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- compounding & extrusion
- materials handling
- service

Simulation of Co-Rotating Fully Intermeshing Twin-Screw Compounding Extruders

Alternatives for process design

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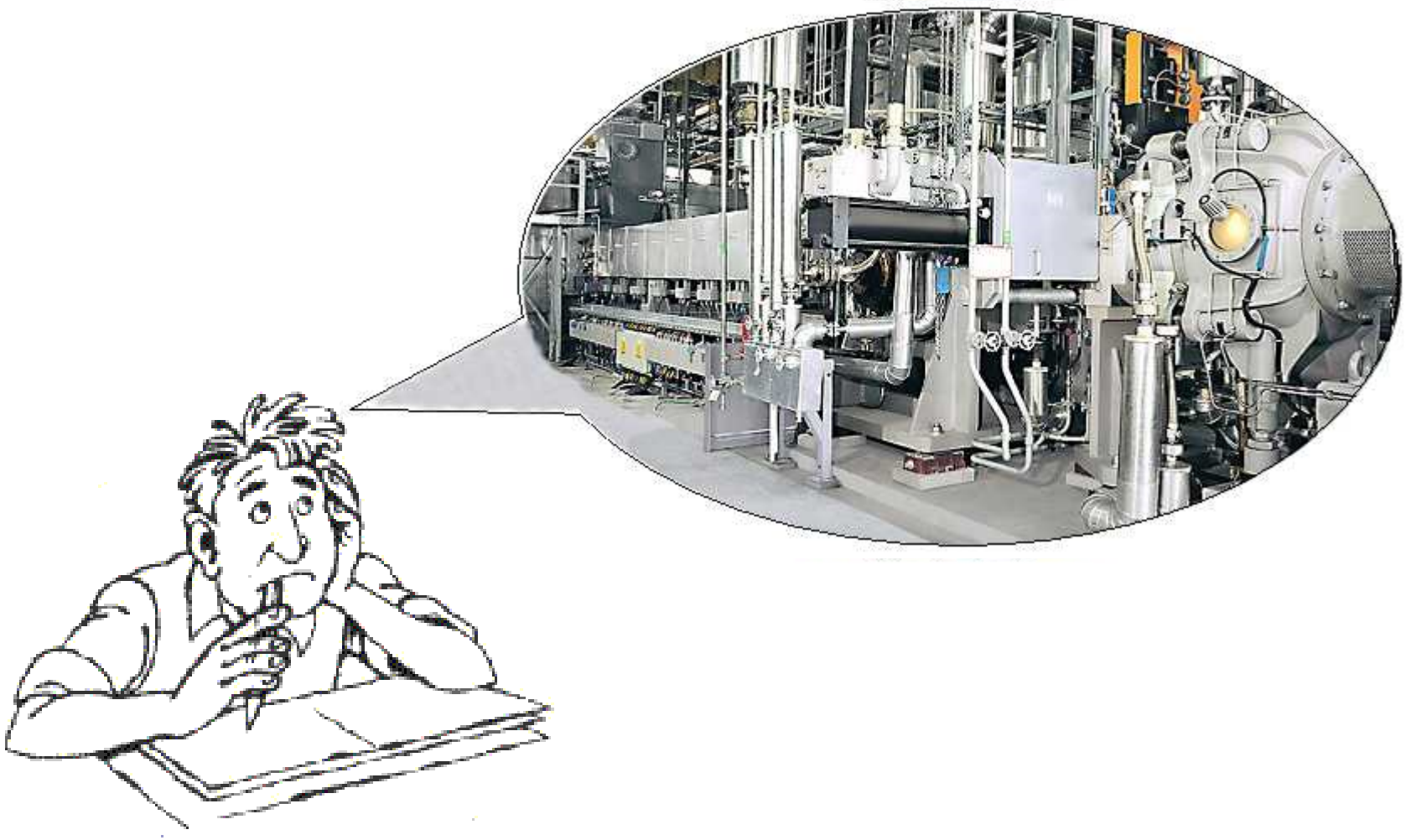
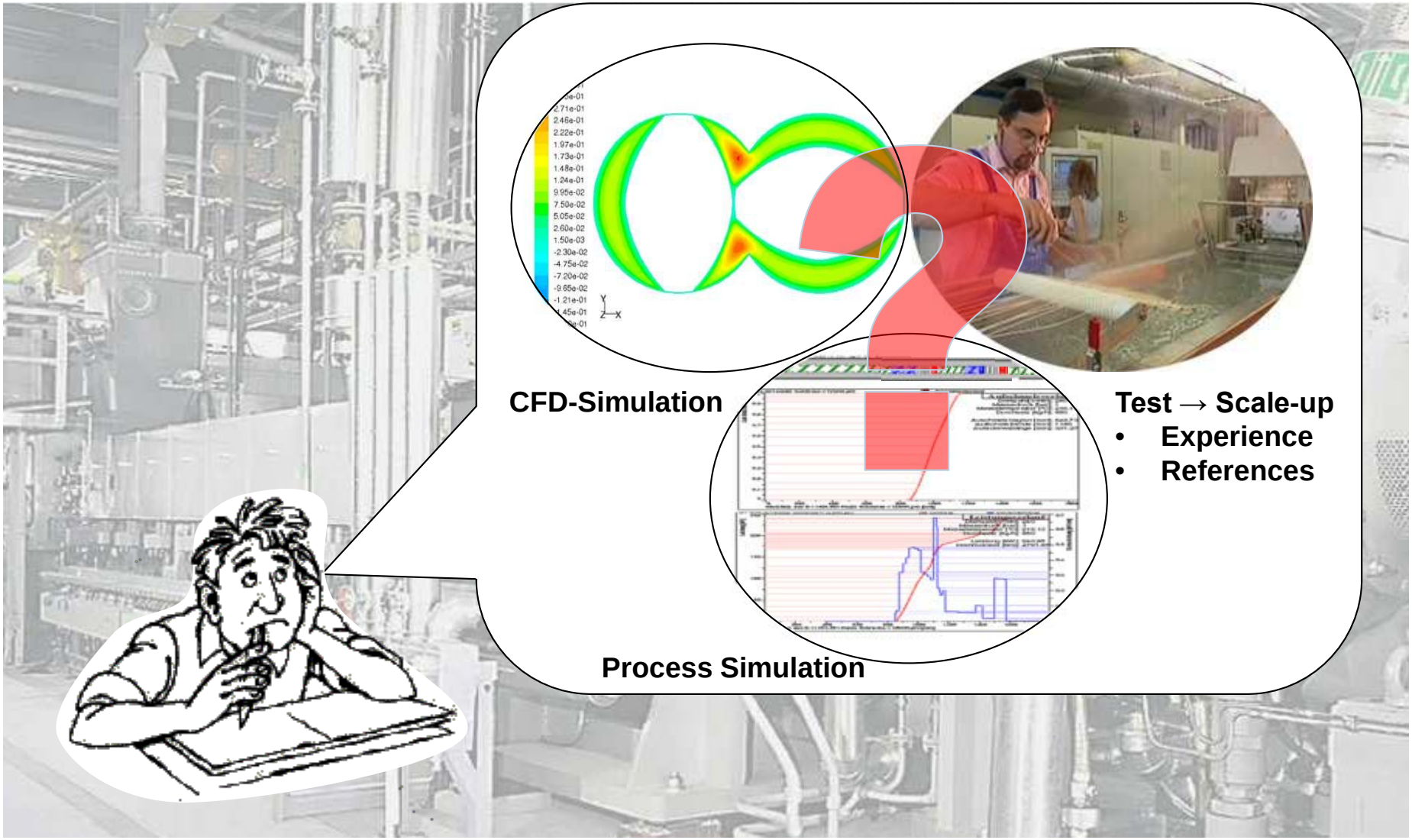
Coperion GmbH, Stuttgart

- **Incentives**
- **Material Properties**
- **1 D Simulation**
- **3 D Simulation**
- **Summary**

Process Design



Process Design



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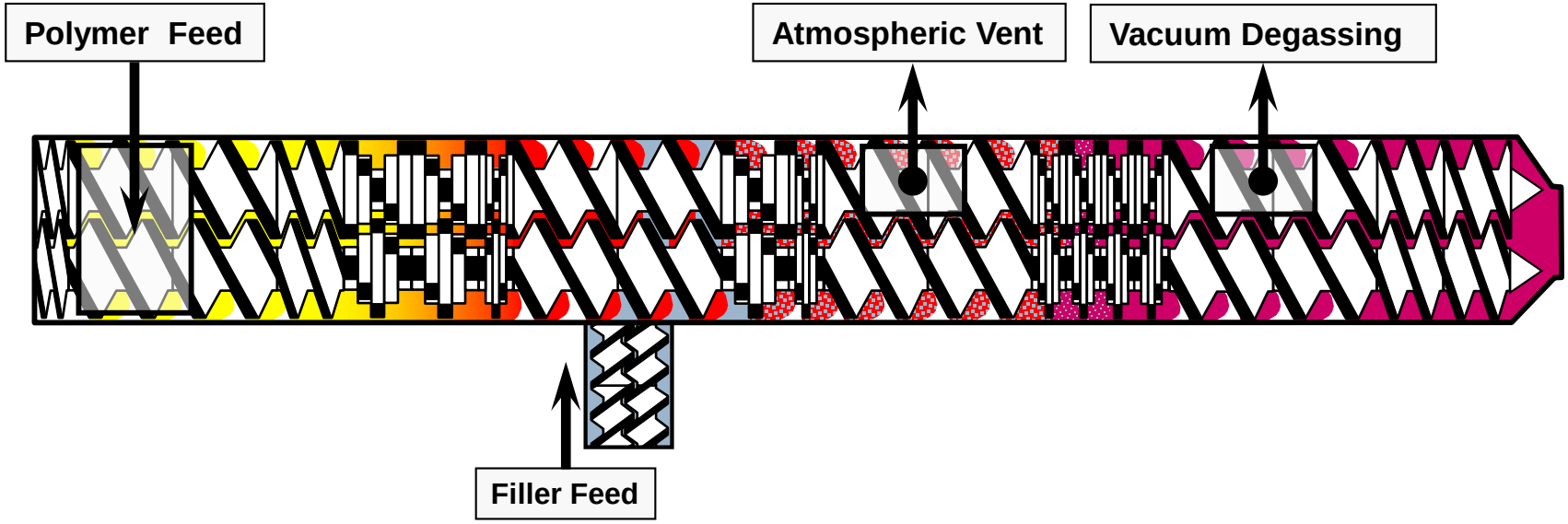
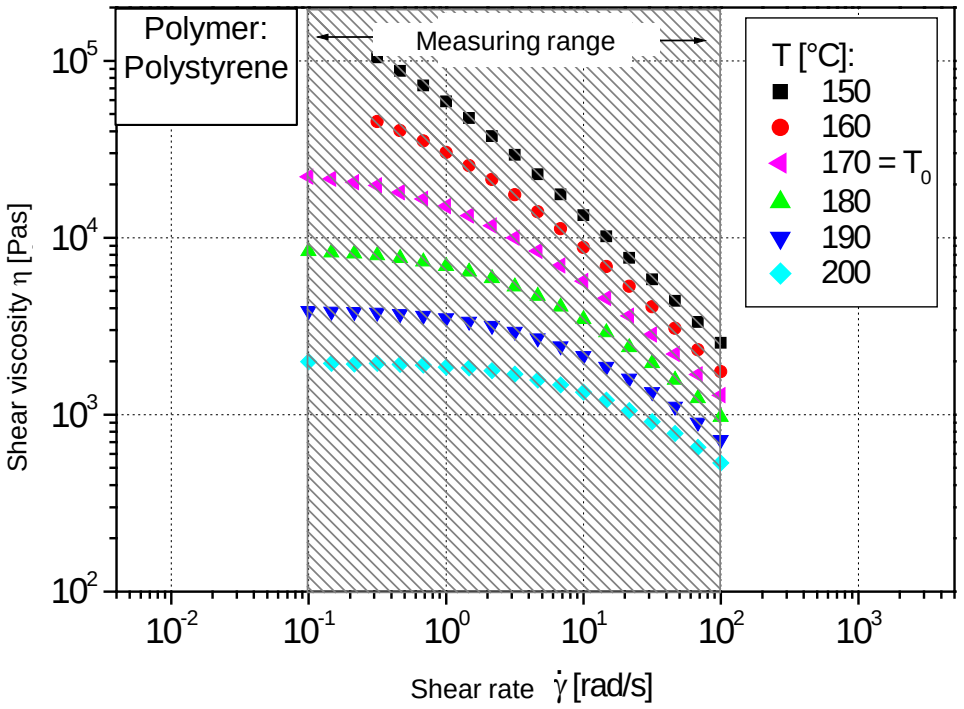
Process Sections of the Twin Screw Extruder



