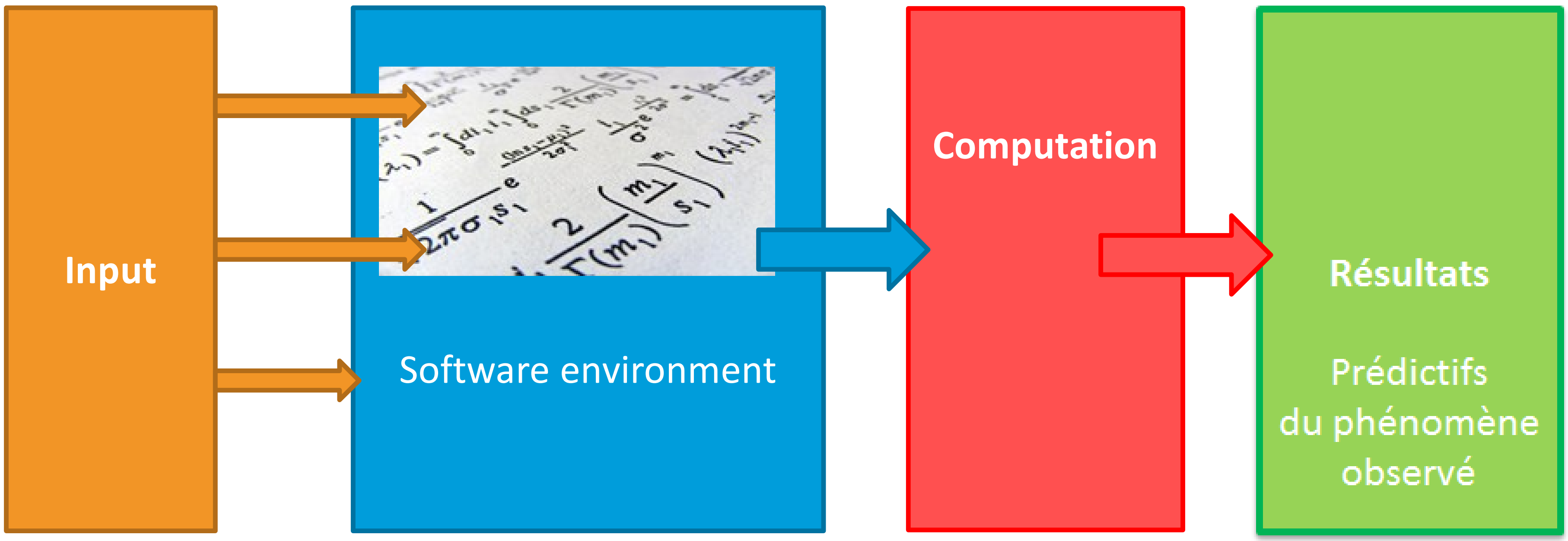
What is simulation ?

- Reproducing a physical phenomena by a model



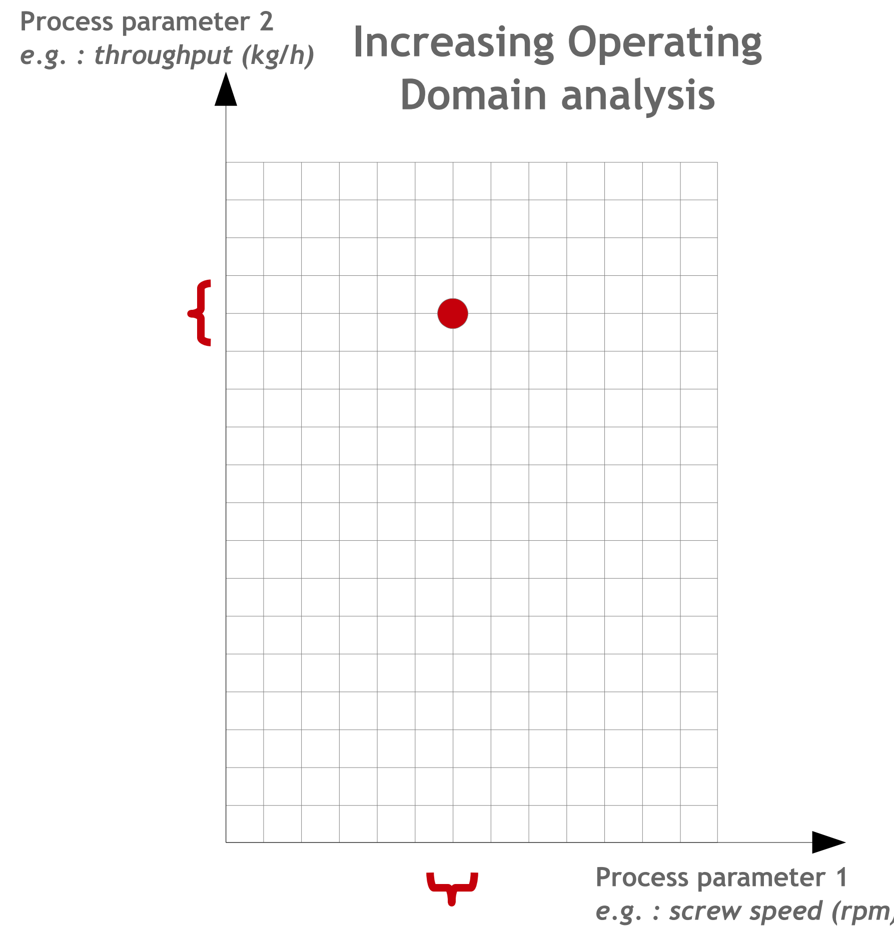
What is simulation ?

- Reproducing a physical phenomena by a model



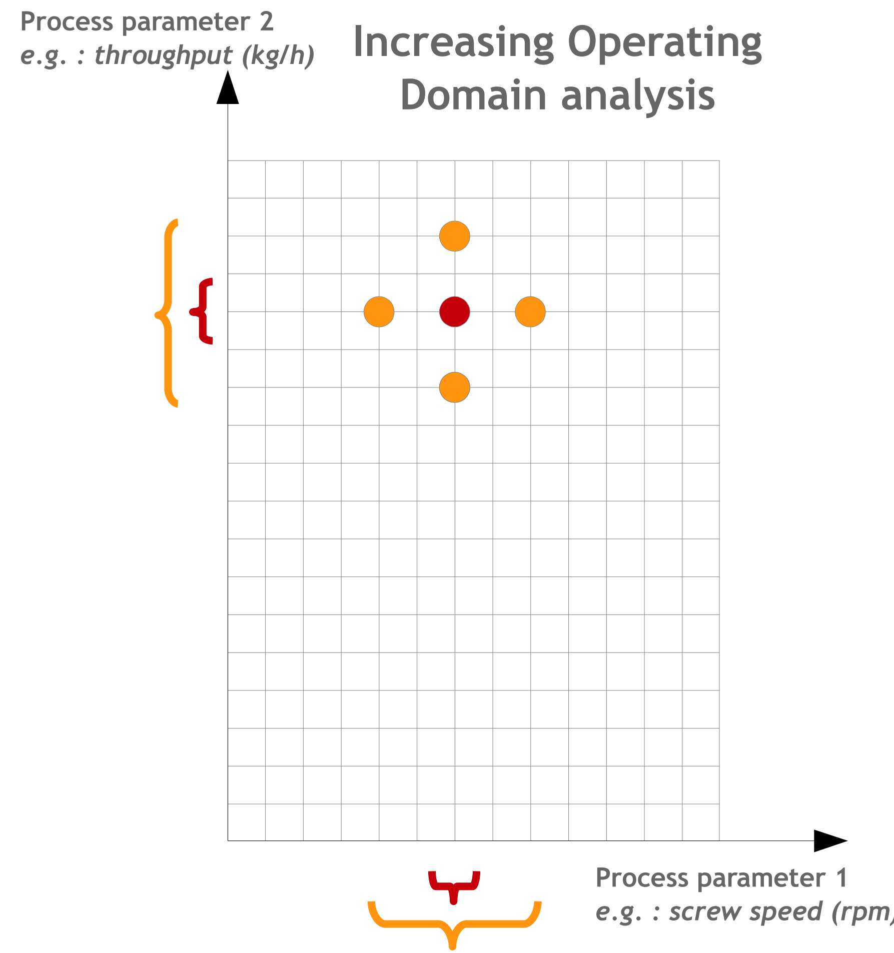
The interest of modeling - different focuses

- 1 Simulation
  - For checking
  - 1 set of operating conditions



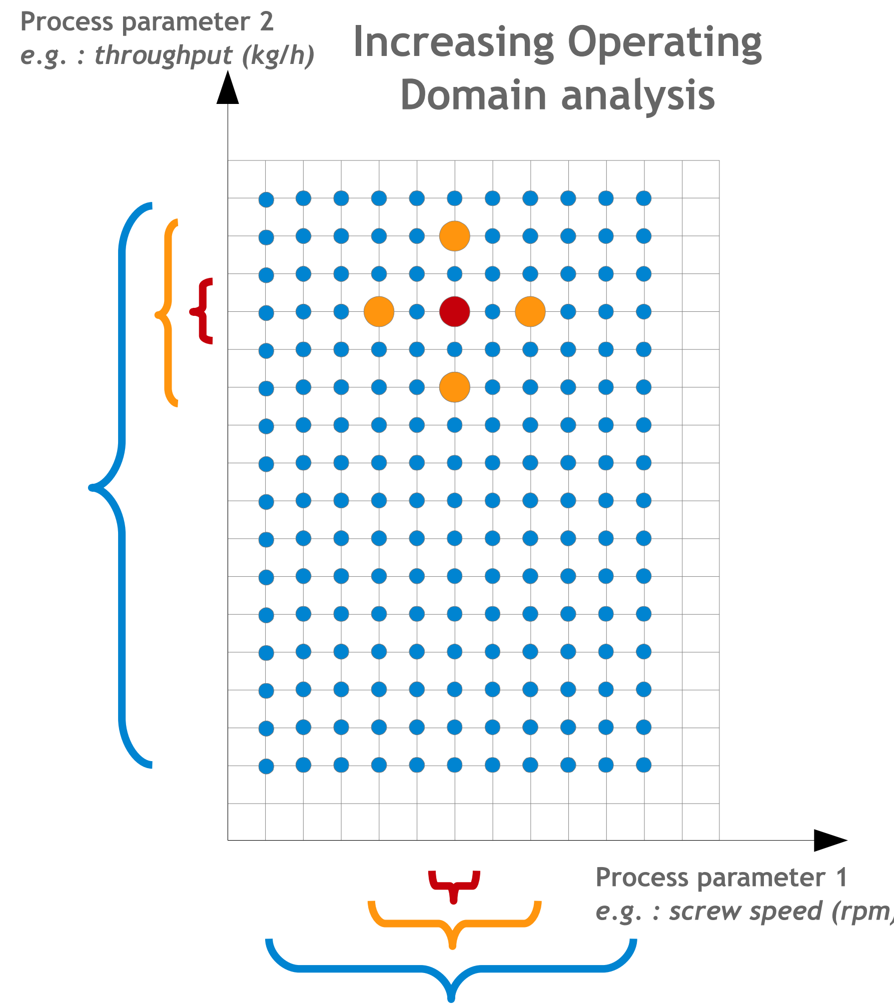
The interest of modeling - different focuses

- 1 Simulation
  - For checking
  - 1 set of operating conditions
- Comparison of simulations
  - For optimizing
  - Few sets of data



The interest of modeling - different focuses

- 1 Simulation
  - For checking
  - 1 set of operating conditions
- Comparison of simulations
  - For optimizing
  - Few sets of data
- 1 DoE / QbD
  - For anticipating
  - Hundred of Simulations
  - Covering a functioning domain
  - Example : new formulation



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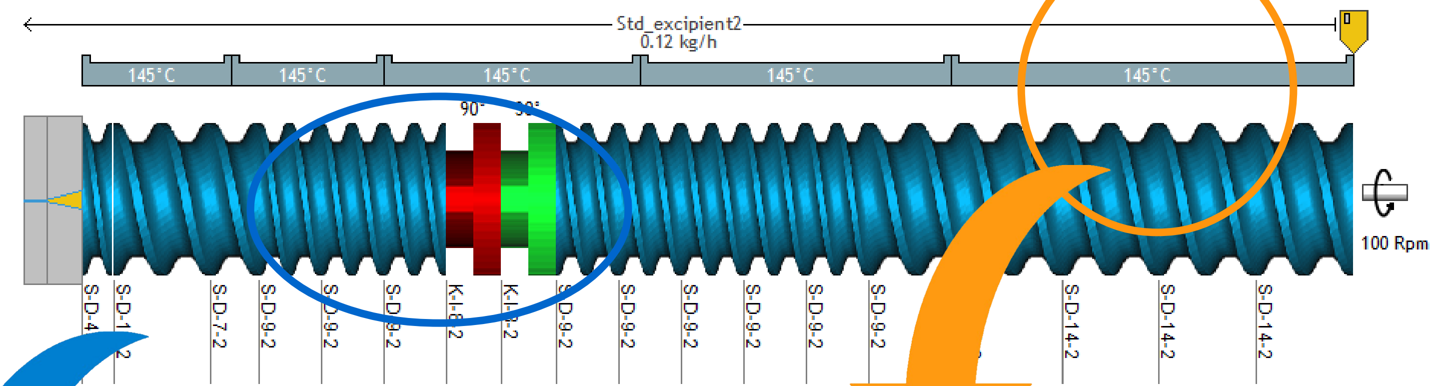
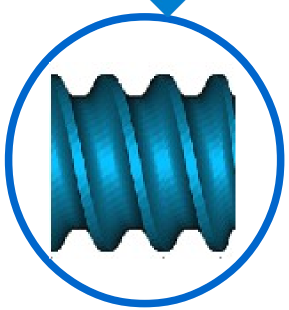
Twin Screw simulation

Control the process to control the Product

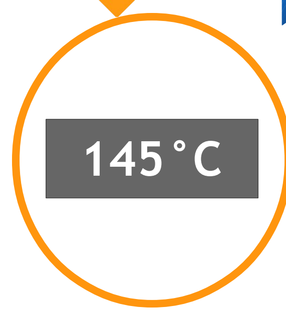
The polymer process in TSE

- Material + additives + energies = Compounds





- **Mechanical** energy
  - Shear Rate
  - Pressure
  - Self heating
  - Viscosity evolution
  - ...