Feeding	Melting	Conveying	Mixing	Venting	Homogen.	Degassing	Metering

Viscosity

Strong dependency on temperature and shear rate



Source: Covestro (Bayer Technology)

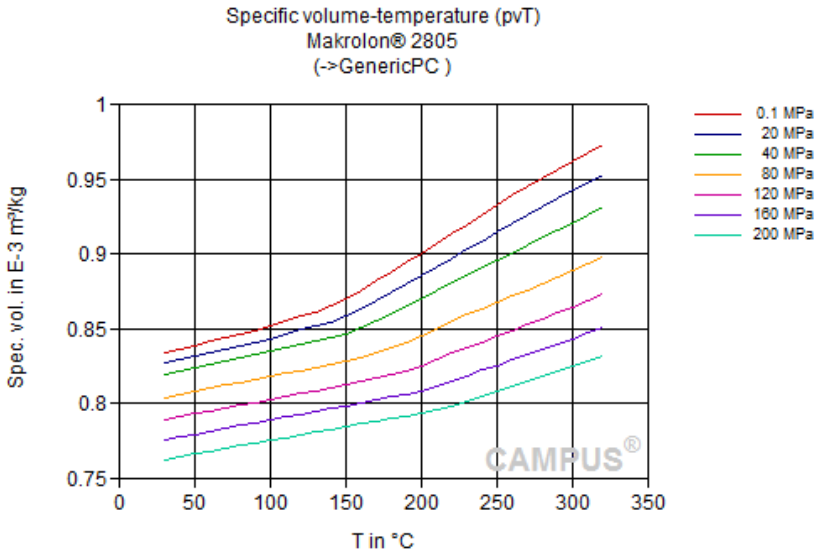
Reality

- Only MVR available
- Measuring of shear thinning inconsistent
- Viscoelasticity: poor measurement leads to false predictions
- Not available for compounds

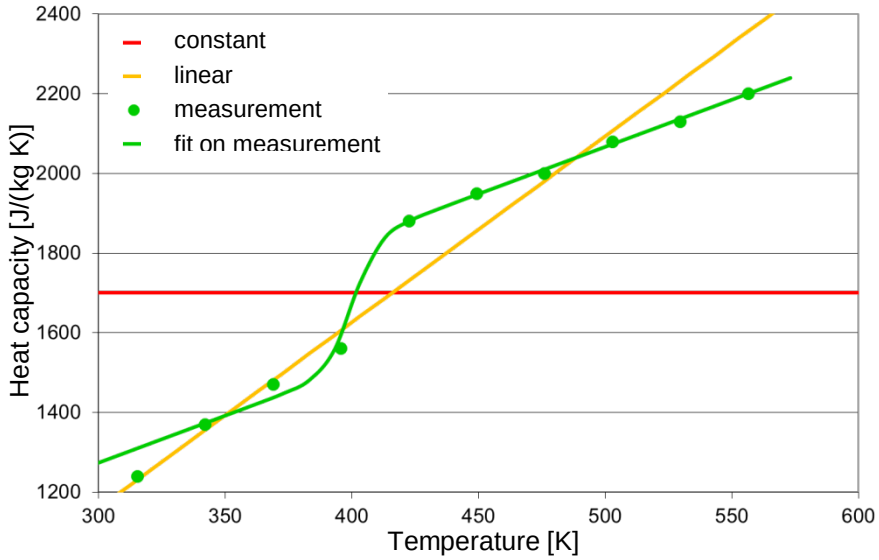
Density and Heat Capacity

Strong dependency on temperature

Density Polycarbonate



Heat Capacity Polycarbonate



Source: Covestro (Bayer Technology)

Reality

- Often only constant data for density and heat capacity
- False prediction for flow rate and temperature

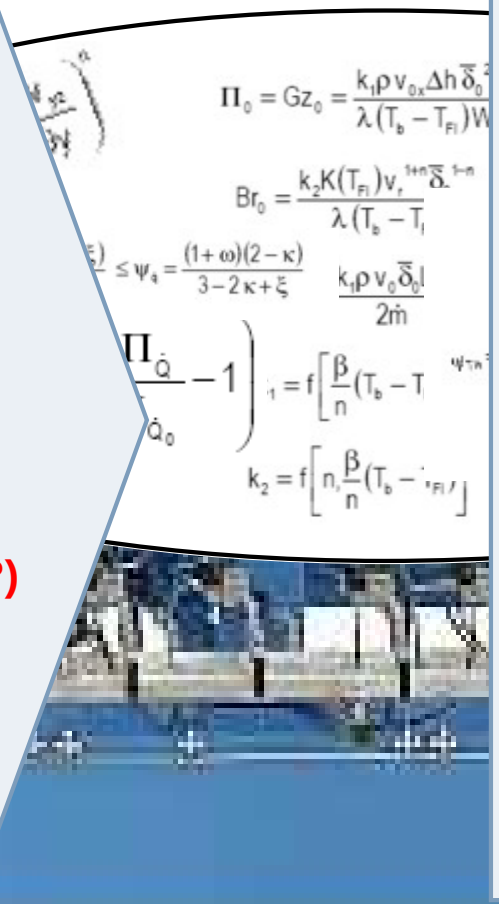
Process Simulation (1D – Modeling)

Geometrical Data
- Process set-up
- Screw design
- Screw pitch, etc.

Process Data
- Screw speed
- Throughput
- Temperature profile
- Discharge pressure etc.

Polymer Data
- Bulk properties
- Viscosity data (Flow curves) (?)
- Heat transfer coeffiecents (?)

Simulation Model for:
- Feed intake (?)
- Plastification, devolatilization (?)
- Pressure built-up



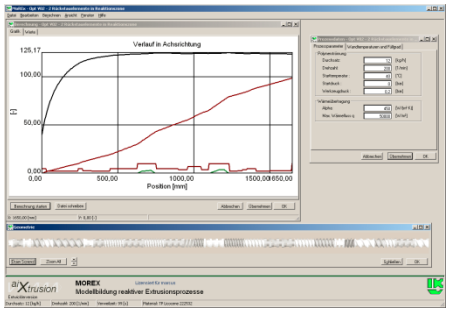
- Feed limit (?)
- Back-up length
- Pressure build-up
- Product quality (?)
- Specific energy input
- Polymer temperature

Process Simulation (1D – Modeling)

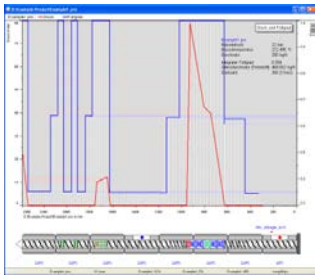
No longer maintained

- Akro: Prof. J. White
- Morex

Morex



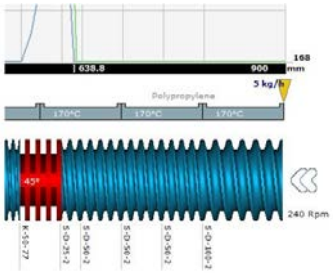
Sigma



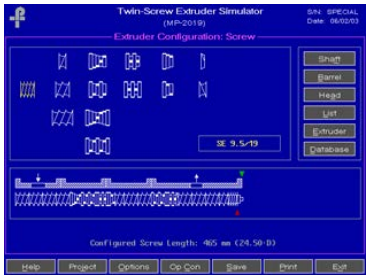
Current

- Polytech WinTxs
- Ludovic
- Sigma
- Company internal:
  Covestro (former Bayer Technology), Coperion

Ludovic



WinTXS



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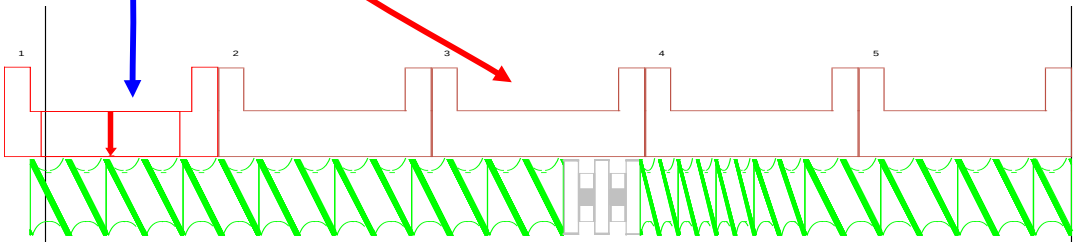
Material Properties Required for Twin Screw Extruder Calculations

With the input data

Material Properties
- Thermal conductivity [W/mK]
- Heat capacity [kJ/kgK]
- Density [kg/m3]
- Viscosity [Pas]

Process Data
- Screw speed [rpm]
- Material feed rate [kg/h]
- Material feed temperature [°C]
- Material pressure at the screw tip [bar]
- Barrel temperatures **T_b** [°C]

Machine Data
- Barrel configuration
- Screw configuration



Using analytical and numerical methods the following are calculated in the process section:
- Material temperature $\mathbf{T_{MAT}}$ [°C]
- Material pressure $\mathbf{P_{MAT}}$ [bar]
- Degree of fill [%]
- Specific energy input **SEI** [kWh/kg]

Note for the calculations:

- **the shaft cooling is not implemented**
- **most of the element types can be calculated**

Material Properties Required for Twin Screw Extruder Calculations

Thermodynamic data

- Crystalline melt / glass transition temperature
- Thermal conductivity
- Thermal conductivity of the solids
- Heat capacity
- Melting enthalpy
- Solid enthalpy

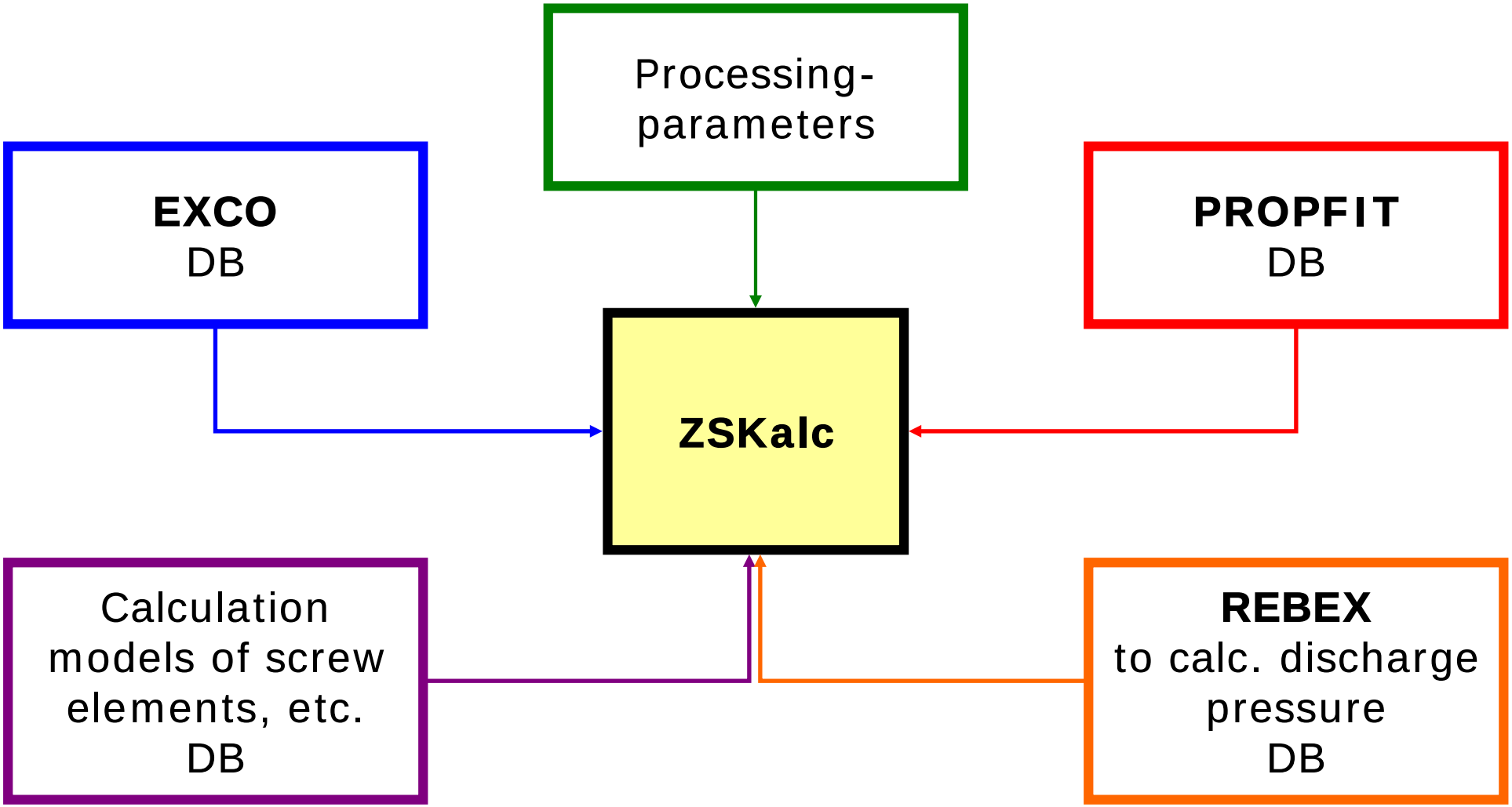
Rheology data (also for blends)