- **Conduction** energy
  - Temperature +/-
  - Melting
  - Viscosity evolution
  - ...

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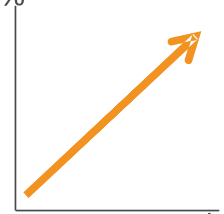
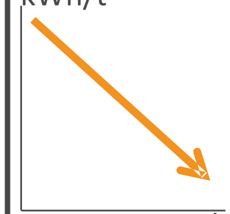
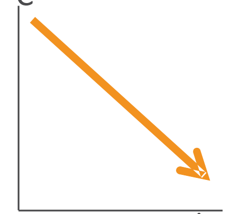
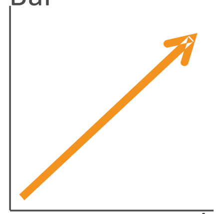
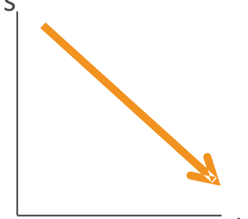
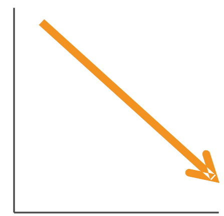
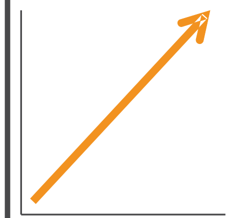
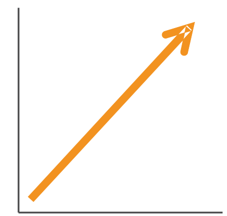
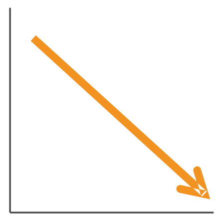
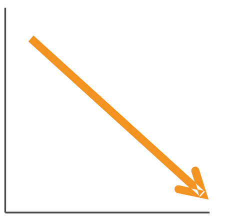
TSE - playing with process parameters

- **With Ludovic® : going further than rules of thumb**

	Torque (%)	SME (kWh/t)	T°C	P (bar)	Residence Time(s)
Throughput (kg/h)	%  Kg/h	kWh/t  Kg/h	°C  Kg/h	Bar  Kg/h	s  Kg/h
Screw Speed (rpm)	%  rpm	kWh/t  rpm	°C  rpm	Bar  rpm	s  rpm

Example of common process parameters impact

Why TSE Simulation

- Controlling the thermo-mechanical history from the material to the product
  - Getting the material sensitivity
  - Getting the process trends
  - Cutting down the trials

Materials + Process/Energies = PRODUCT

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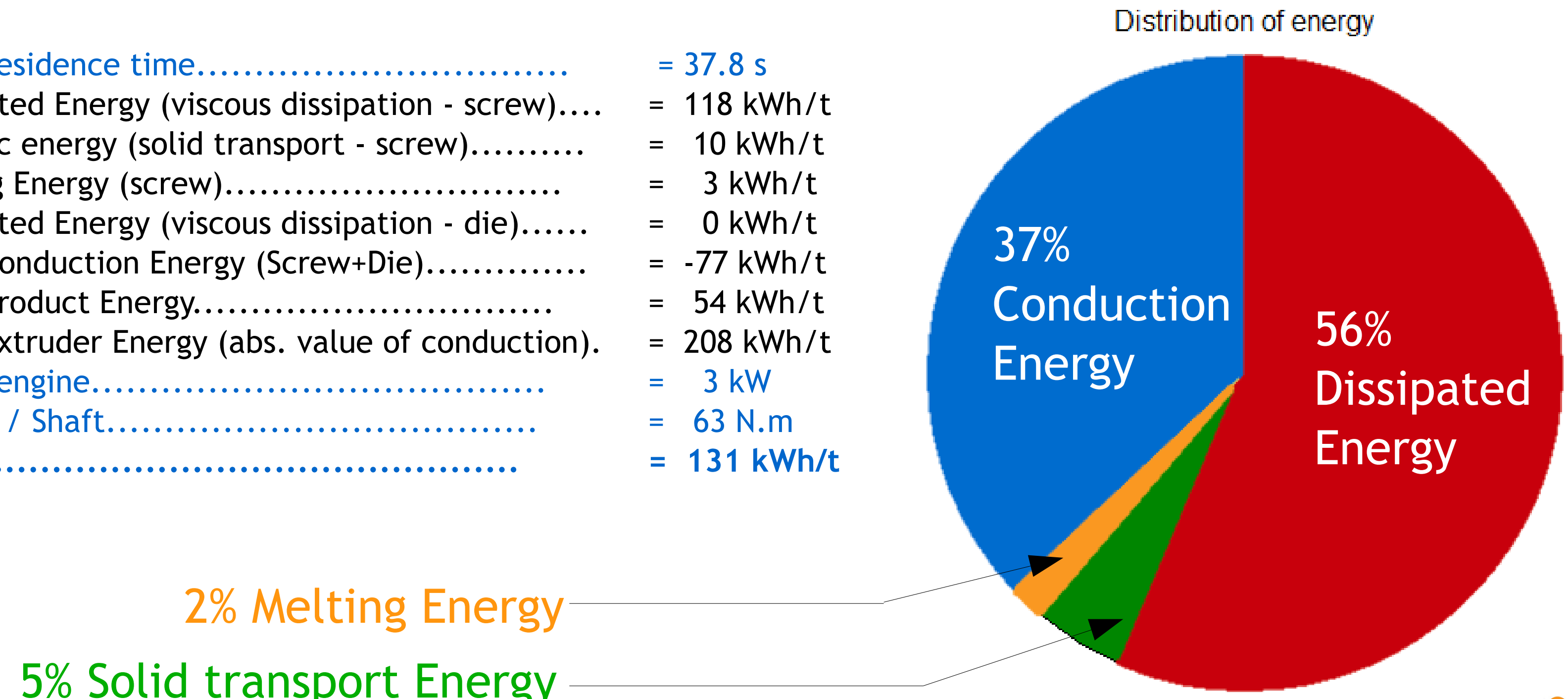
Controlling the process

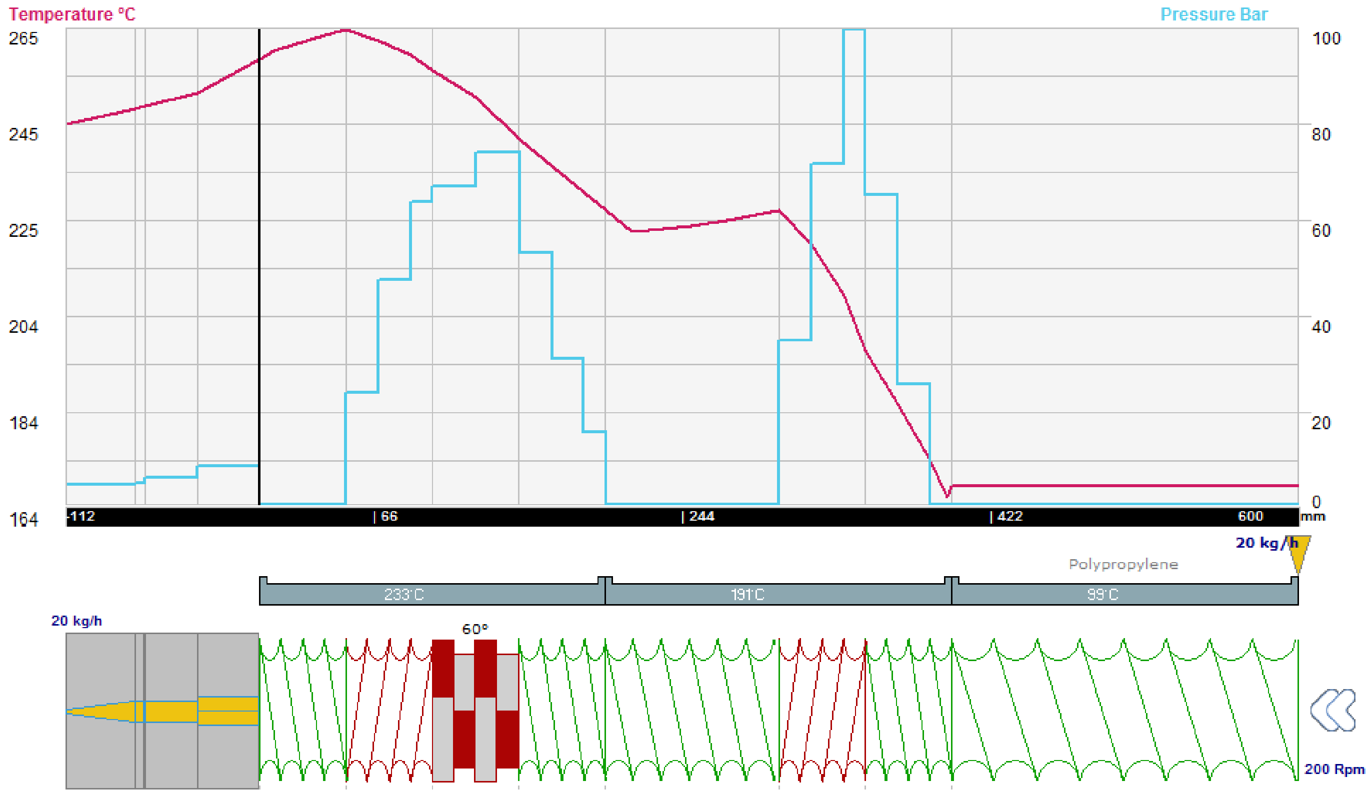
- Hands on the energy balance
  - Checking the machine capabilities
  - Checking the mixing efficiency of the process

Mean residence time................................	= 37.8 s
Dissipated Energy (viscous dissipation - screw)....	= 118 kWh/t
Specific energy (solid transport - screw)..........	= 10 kWh/t
Melting Energy (screw)............................	= 3 kWh/t
Dissipated Energy (viscous dissipation - die)......	= 0 kWh/t
Total Conduction Energy (Screw+Die).............	= -77 kWh/t
Total product Energy..............................	= 54 kWh/t
Total extruder Energy (abs. value of conduction).	= 208 kWh/t
Power engine..	= 3 kW
Torque / Shaft......................................	= 63 N.m
SME..	**= 131 kWh/t**



Controlling the Product

- Thermo-mechanical evolution
  - Displayed along the screw profile
  - Describes the material history

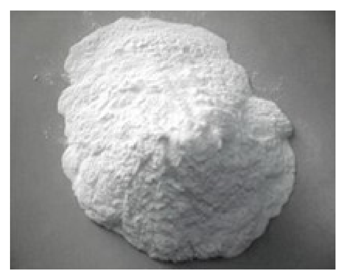


4 Leistritz Experiments

Experiments vs Simulations

- Background
  - During a workshop at Axel'one platform (1)
  - Goal : showing the reliability of the Ludovic® results

- The Configuration
  - Leistritz ZSE 18 MAXX 44D
  - PP (H7020) + CaCo3



(1) https://www.axel-one.com/ppi-plateforme-procedes-innovants

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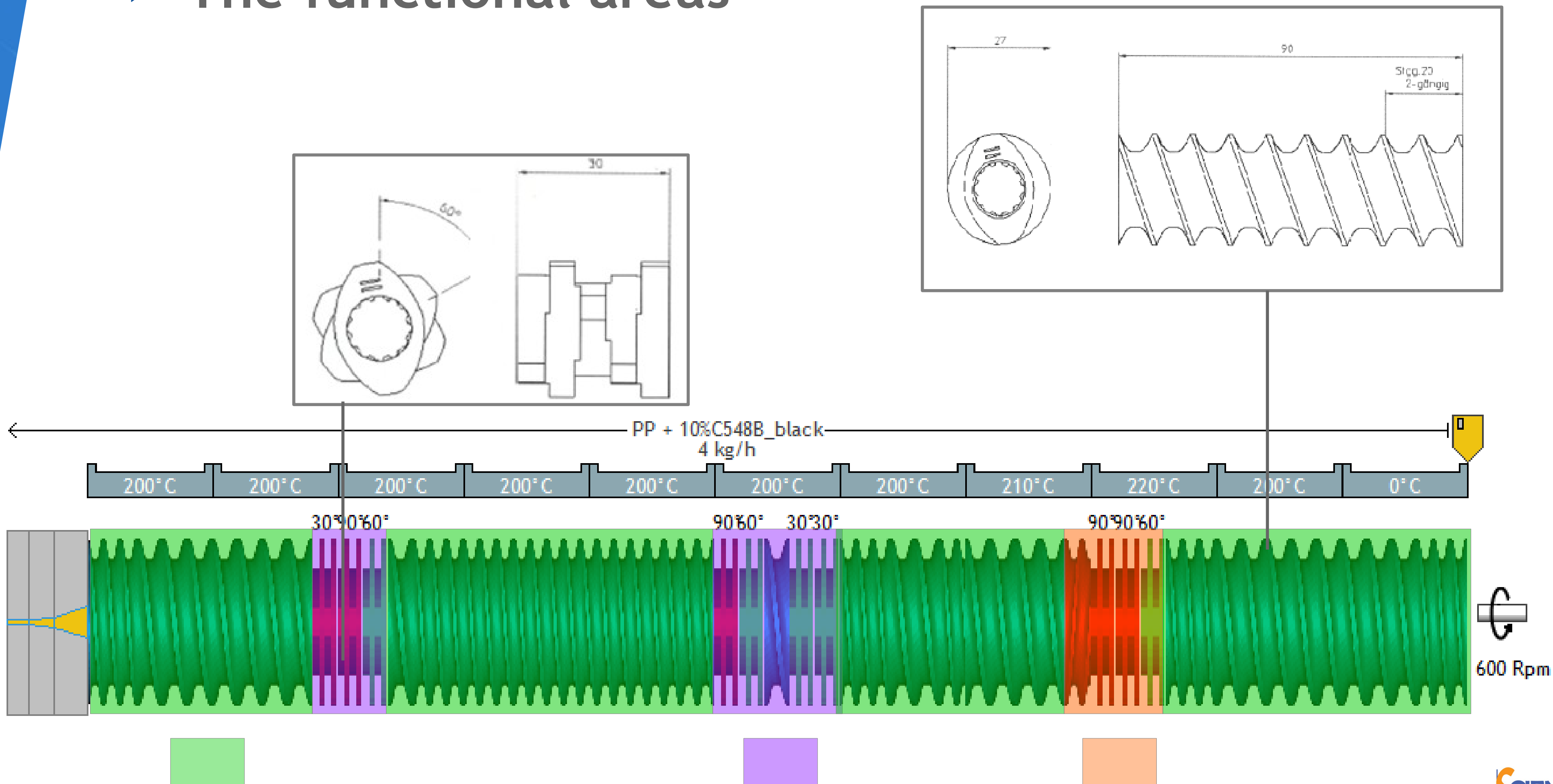
The ZSE 18 - the screw profile