- Viscosity data to get Carreau / Power-Law parameter and
- Temperature shift using Arrhenius / WLF

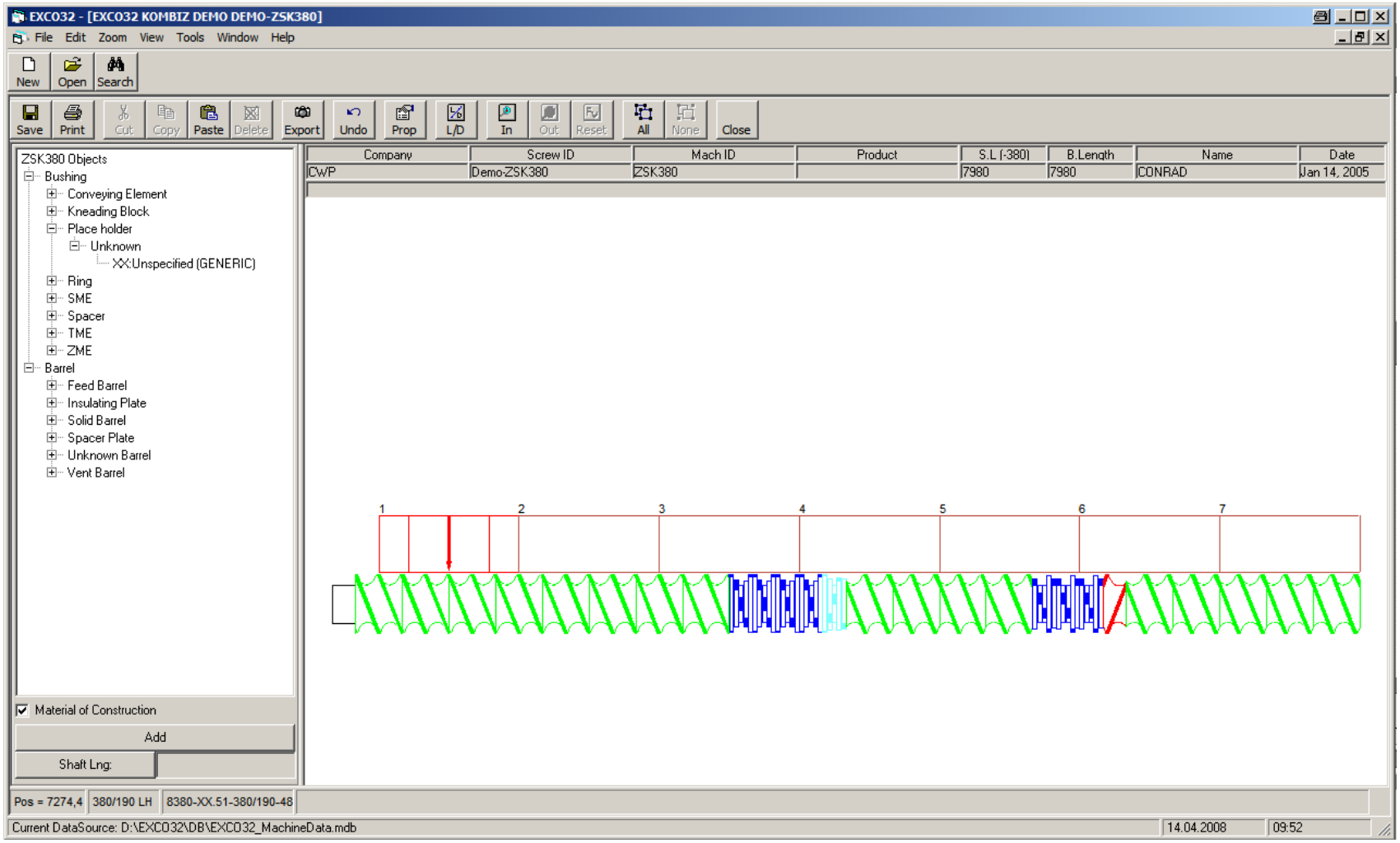
Densities

- Melt density
- Particle diameter
- Solid density
- Bulk density

Coperion Data Structure for Twin Screw Extruder Calculations



Coperion Data Structure: Screw Configuration Database EXCO



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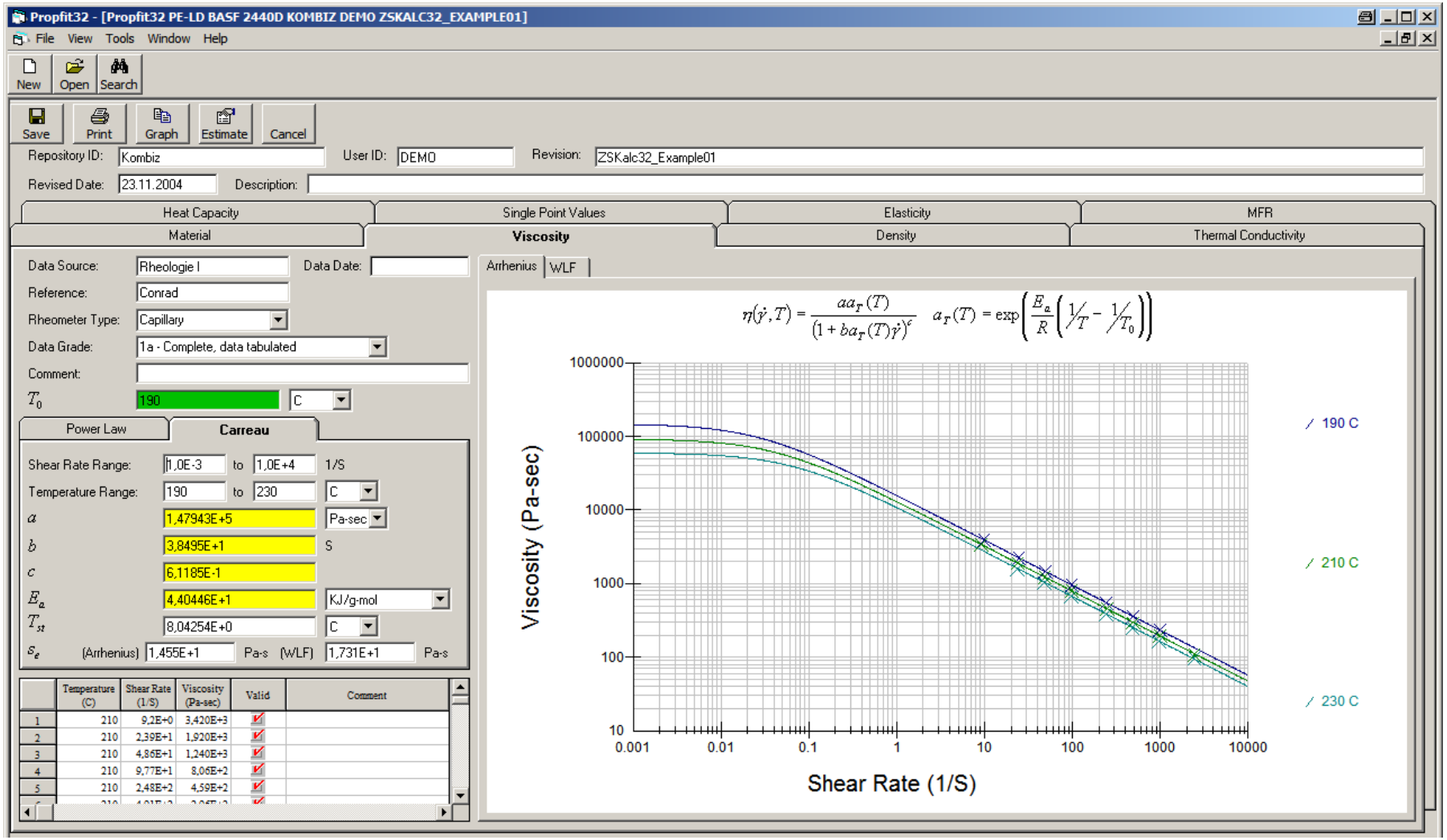
Coperion Data Structure: Material Database PROPFIT



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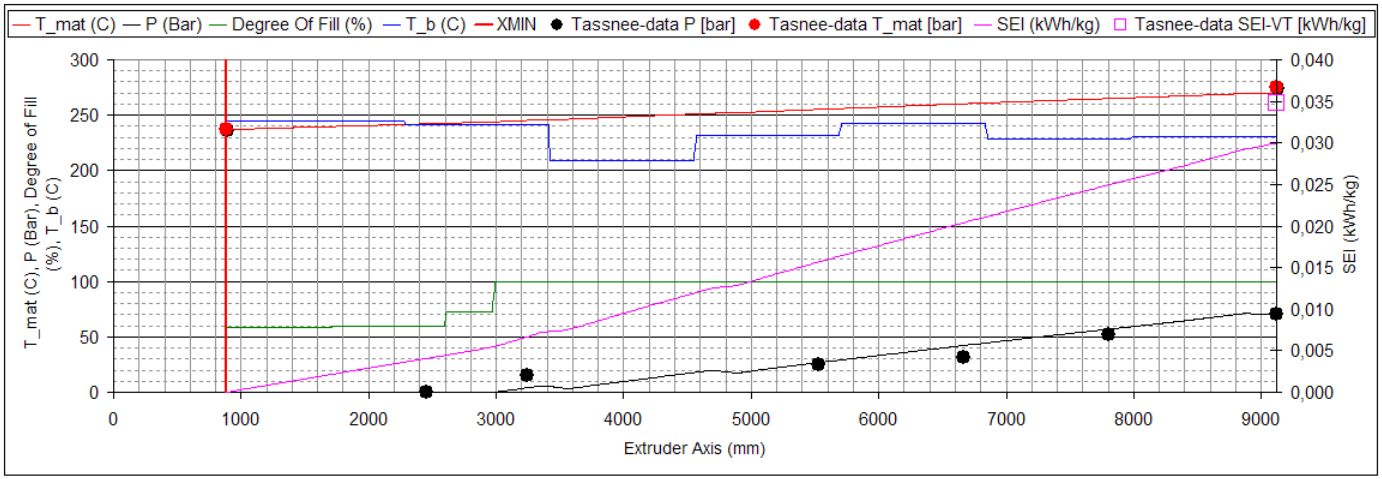
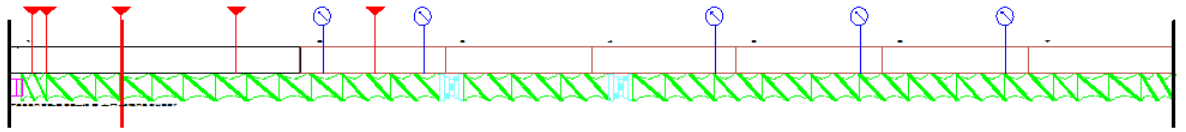
Coperion Example of simulation: ZSK380