- The functional areas

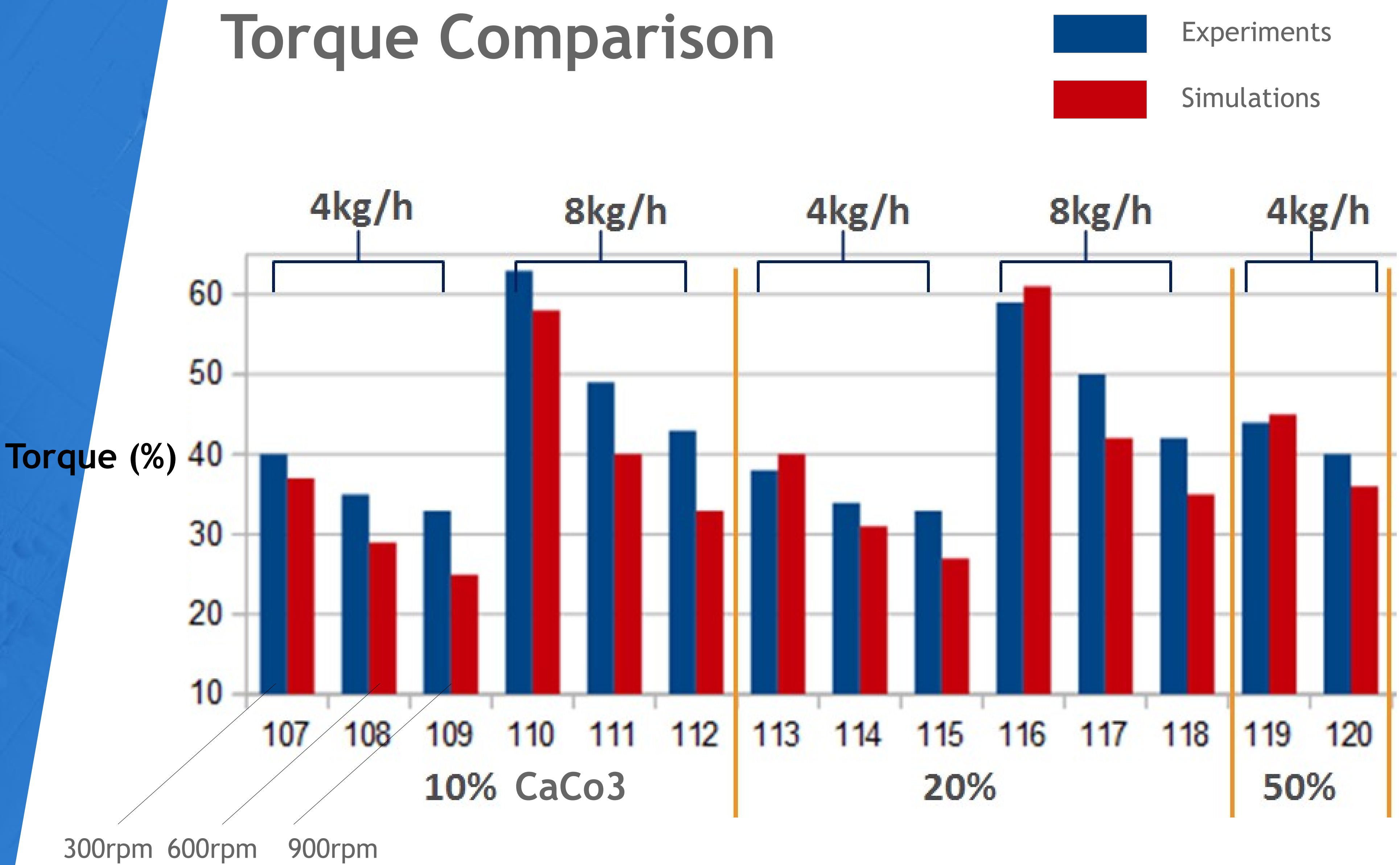


Conveying zone

Mixing zone

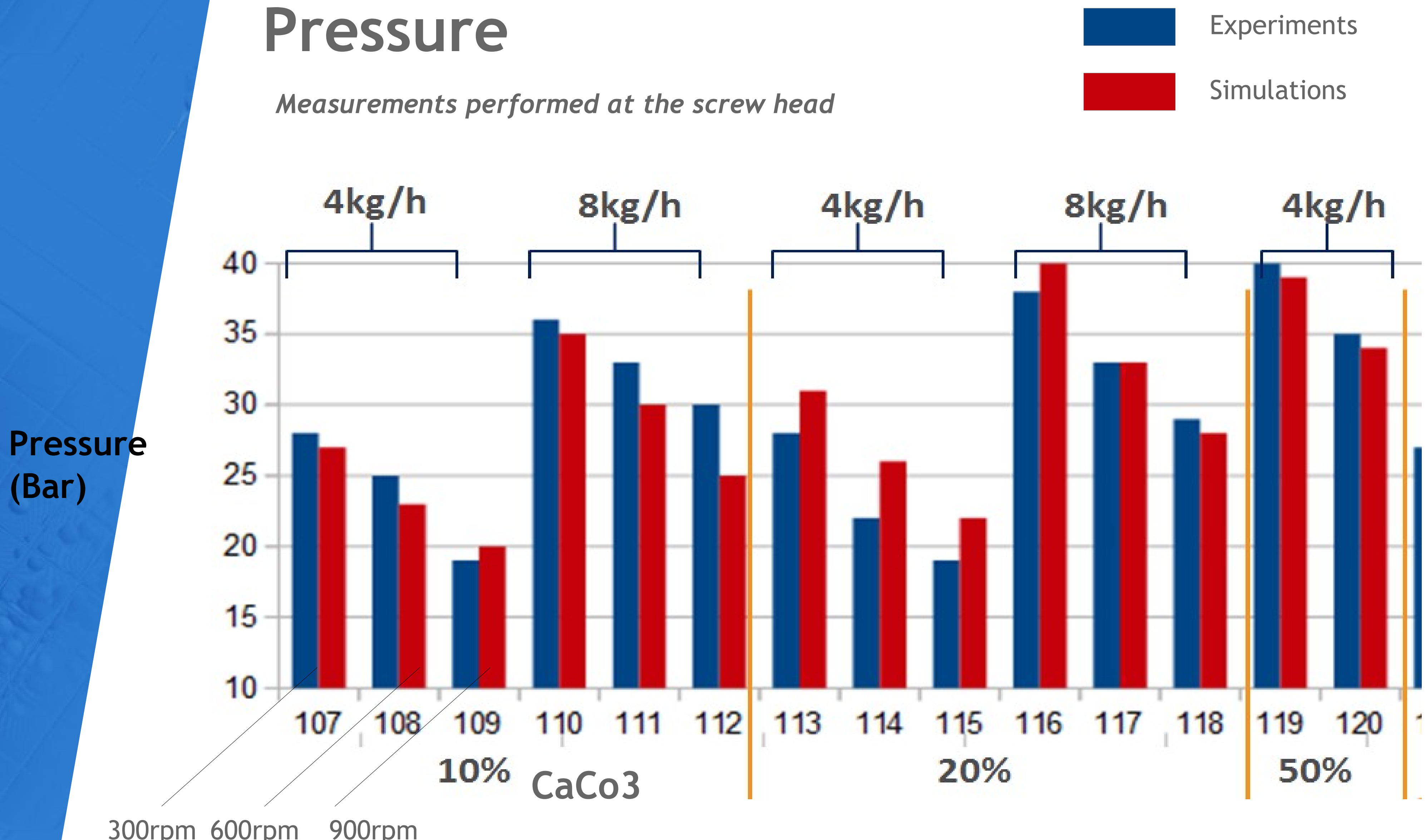
Melting zone

Torque Comparison



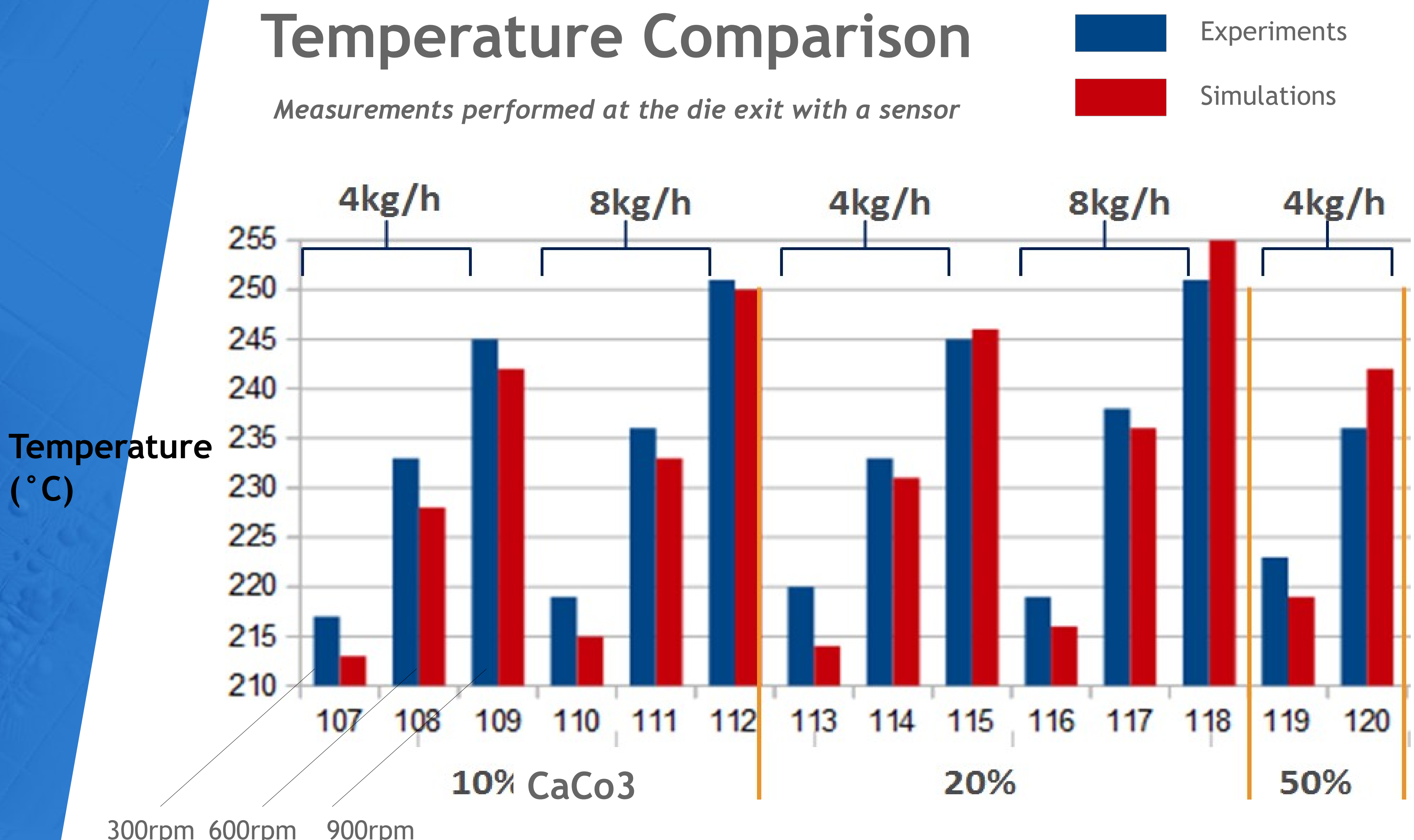
Pressure

Measurements performed at the screw head



Temperature Comparison

Measurements performed at the die exit with a sensor



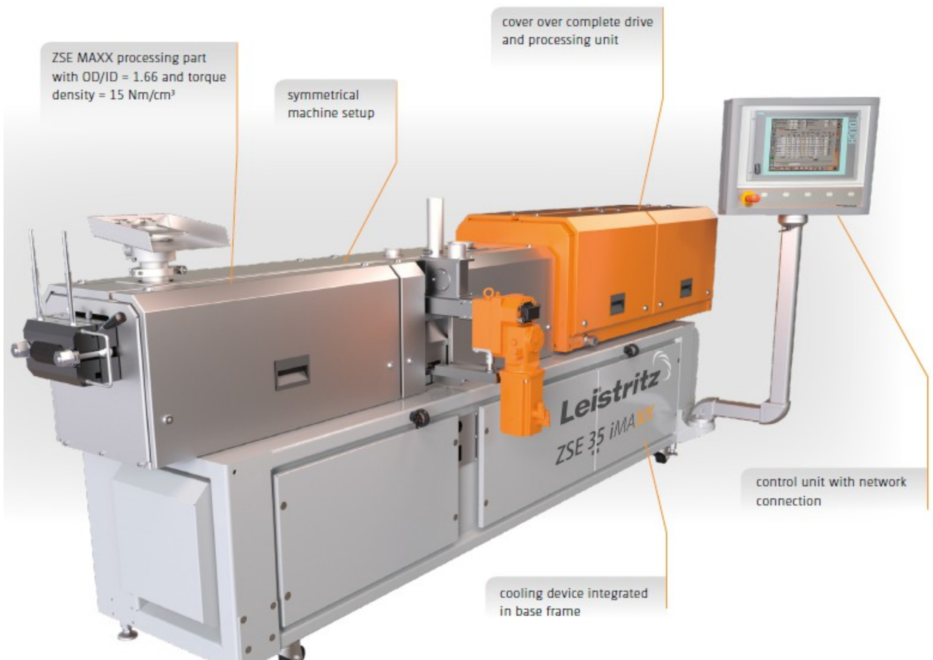
Performing a scale up

From ZSE18 to ZSE35iMAXX machine

Control the process to control the Product

The targets

- From a ZSE 18 mm
- To a ZSE 35iMAXX



Example of a ZSE 35 iMAXX

Scale up

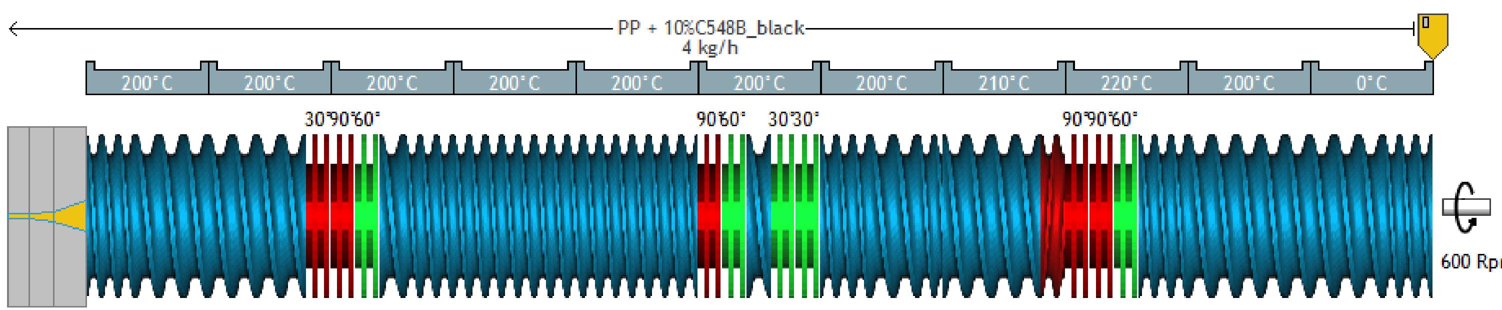
Methodology

- 1. Lab scale preparation
- 2. Industrial scale definition
  Screw design
  Best Trends
- 3. Industrial scale OPTIMIZATION

1. Scale up - from the lab scale

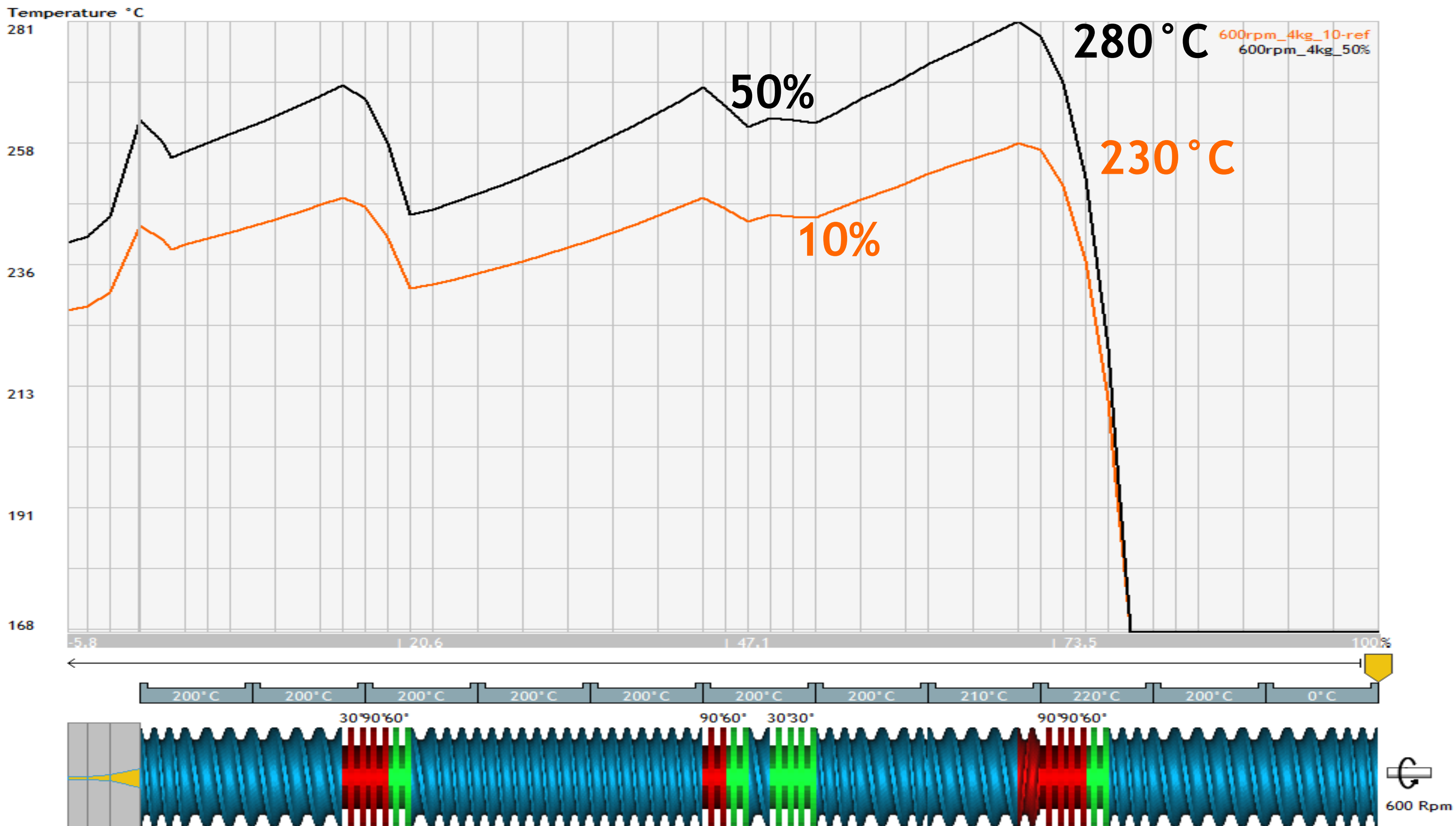
Step by step

- 1. Define the best configuration in **ZSE18** between :
  - 2 materials
    - PP + 10% CaCo3
    - PP + 50% CaCo3
  - Rotation speed [300;600;900] RPM
  - Throughput = 4 kg/h



1. Scale up - from the lab scale

ZSE18 scale : temperature profile at 600 RPM



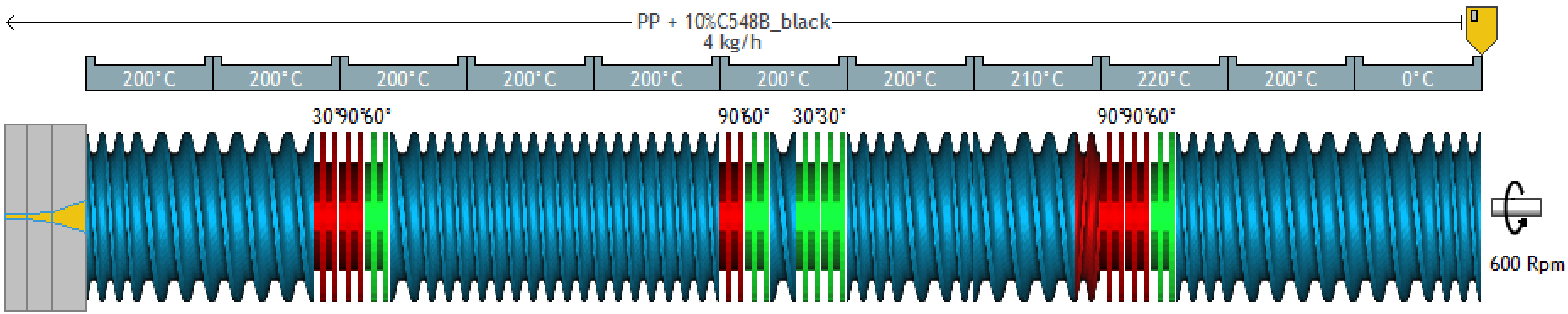
For 600 RPM : Temperature : 230°C - 280°C

The temperature of product PP + 50% CarCo3 is too high

1. Scale up - from the lab scale

Step by step

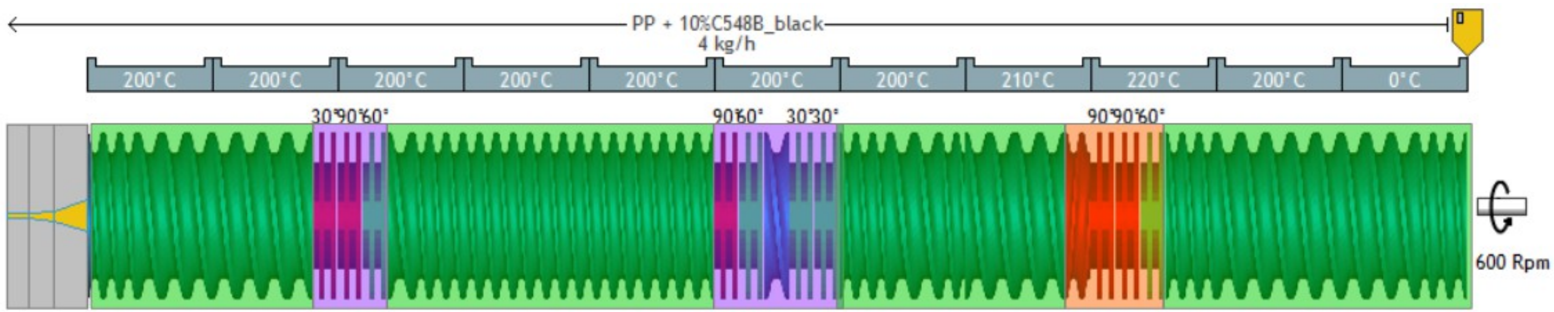
- 1. Best configuration in **ZSE18** :