46.000 kg/h, 86 rpm, PE-LD, 2440D

Comment	Tasnee: Grade 2420D, Run @ 07:00 / 2009-07-13	
Screw from EXCO32	KOMBIZ:CONRAD-ULRICH:TASSNEE-S02_KB-LH_TRANSD	
		Rebex [bar]
	AV 380/350	4,8 bar
	Flange	0,4 bar
	UG 1000 - GKG	11,8 bar
	UG 1000 - LP	59,5 bar
Boundary Values		76,4 bar
Parameter	**Definition or Value**	safety
DIRECTION of calculation	FORWARD	-8,4 %
PRESSURE [bar]	70,00	<=> 70,0 bar
Screw Speed [RPM]	86	
TEMPERATURE [°C]	237	
XMIN [mm]	880	
Product Flow		
Material Properties	**Position [mm]**	**Feed Rate [kg/hr]**
PE-LD:BASF:2440D:KOMBI	880	45911
Operating Conditions		
Parameter	**Position [mm]**	**Definition or Value**
Barrel Temperature (C)	0	245
Barrel Temperature (C)	2280	241
Barrel Temperature (C)	3420	209
Barrel Temperature (C)	4560	232
Barrel Temperature (C)	5700	243
Barrel Temperature (C)	6840	229
Barrel Temperature (C)	7980	231
h(W/m^2C)	0	0,00
Heat Transfer Model	0	JKR

Input data





Simulation Results

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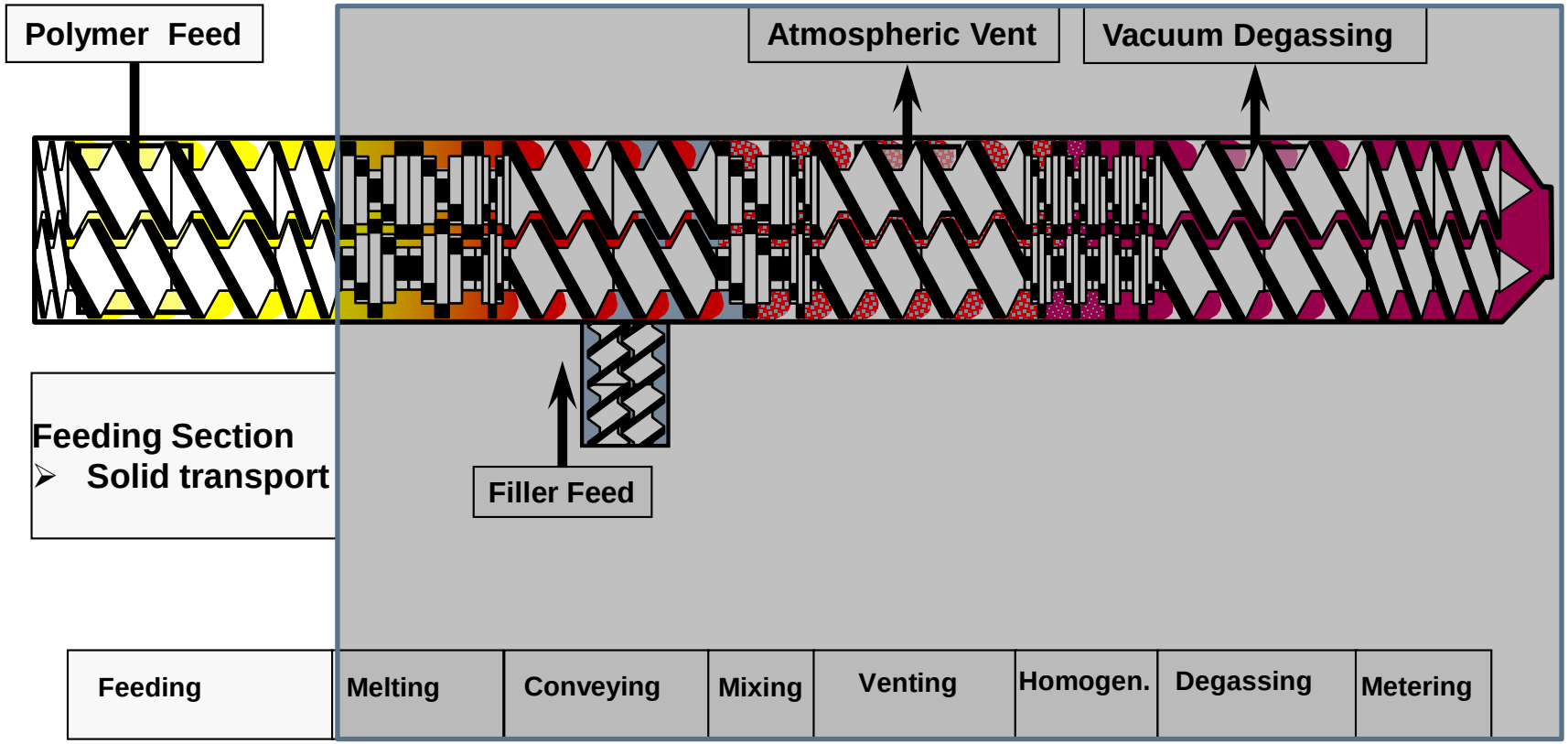
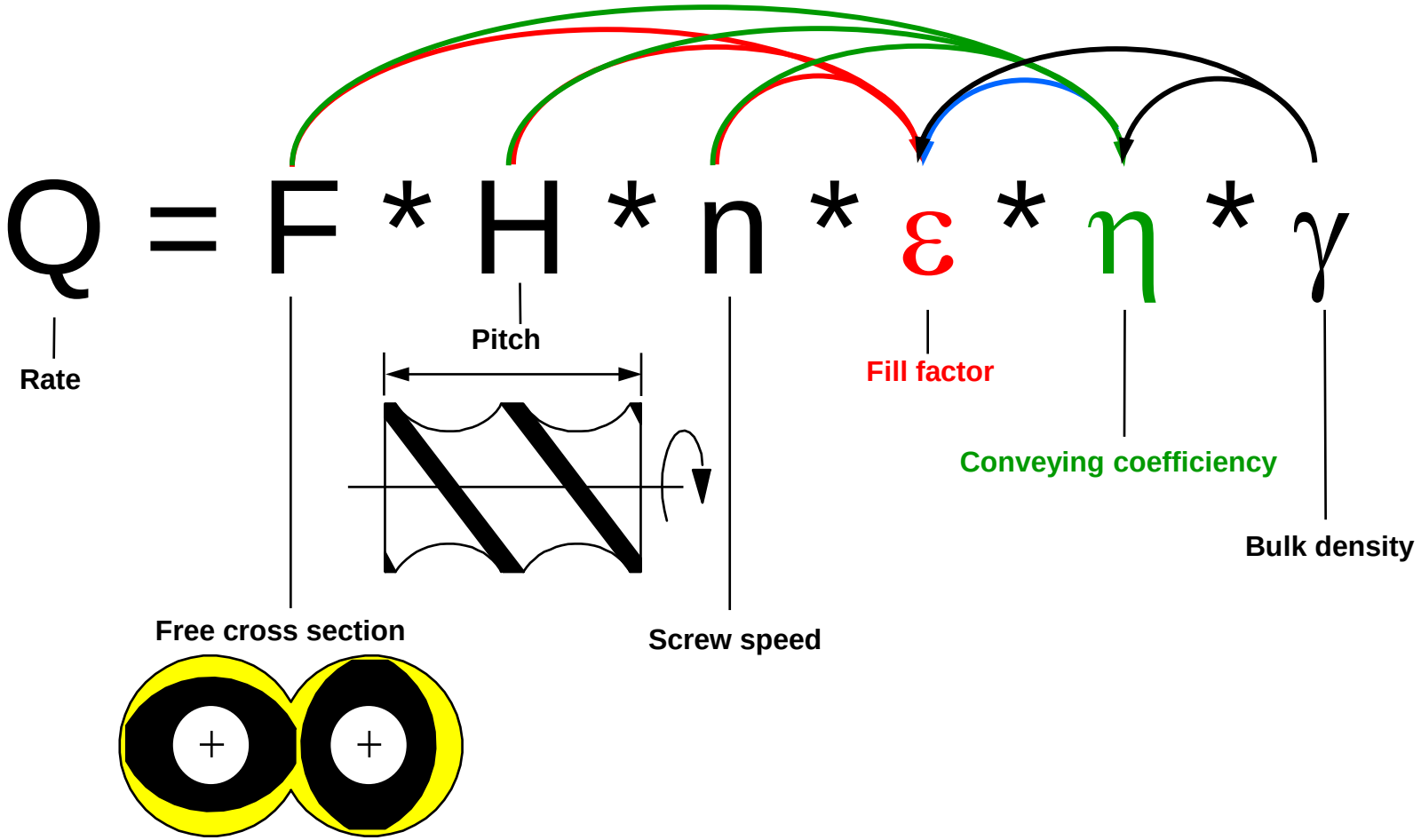
Simulation: Feed Intake Zone



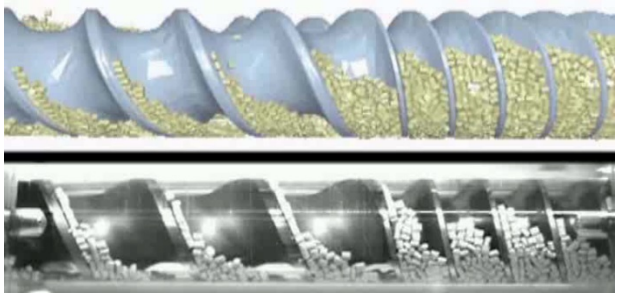
Simulation: Feed Intake Zone

Conveying capacity

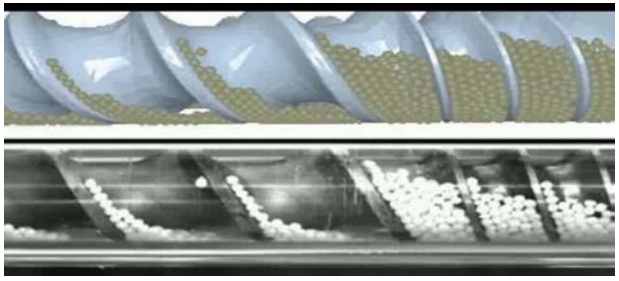


Simulation: Feed Intake Zone

Artificial neural networks



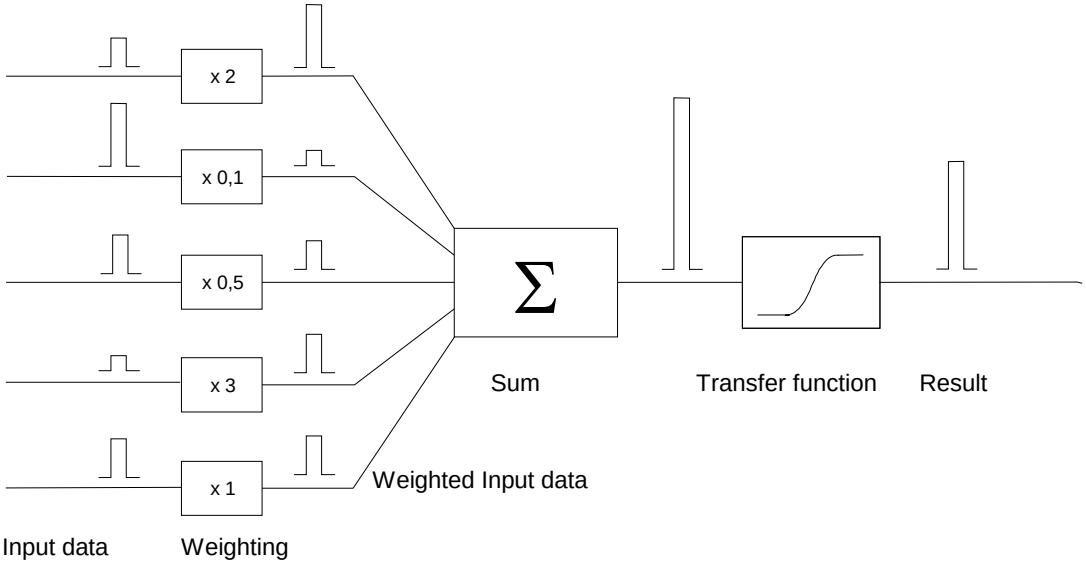
Cylindrical pellets



Spherical pellets

Powder, preblend, etc. ????