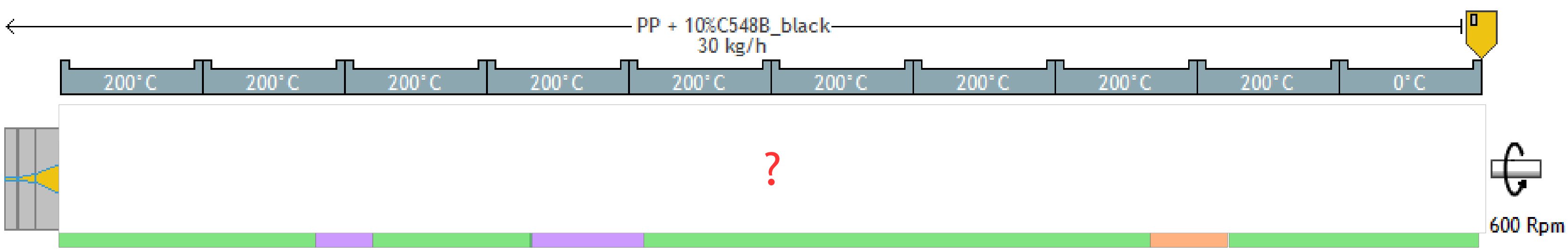
- Material : **PP + 10% CaCo3**
- Identified optimized process parameters at lab scale :
  - **RPM = 600 tr/min**
  - **Q = 4 kg/h**
  - **$T°_{barrel}$ = 200°C**

2. Scale up - to the industrial line

Build the ZSE35 configuration



ZSE18 44D



ZSE35 48D

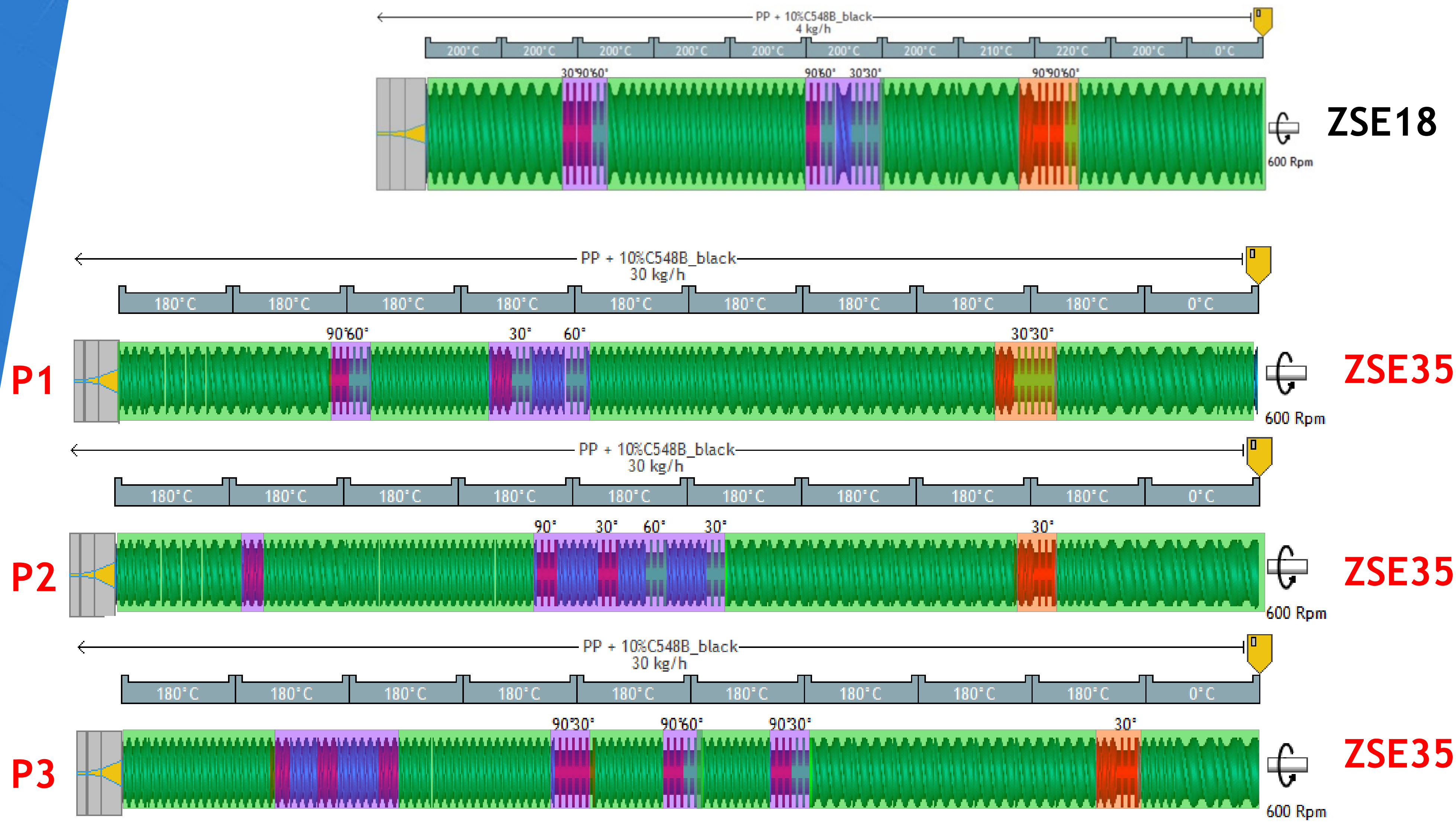
Conveying zone

Mixing zone

Melting zone

2. Scale up - to the industrial line

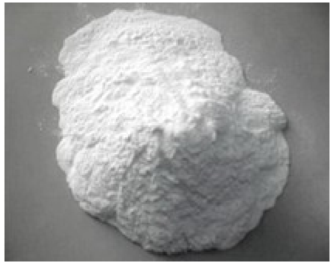
Build the industrial configuration

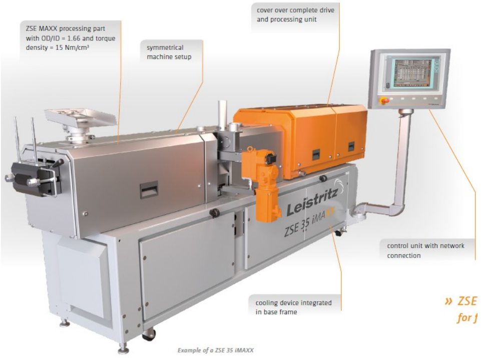


2. Scale up - to the industrial line

Define the process parameters (RPM, Q, T°) (estimation)

- Constraints on Products characteristics :
  - Temperature : max 260°C
  - SME ~ 260 kWh/t, > 200 kWh/t
  - Residence time : as close as possible
  - Maximize throughput
- Constraints on extruder for ZSE35:
  - Torque max (per shaft) : 694 Nm
  - Motor Power (kW max) : 91,8
  - Screw speed max : 1200 rpm





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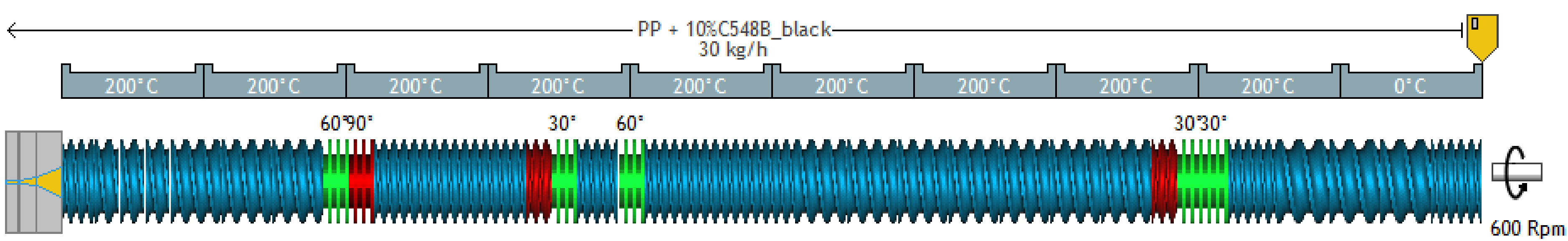
2. Scale up - to the industrial line

Define the process parameters (RPM, Q, T°) (estimation)

- 600 RPM
- Regulation temperature = 200°C
- Throughput estimation :

$$Q_{ind} = Q_{lab} \left(\frac{D_{ind}}{D_{lab}} \right)^3 \qquad Qind = 4 \left(\frac{35}{18} \right)^3 \sim 30 \text{ (kg/h)}$$



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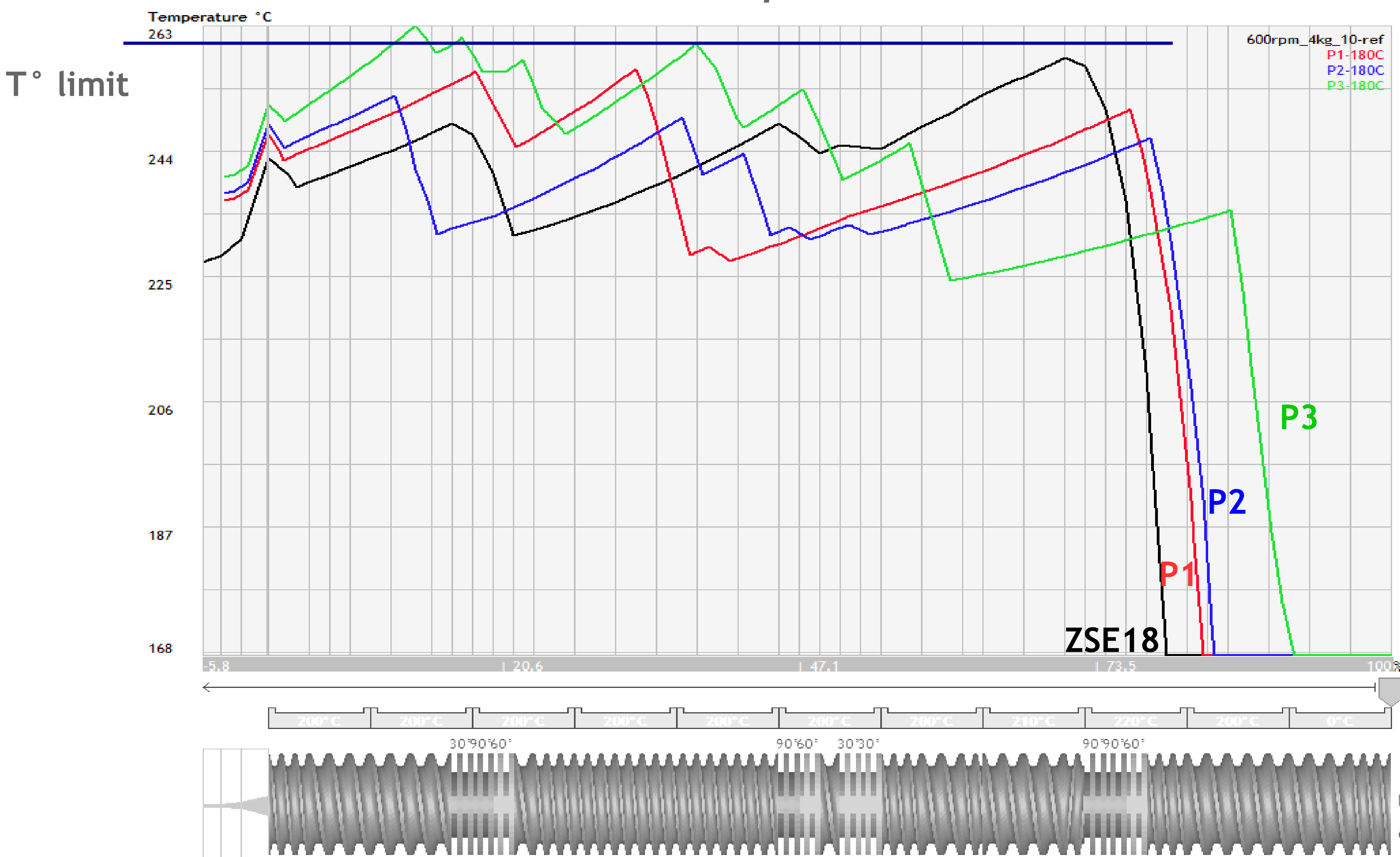
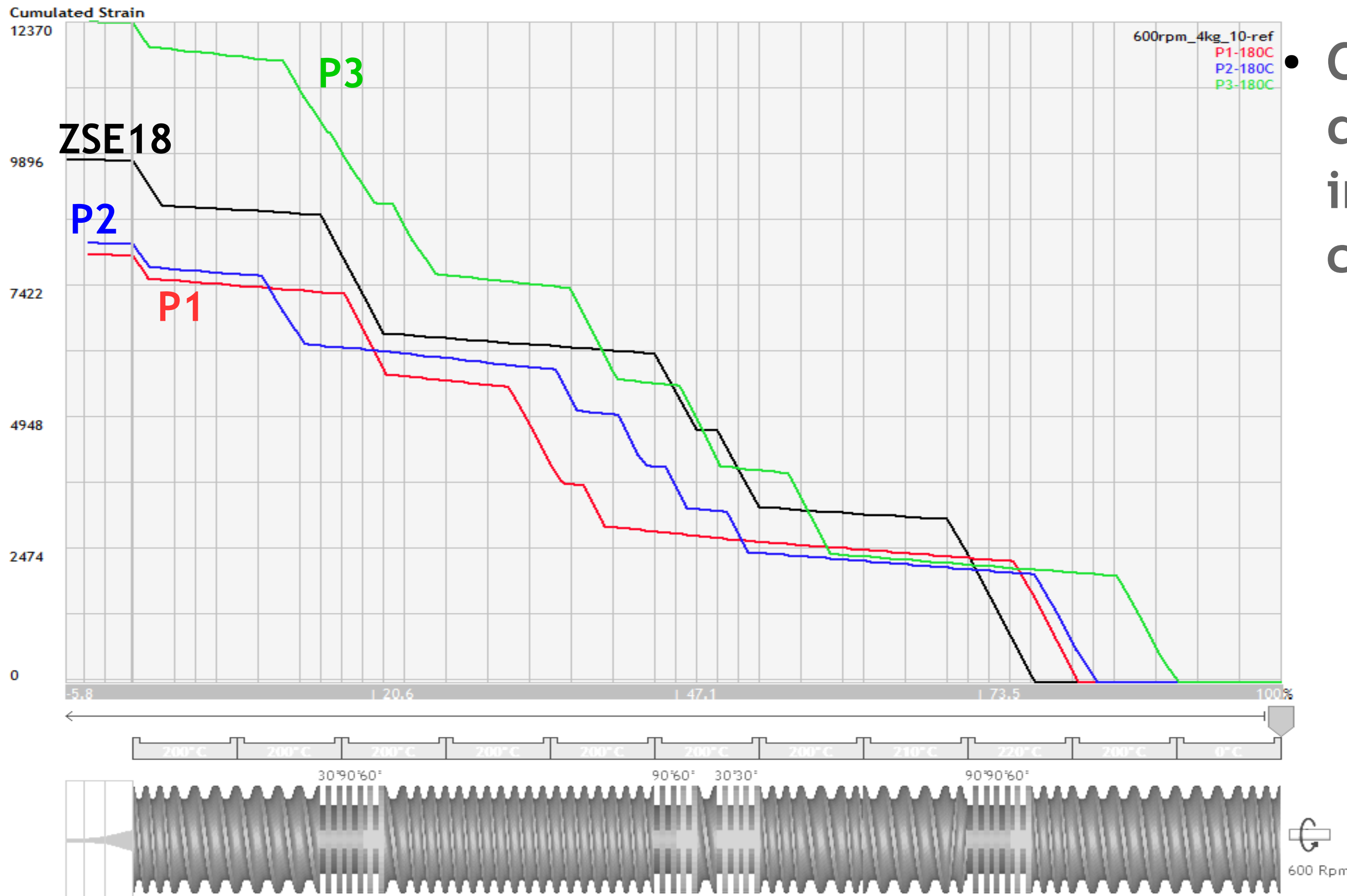
2. Scale up - to the industrial line

Lab scale vs industrial scale - Temperature



2. Scale up - to the industrial line

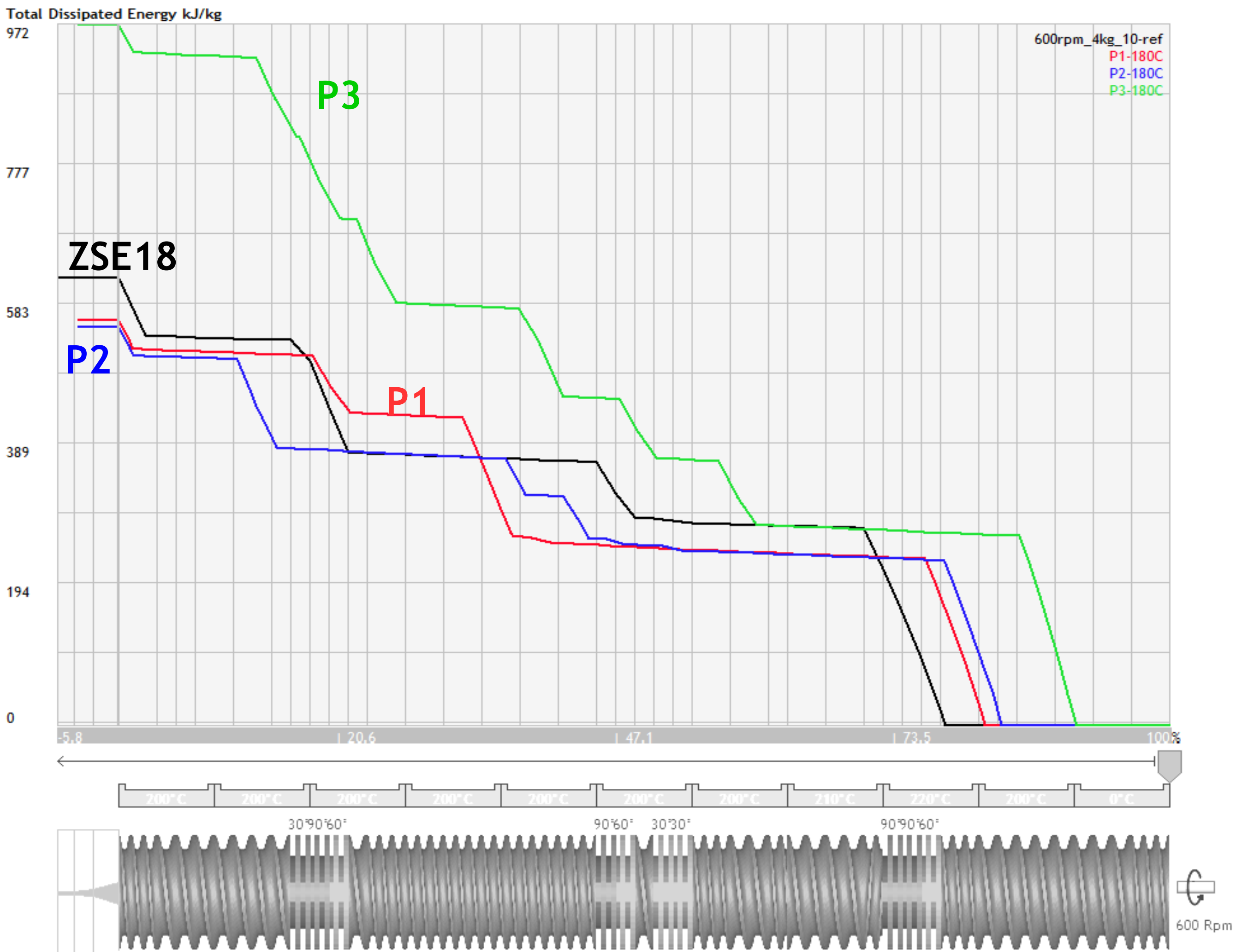
Lab scale vs industrial scale - cumulated strain



- Cumulated strain is a quantitative mixing index for compounding

2. Scale up - to the industrial line

Lab scale vs industrial scale - dissipated energy



- Dissipated energy is a quantitative mixing index for coumpounding

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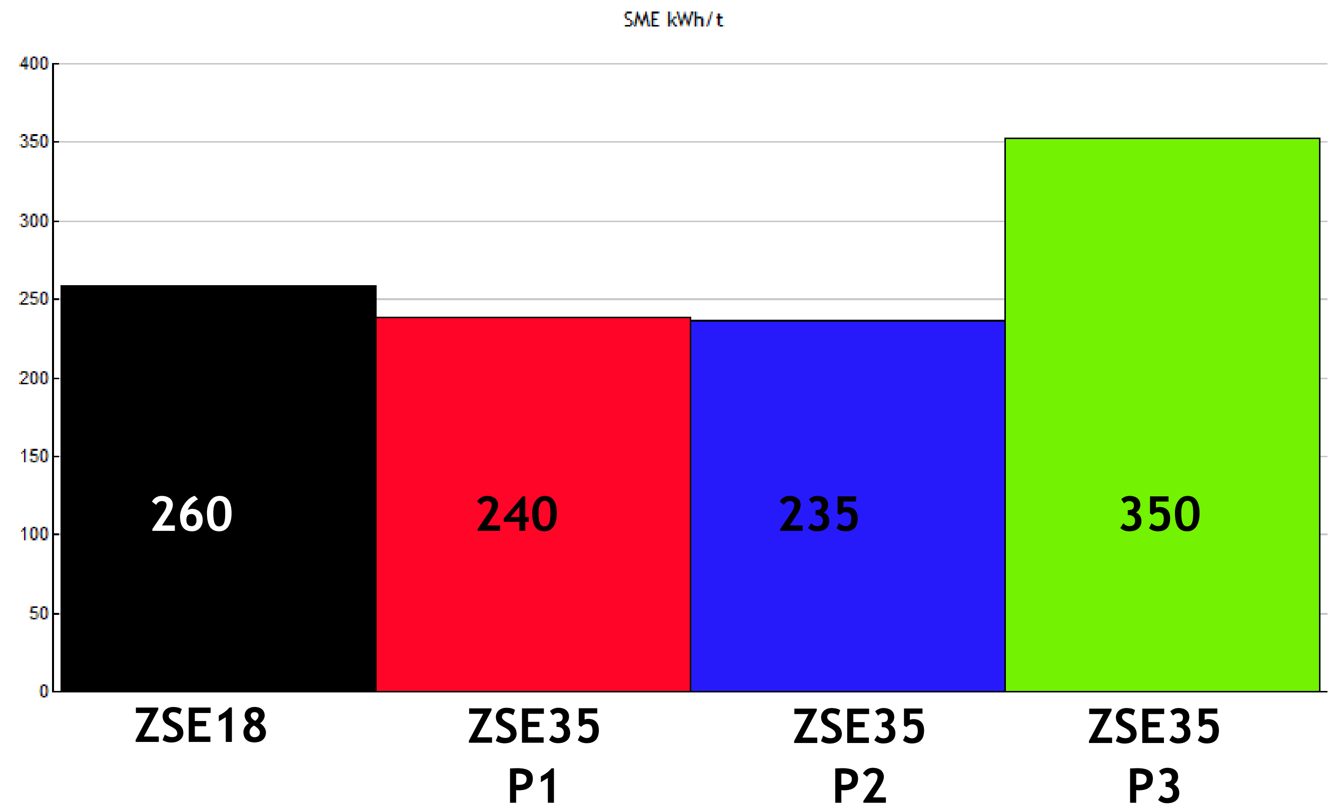
2. Scale up - to the industrial line

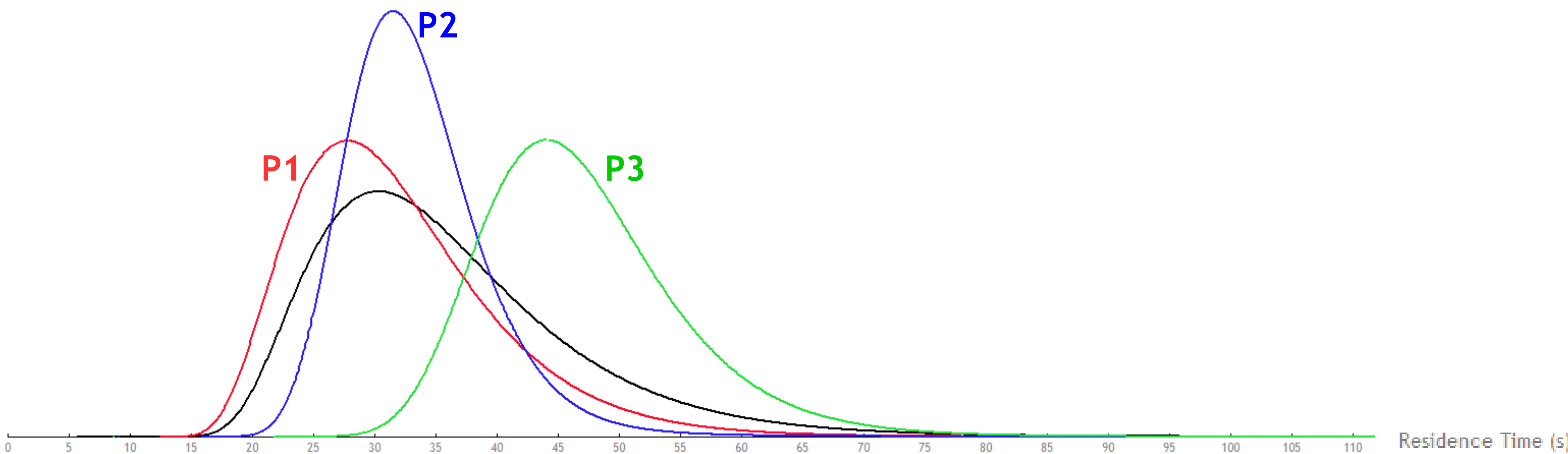
ZSE18 vs industrial scale - SME



- *The SME in industrial scale for **P1** & **P2** is lower than the **lab** scale but still ok according to criterion*
  *The SME for **P3** is larger than lab scale, so criterion respected*

2. Scale up - to the industrial line

ZSE18 vs industrial scale - RTD



- The residence time distribution is quite close from the **ZSE18** scale for **P1** & **P2**.
  RTD is a little bit longer for **P3**.