- Simulation Model by ATLAN-tec
- Algorithm: Rummelhart – Error – Backpropagation
- Model to be trained by real data
- The more input data, the more accurate the result



Simulation: Feed Intake Zone

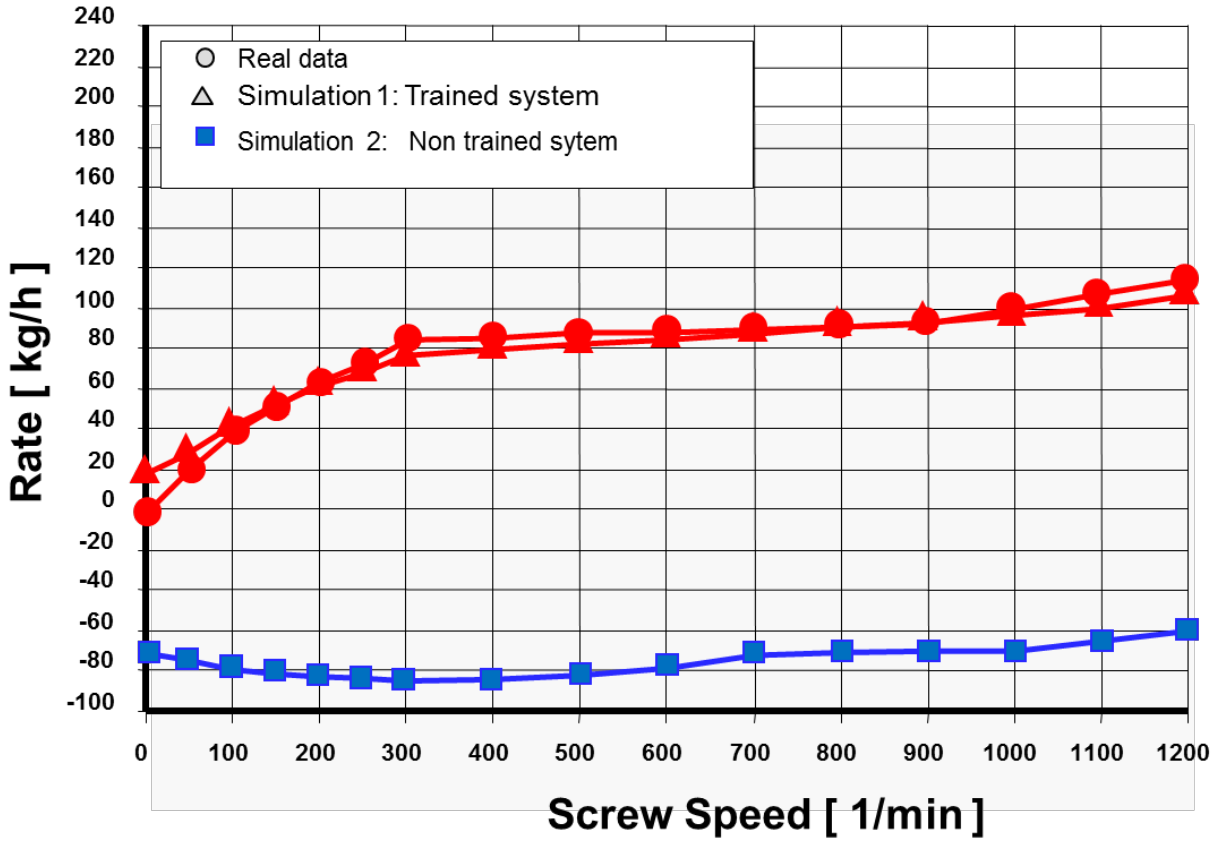
Conveying capacity

Input Data:

- Screw speed
- Bulk density
- Density
- Compression ratio
- Specific surface

Result:

- Feed intake rate



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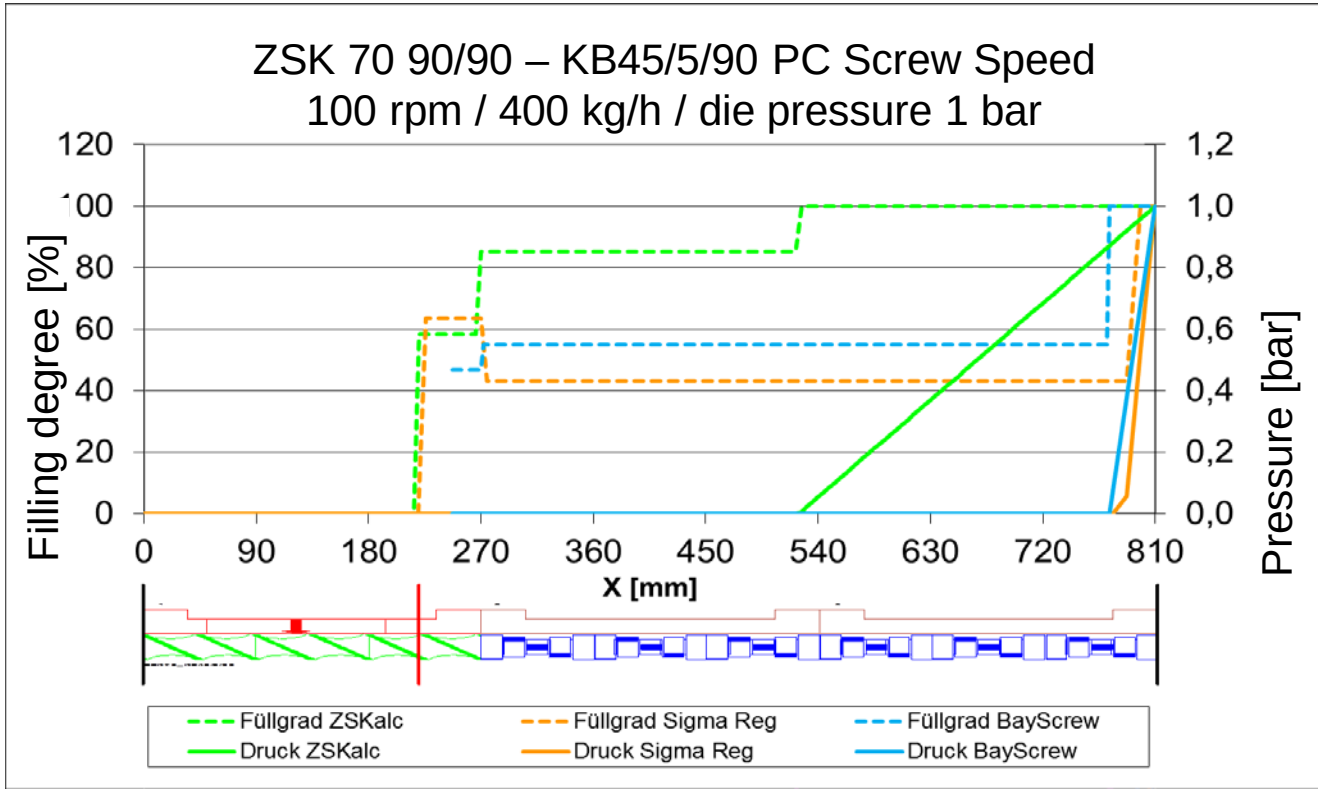
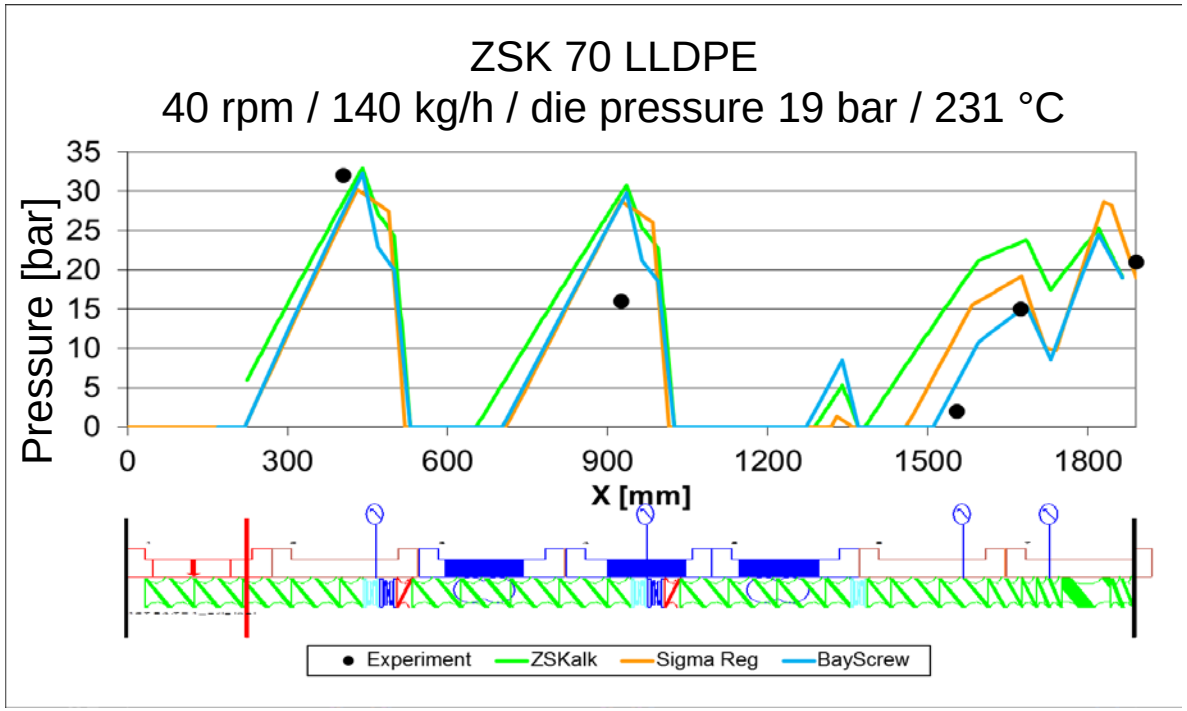
Simulation: Process Sections

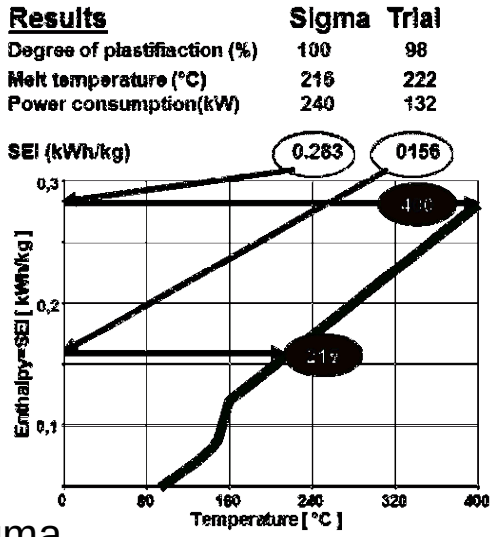


- Experience: Conveying efficiency of kneading elements lower than of conveying elements → degree of fill higher in partially filled section
- ZSKalc, BayScrew: ok - Sigma: not ok
- Absolute degree fo fill depends on density applied

Simulation: Complete Process



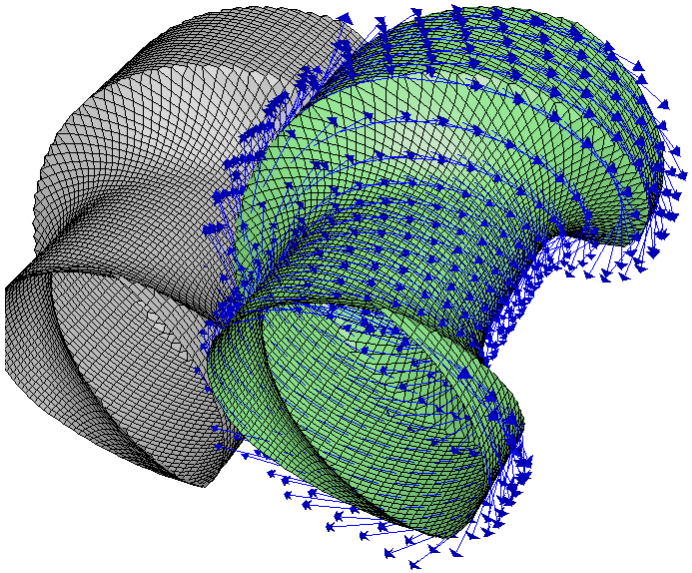
- Simulation results such as SEI [kWh/kg] and melt temperature [°C] have to correlate !

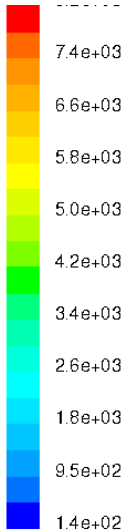


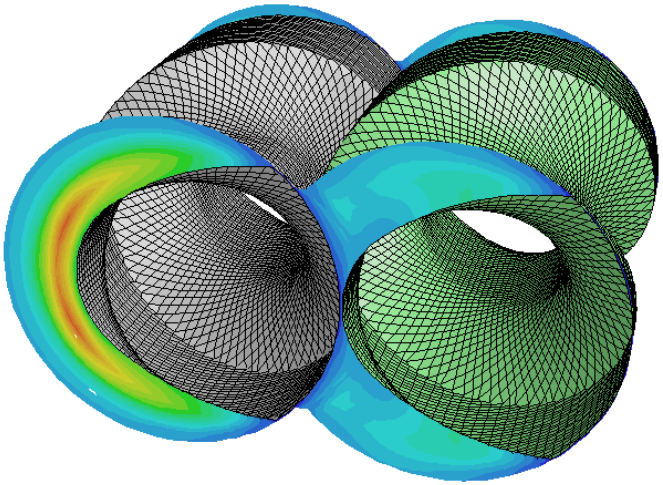
- In general: good results for pressure using ZSKalc, BayScrew and Sigma
- Sigma: 2 of 4 tested models for pressure simulations failed

Numerical Technique to Simulate Various Process Conditions

Delivers local process conditions







Finite Element Method

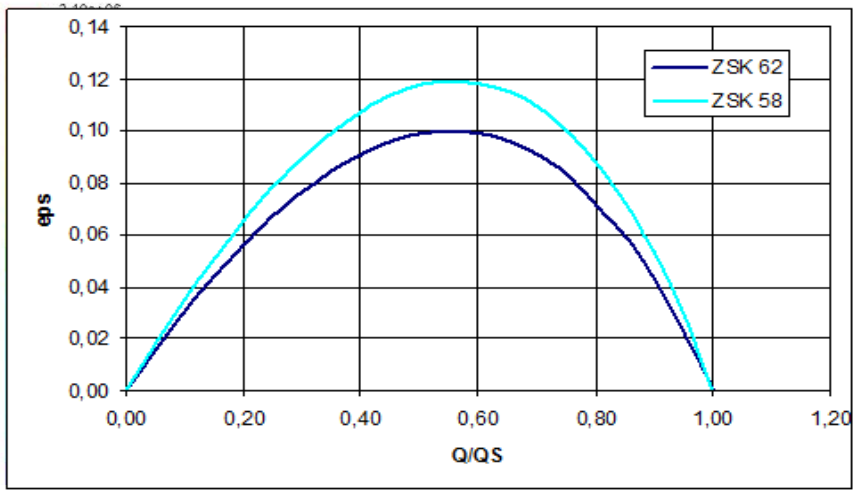
- Transformation of coordinates
- Input: Throughput, pressure difference or throughput
- Unknown clearances / wear can falsify the result

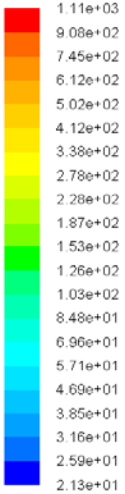
Results

- Good graphical and numerical analysis
- Local distribution of pressure and velocity
- Viscosity / shear rate

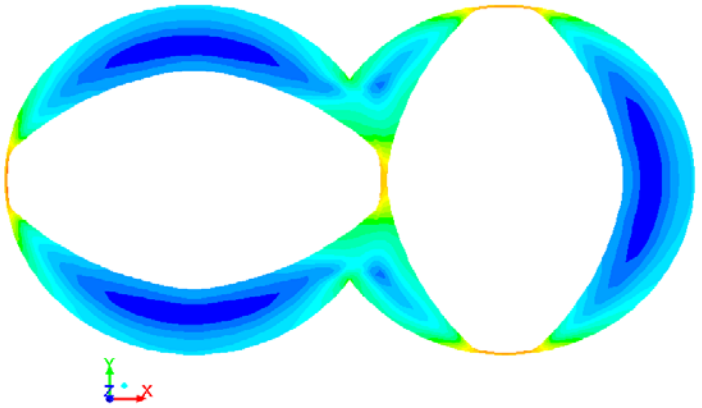
Numerical Technique to Simulate Various Process Conditions

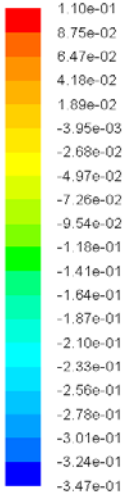
Example – ZSK – Dynamic – relative pressures [Pa]



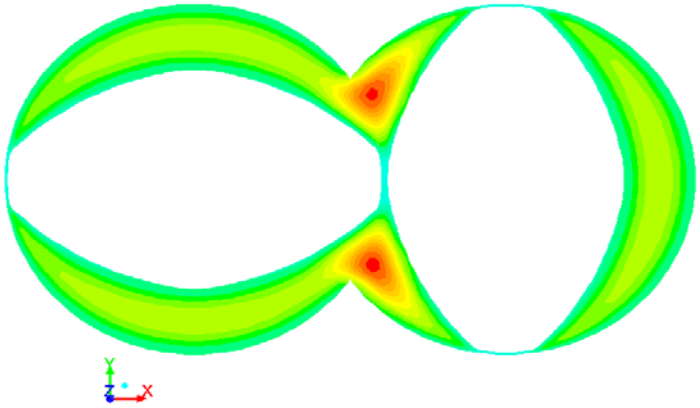


Shear Rate

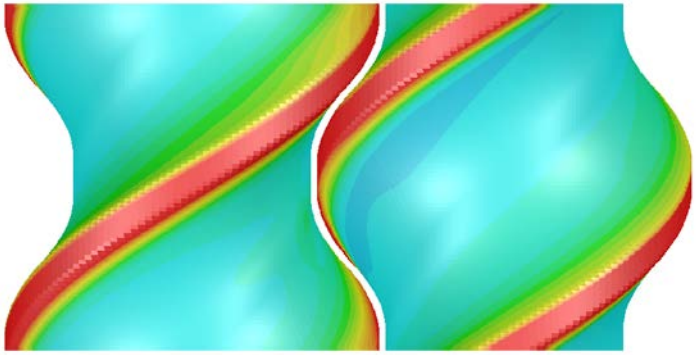




Axial Velocity



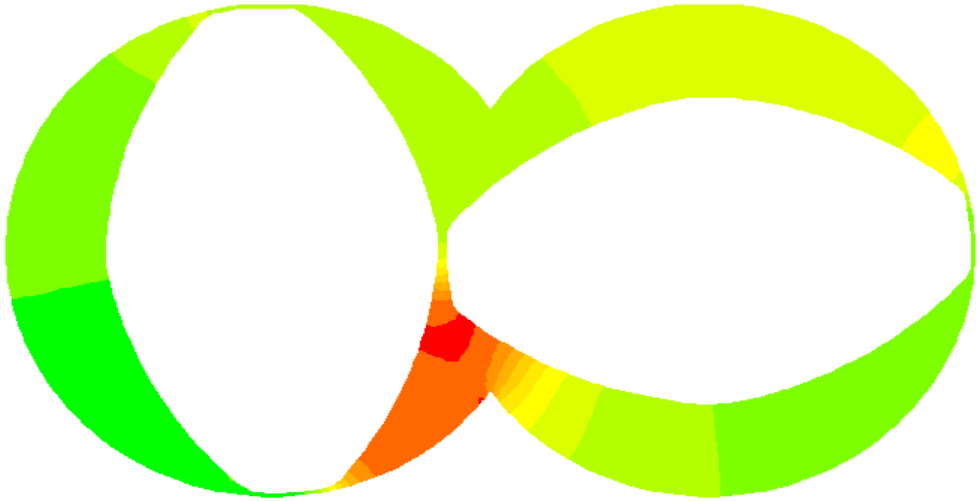
Temperature

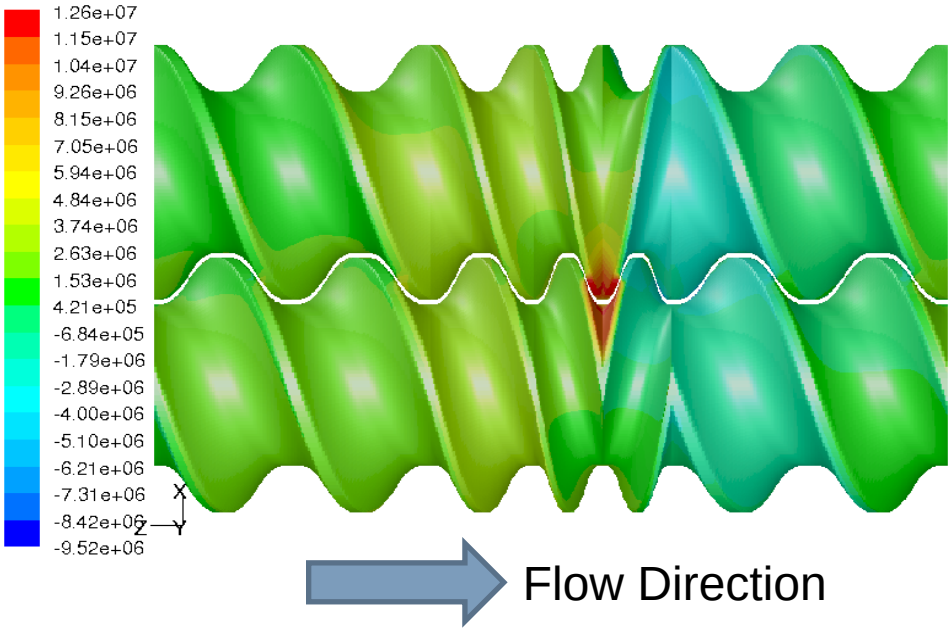


Source: Covestro (Bayer Technology)

Numerical Technique to Simulate Various Process Conditions

Local screw section





- Pressure maximum at intermeshing zone
  - Average pressure: +38 bar
  - Pressure peak: +126 bar
- Transition from right hand to left handed screw elements impacts lower enclosed volume