3. Scale up - process optimization

Which industrial configuration for optimization ?

	P1	P2	P3
Temperature	✓	✓	~
SME	~	~	✓
RTD	✓	~	~
Cumulated strain	~	~	✓
Dissipated energy	~	~	✓

- **Selection of P3 to optimize process parameters using DoE**

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3. Scale up - process optimization

Which industrial configuration for optimization ?

- Regarding the results comparison between ZSE18 and the 3 proposed configurations at scale ZSE35 :
  - P1 provides a good SME & RTD close to ZSE18 one. T°C profile is a little bit high but still acceptable. Cumulated strain too low
  - P2 provides a good SME. Mean residence time is close to ZSE18 one but the distribution is quite different. T°C profile is a little bit high but still acceptable. Cumulated strain too low
  - P3 provides a high SME & RTD a little bit too long comparing to ZSE18 one. T°C profile is a little bit too high but still acceptable. Good cumulated strain

- Selection of P3 to optimize process parameters using DoE

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3. Scale up - process optimization

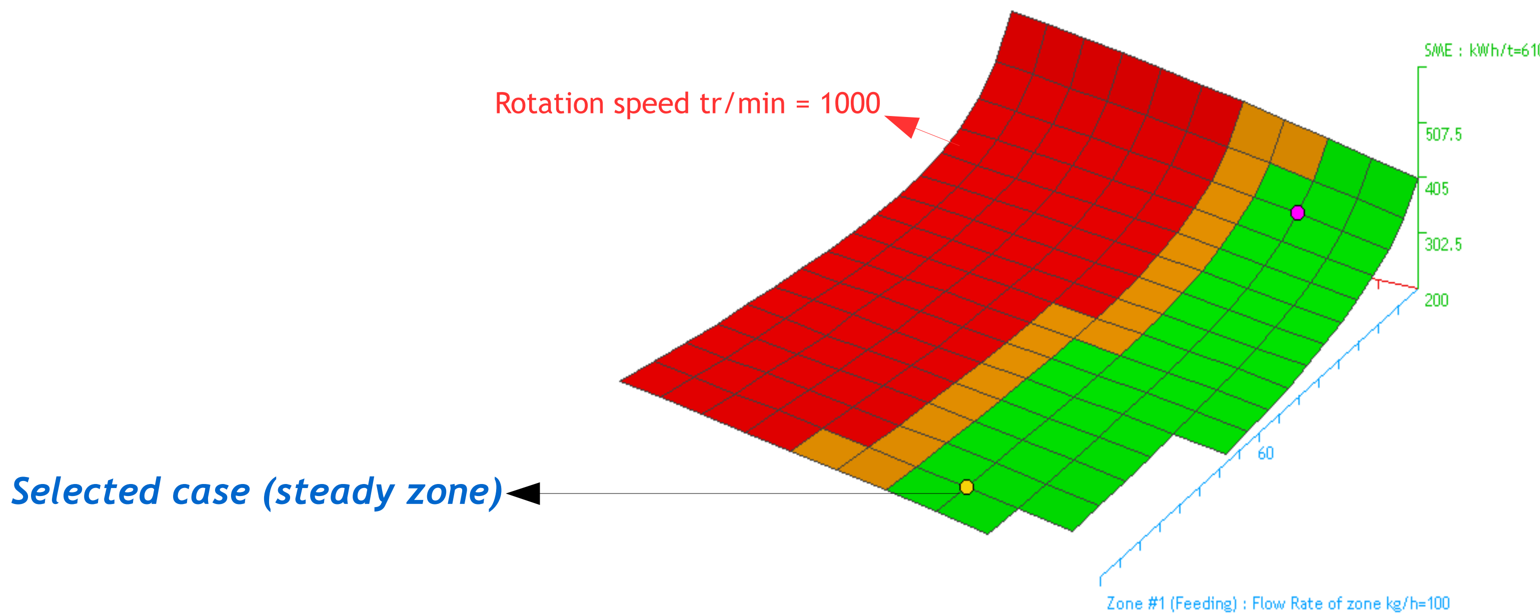
ZSE35 optimization

- DoE settings up
  - Process parameters
    - Throughput : [20;100] kg/h / 17 steps
    - RPM : [500;1000 RPM] / 11 steps
  - Observed Results
    - RTD
    - SME
    - Dissipated energy
    - Cumulated strain
    - Torque
    - Temperature max

3. Scale up - process optimization

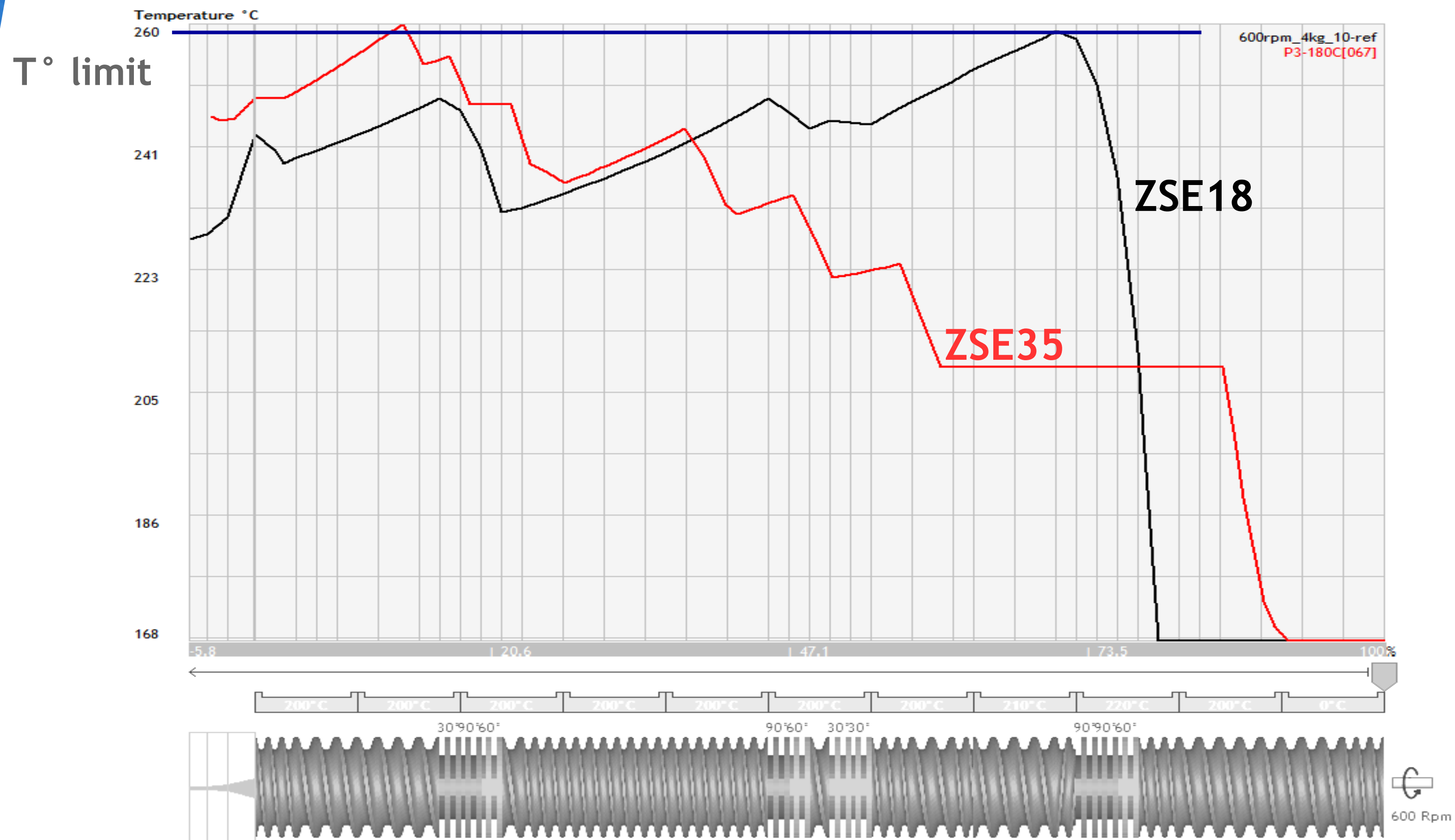
ZSE35 optimization

Active	Result	Criterion	Value (x / y)	Range
☑	SME : kWh/t	>= X	200	[202.42 , 607.57]
☐	RTD - Mean : s	<= X		[17.45 , 67.35]
☐	RTD - Variance :	<= X		[8.71 , 176.4]
☑	Temperature (Max) : °C	<= X	260	[245.4 , 308.9]
☑	Torque / Shaft : N.m	<= X	694	[58.02 , 166.94]
☐	Dissipated Energy (viscous dissipation - screw) : kWh/t	<= X		[118.89 , 524.51]
☐	Cumulated Strain (Pos=-63) :	<= X		[4821.13 , 28068.67]