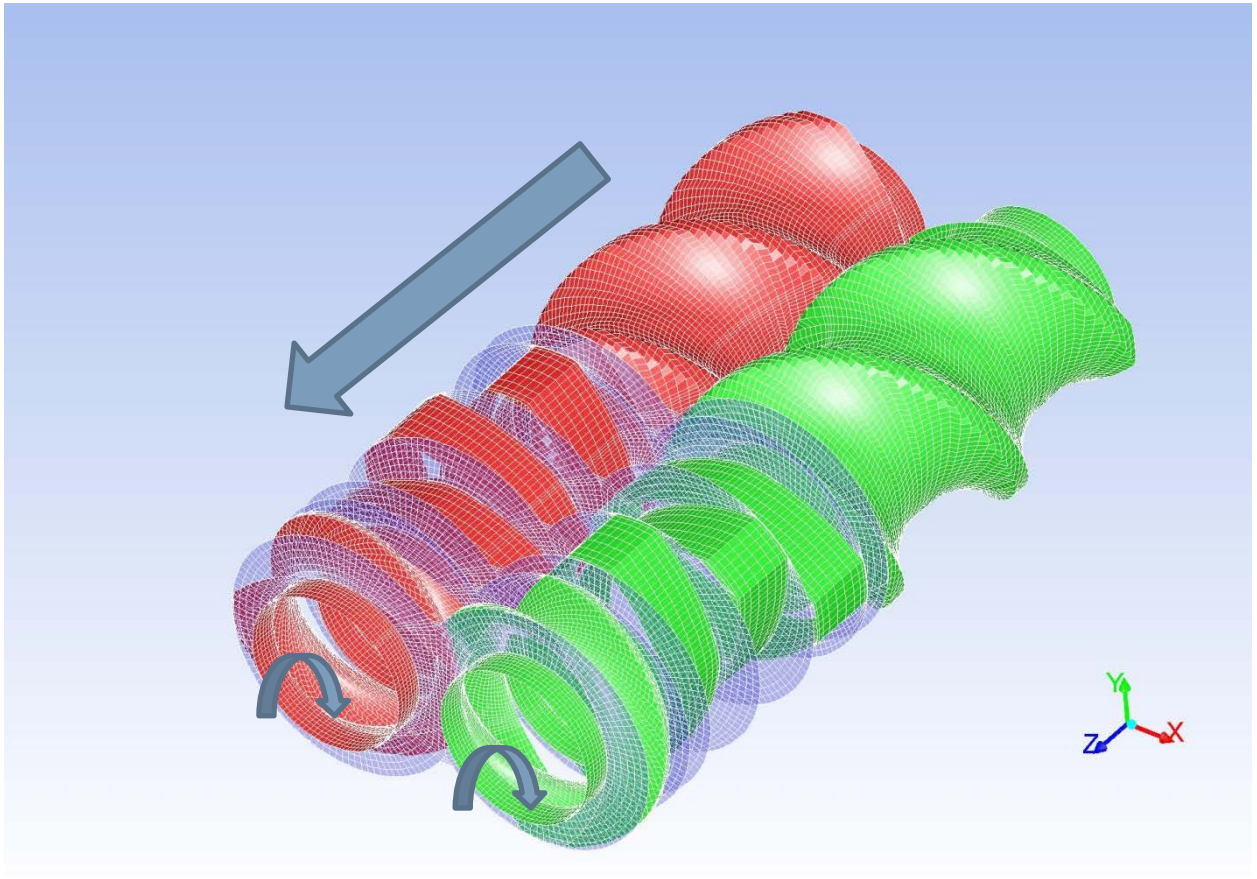
  → polymer melt is forced over small clearances

  → local pressure maximum

Source: Covestro (Bayer Technology)

Numerical Technique to Simulate Various Process Conditions

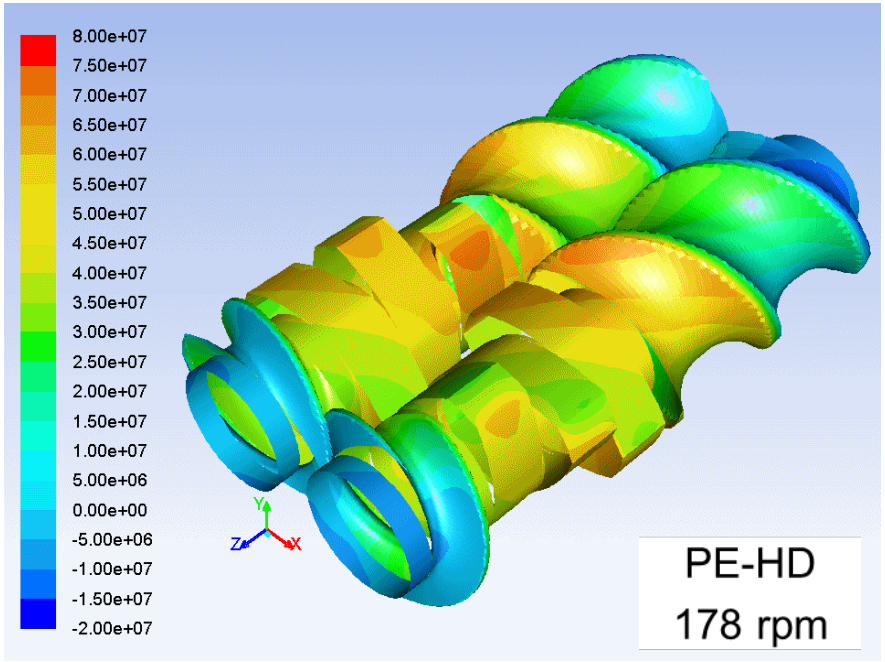
Example – ZSK – Dynamic – relative pressures [Pa]

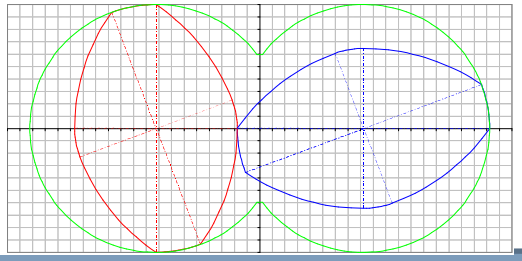


- Ring 5 mm
  - 60/60
  - Ring 5 mm
  - KB 45/3/50
  - Ring 5 mm
  - 20/10 Li
- Ring 5 mm

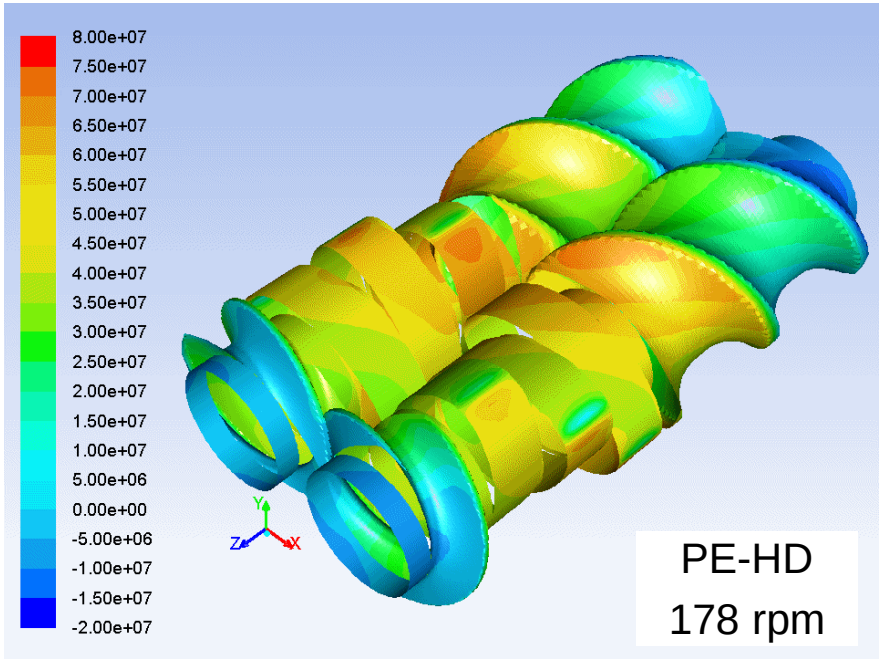
Numerical Technique to Simulate Various Process Conditions

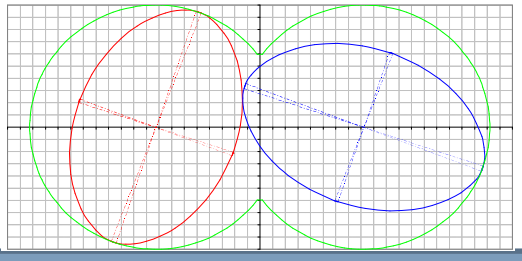
Example – ZSK – Dynamic – relative pressures [Pa]





Standard 2 lobe kneading discs





improved 2 lobe kneading discs

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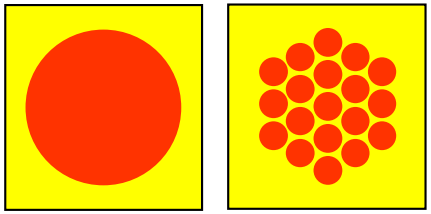
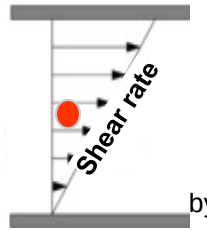
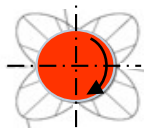
Dispersive and Distributive Mixing

Dispersive mixing = Deagglomeration



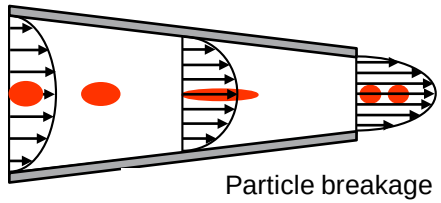
Shear flow





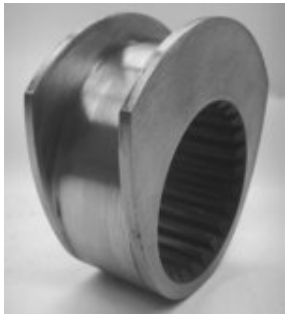
Particle breakage by “centrifugal force”

Elongational flow

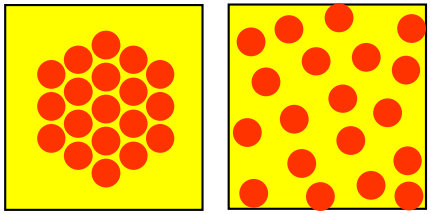


Particle breakage by “overexpansion”

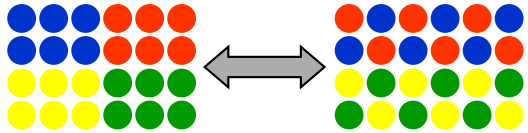
Example: Elongational element



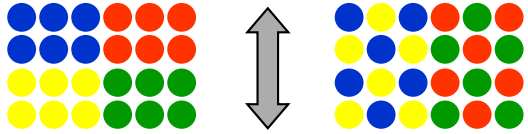
Distributive Mixing = Equal concentration



Longitudinal mixing ⇨ in axial direction



Cross mixing ⇨ vertical to axis

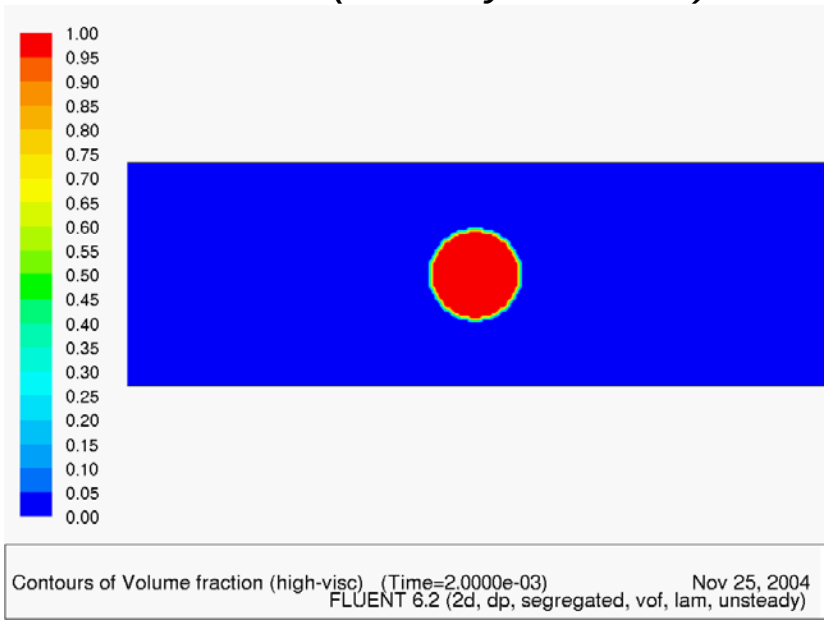


Example: Mixing element

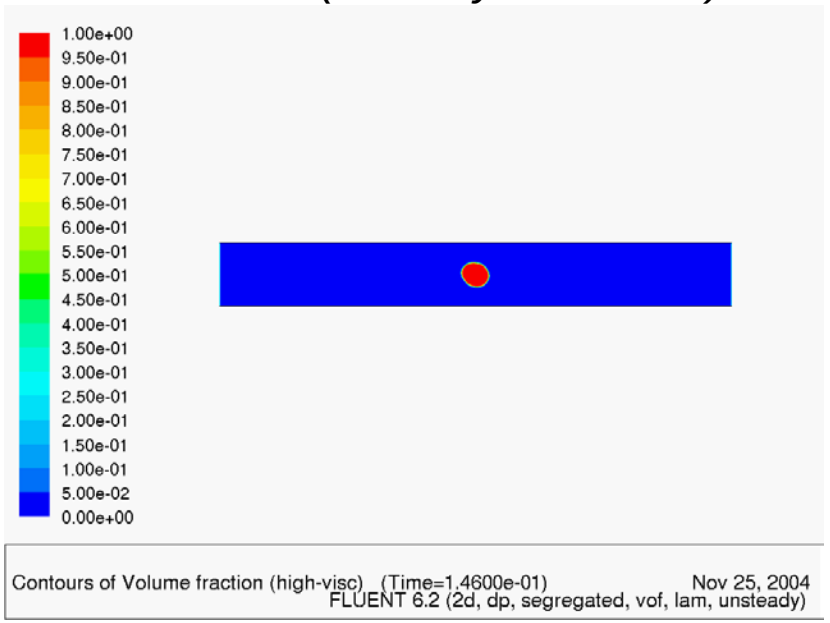
Gel Dispersion in Different Screw Geometries

Dispersion of droplets in shear flow

Shear flow (viscosity ratio 1/10)



Shear flow (viscosity ratio 1/100)

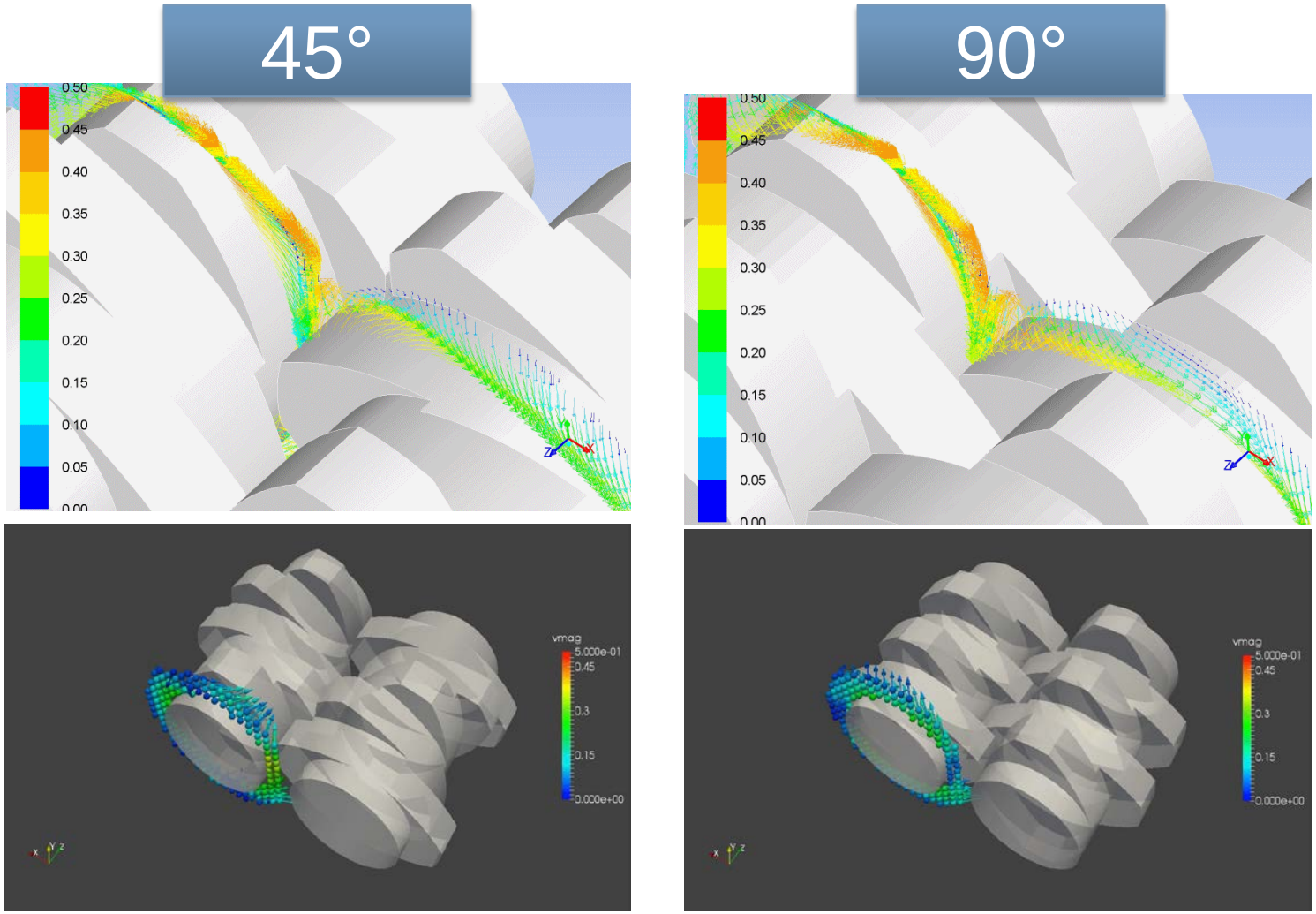


Gel Dispersion in Different Screw Geometries

Velocity profile and particle flow in kneading blocks

Velocity profile in cross section

Particle flow



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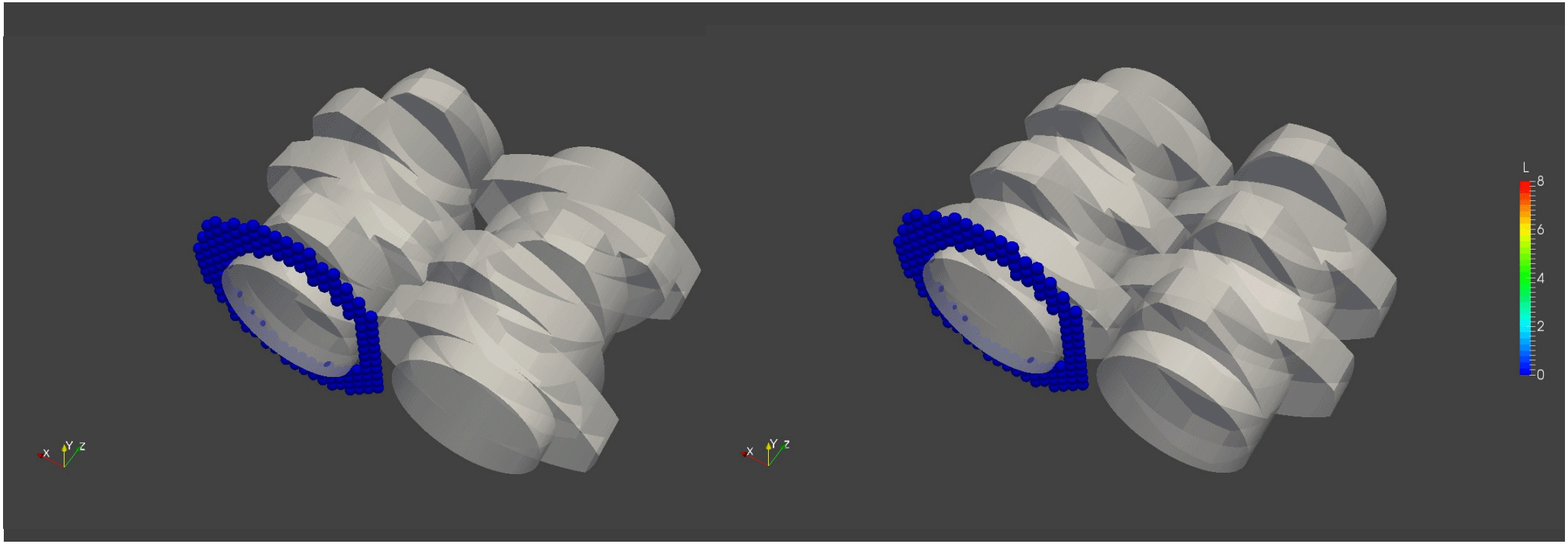
confidence through partnership

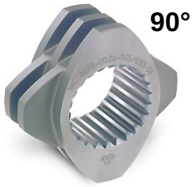
Gel Dispersion in Different Screw Geometries

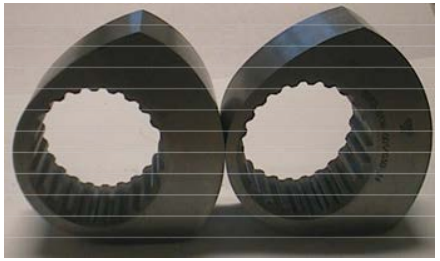
Particle dispersion in kneading blocks

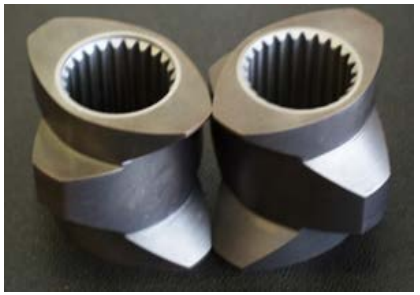


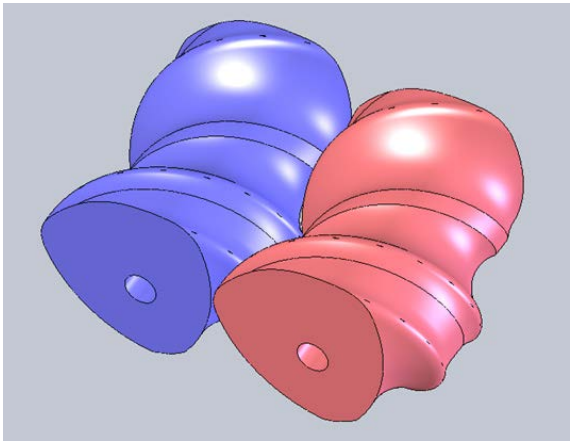
- Color change indicates number of breakdowns

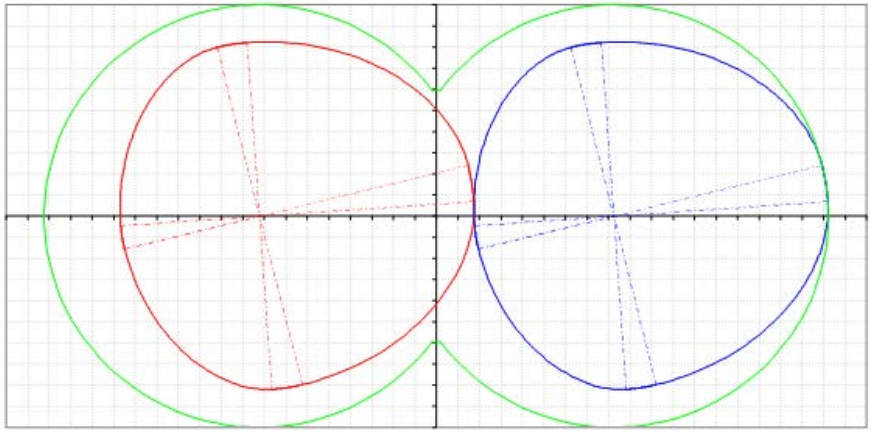
Screw Elements for Dispersive Mixing

Type of element		Mixing effect	Shearing
 X°	 90°		
 X°	 90°		









Summary

- Using 1 D and 3 D modelling can be used to minimize the risk for process design and the scale-up. The result can only be accurate if the required parameters are provided. Finally a comparison with operation or trial data is strongly recommended.
- 3 D modelling delivers local details of a process section whereas 1 D modelling can provide tendencies of process characteristics, e.g. the influence of screw speed on the specific energy input. The optimum screw configuration in the pressure built-up zone can be designed more effectively.
- 3 D modelling will support the design and understanding the function of new screw elements.

Thank you very much for your attention.