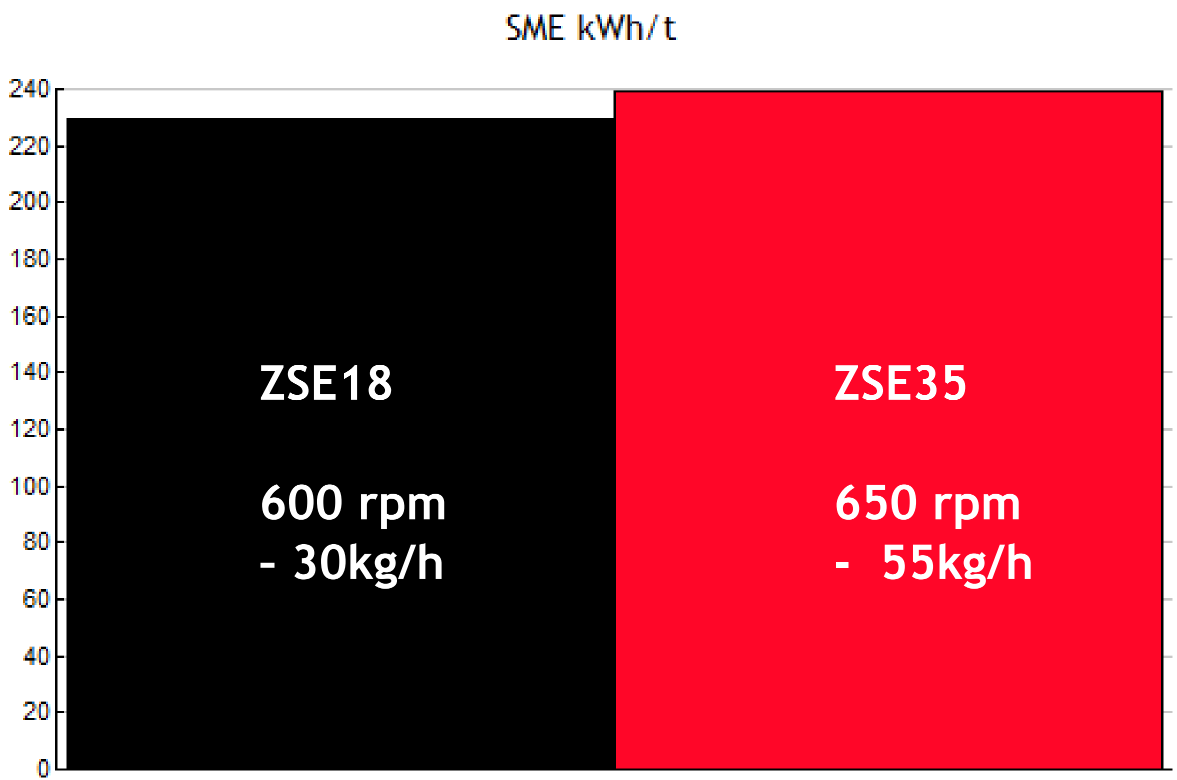
3. Scale up - process optimization

ZSE35 optimization - comparison with ZSE18



3. Scale up - process optimization

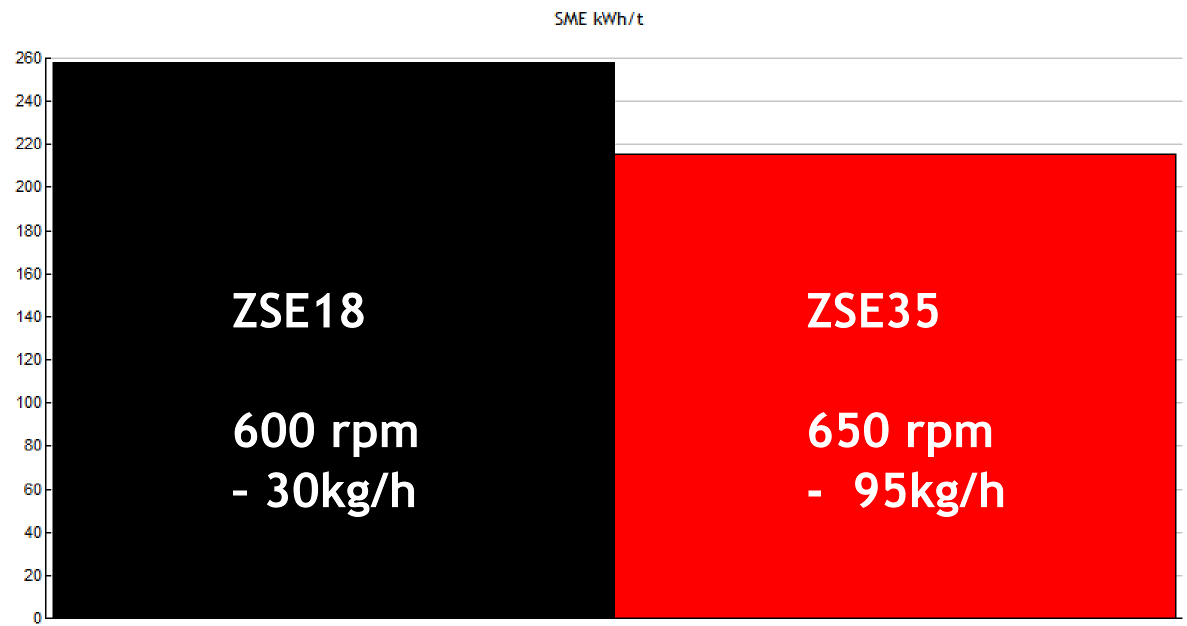
ZSE35 optimization - comparison with ZSE18



Same target in terms of SME

3. Scale up - process optimization

ZSE35 optimization - comparison with ZSE18



Industrial conditions : increasing the throughput

SME > 200 kWh/t : criterion is respected

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Scale up - Conclusion

From ZSE18 to ZSE35 scale

- Identification of the key targets
- Easiness in the screw profile translation
- Screening the functioning domain
- Optimizing the conditions

In a virtual way !!

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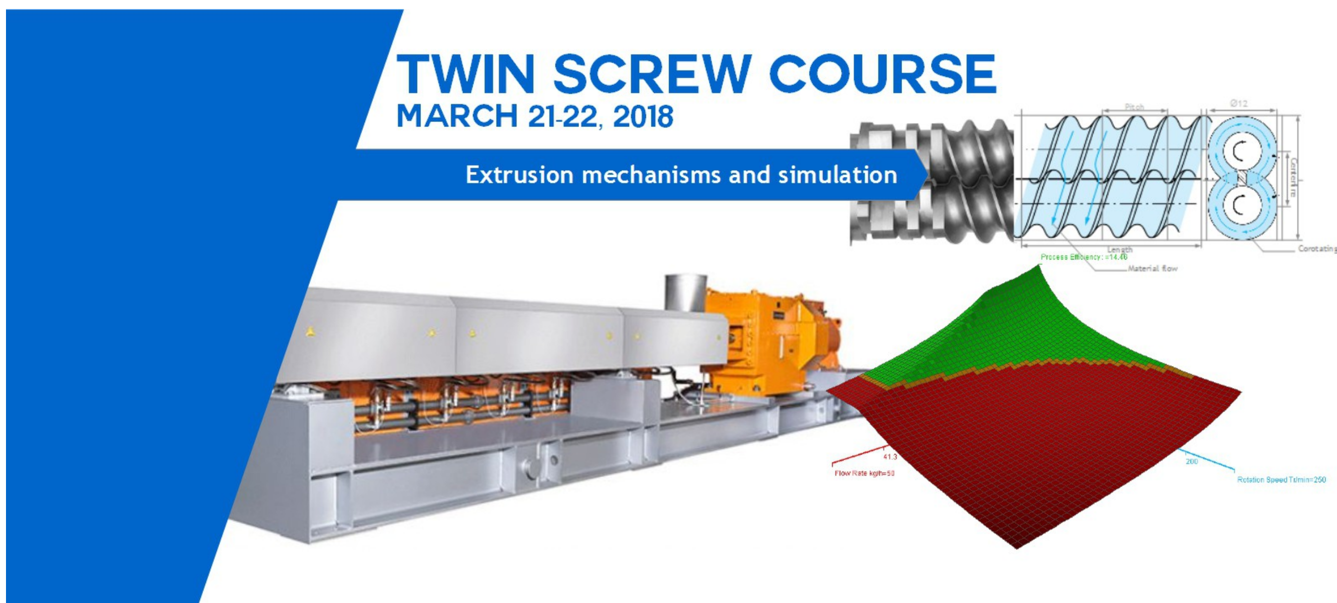
Ludovic® - driving the process efficiency

- Experiments constraints
  - Experiments costs
  - Measures difficulty
  - Mechanics knowledge
  - Time consuming

- Ludovic® answers
  - Virtual trials
  - Models for input
  - Readable results
  - Only a few minutes

Going further with Ludovic®

- Twin Screw Course (TSC)
  - On March 21-22, 2018
  - On the French Riveira (Sophia Antipolis)
  - 2 day course on Twin Screw mechanisms and simulation



Thanks for your attention

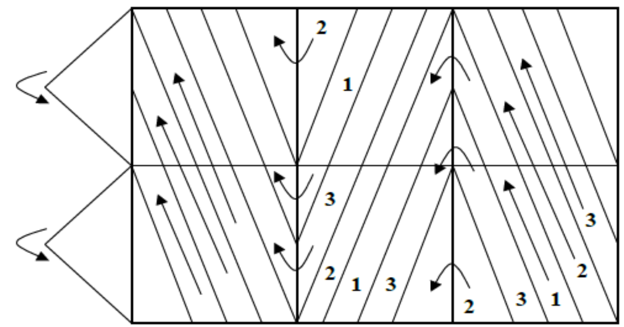
Http://www.scconsultants.com
Http://www.mixingsimulation.technology

5 Ludovic® functioning

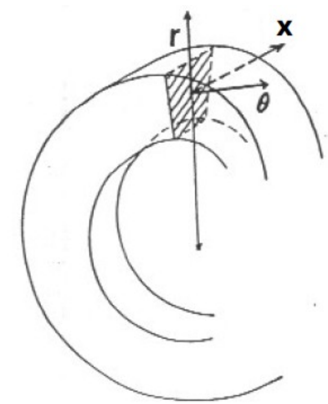
- The model
- The advantages

The model

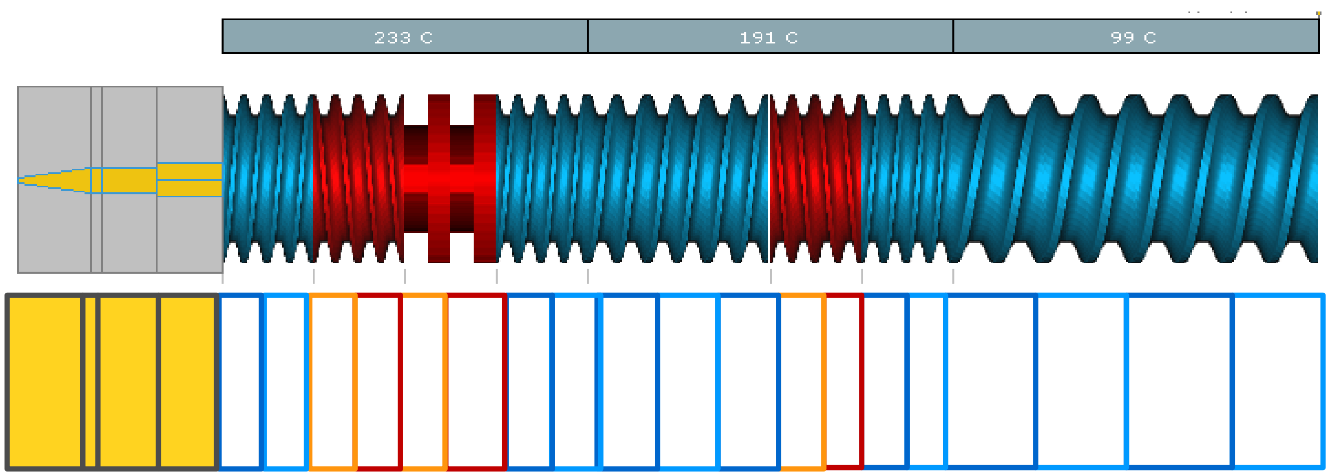
- Flat geometry modeling
  - Screw partition in computation domains
  - C-Chamber areas
  - Robust model
  - Fast computation



Flattened geometry for a two-flight screw



C-chamber scheme for a conveying element



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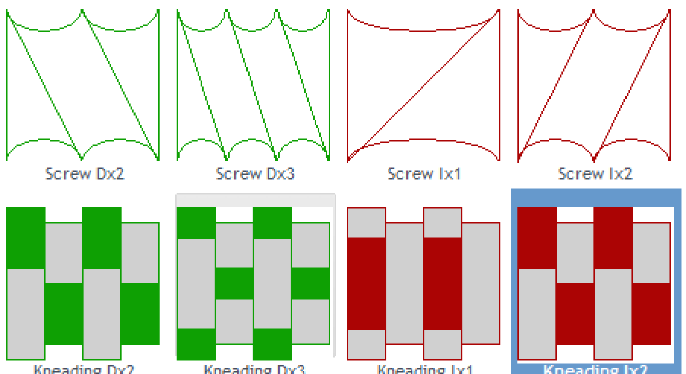
Dedicated to corotating TSE

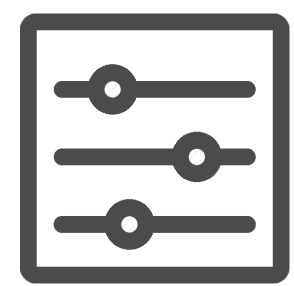
- Dedicated environment
  - Customizable screw elements
  - Products library
  - 3 Tabs technology for simulation definition

1 Screw Design



2 Product selection

3 Parameters



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6

Ludovic® solutions

- Quick adaptation
- Fast ROI
- Including support

Ludovic® benefits

- Speeding up the time to market !
  - Saving 30% time
  - Saving 50% materials and trials
  - Controlling the process
  - Optimizing the product

6 trials

- 3 days (prep. + trials + cleaning)
- 2 persons
- 200 kg material

- **Total human cost : ~4 200,00€**
- **Material cost : 400,00€**

90 simulations

- 3 hours (prep. + trials + cleaning)
- 1 person
- 0 kg material

- **Total human cost : 300,00€**
- **Material cost : 0,00€**

SCIENCES COMPUTERS CONSULTANTS

For more details

A global Computer Software for Polymer Flows in Corotating Twin Screw Extruders	B. Vergnes, G. Della Valle, L. Delamare	**1998**	Polymer Engineering and Science
Twin screw extruder simulation programs - What can they offer ?		**2002**	Plastics Additives & Compounding Volume 4, Number 2, February 2002 , pp. 22-26(5
Effect on processing conditions on the formation of polypropylene/Organoclay Nanocomposites in a twin screw extruder	W.Lertwimolnum, B. Vergnes	**2006**	Polymer Engineering and Science
Modeling of coupling between specific energy and viscosity during twin screw extrusion of starchy products	F. Berzin, A. Tara, B. Vergnes, Ch. David	**2009**	ANTEC 2009
Rational Development of Solid Dispersions via Hot-Melt Extrusion Using Screening, Material Characterization, and Numeric Simulation Tools	D.E. Zecevic; K.G. Wagner	**2013**	Wiley Online Library (wileyonlinelibrary.com) DOI 10.1002/jps.23592

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