# SIMULATION OF CO-ROTATING FULLY INTERMESHING TWIN-SCREW COMPOUNDING EXTRUDERS: ALTERNATIVES FOR PROCESS DESIGN

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## Abstract

The co-rotating fully intermeshing twin-screw extruder is the primary production unit for compounding polymer based materials. It also has had a long term presence in processing material in the chemical and food industry and more recently in pharmaceuticals. The layout of a co-rotating twin-screw compounder for a specific processing task is primarily based on 1) the experience of the process development engineer, and 2) tests run on a lab-scale unit. Additionally, scale-up to a much larger extruder is very often required as part of the development process. Traditionally this scale up has been based on experience and classical scale-up rules.

In addition to experience and lab tests, good simulation software can help guide the development engineer in the design of initial compounding extruder configuration as well as scale-up to a commercial unit. The overall objective being to minimize risk (cost). Know-how based on experience, trials in the laboratory, production and simulation software are the preferred combination for the layout of an extrusion process.

## Introduction

It has been a long standing industry goal to be able to simulate the entire compounding process from feed intake, through plastification and downstream mixing zones until the pressure built-up zone. Nevertheless, not all process sections can be described sufficiently by simulation software. This is due to several reasons such as high complexity of the computation as well as missing feedstock and product characteristic data. This later point is particularly relevant when it comes to polymer compounds containing different components such as additives, fillers, etc. However, in spite of shortcomings, 1 D and 3 D modeling is used to describe the process and can support the process engineer for the layout and scale-up of a compounding process.

## Background

Co-rotating and fully intermeshing twin screw extruders, with one screw wiping the other, and both wiping the 8–shaped barrel inside, are defined by two characteristic dimensions: diameter ratio $D_o/D_i$ and specific torque $Md/a^3$, Figure 1.

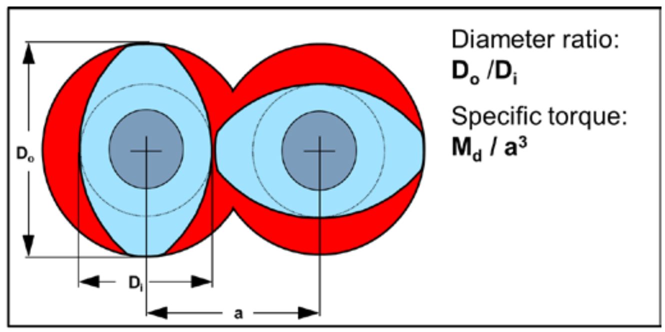


Figure 1: Character dimensions of Twin-screw Extruder

Figure 2 shows a typical set-up for compounding engineering polymers. Materials contained in the formulation are fed at precisely defined locations along the length of the process section. During the compounding process the blended ingredients pass through each of the different unit operations along the length of the extruder.

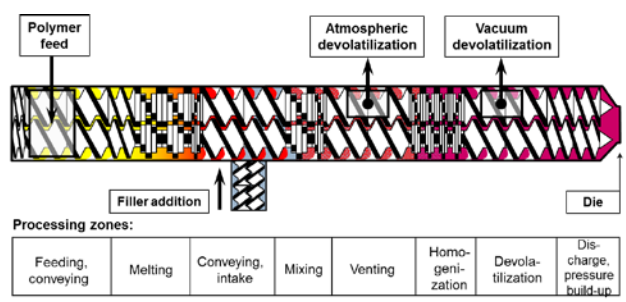


Figure 2: Process section for Compounding

For each new compounding process, the feed sequencing and unit operation need to be defined. In addition to experience and lab tests, 1 D and 3 D modeling programs are available for use to describe the process and can support the process engineer for the layout and scale-up of a compounding process. Comparison of the simulation results to real process data is strongly recommended.

One of the issues related to using simulation software is that exact conditions required to start the simulation are difficult to describe at a specific location. Therefore each unit operation has to be described separately: Feeding section, plastification, mixing, degassing and pressure built-up zone. Suitable characteristic data of all raw materials as well as of the final polymer melt are essential parameters required to use simulation software. The most important data are 1) melt density, 2) heat transfer coefficient as a function of temperature, and 3) the viscosity curve over a shear rate range from 1 1/s to 1000 1/s. The geometrical data of the co-rotating twin screw compounder is given by the individual machine supplier.

## Simulation: 1D

For 1 D modeling the two most widely used commercial simulation software packages are Sigma and Ludovic. Coperion developed its own proprietary software in the late 1970s called ZSKalc. These software packages are mainly used to 1) simulate temperature profile, 2) filling degree, and 3) pressure built-up capability along the length of the process section.

The Coperion ZSKalc simulation software hierarchy is illustrated in Figure 3. Input data required are 1) machine configuration (barrels and screw), 2) process parameter (screw speed, material feed rate, material feed temperature, material pressure at the screw tip, barrel temperatures), and 3) material properties. The resultant output, material temperature, material pressure, degree of fill and specific energy input is calculated by using both analytical and numerical methods.

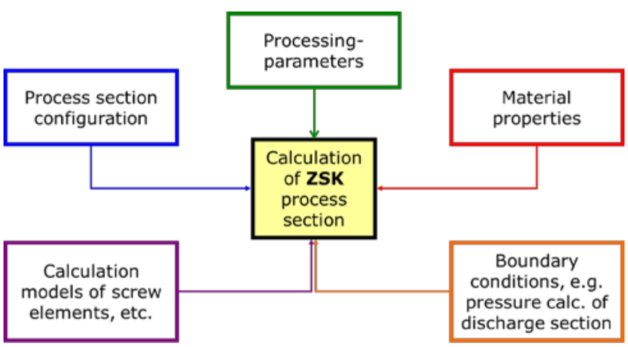


Figure 3: Data structure for ZSK calculations

## Simulation: 3D

Using 3D-Modeling (finite element method) as a numerical technique is also used to simulate various process conditions. It delivers local details of a compounding process as shown in Figure 4. The pressure distribution is depicted by gradation of colors from high pressure (orange) to low pressure (blue). The pressure drop downstream of the reverse conveying screw element can be clearly seen as well as the pressure peak in the intermeshing zone.

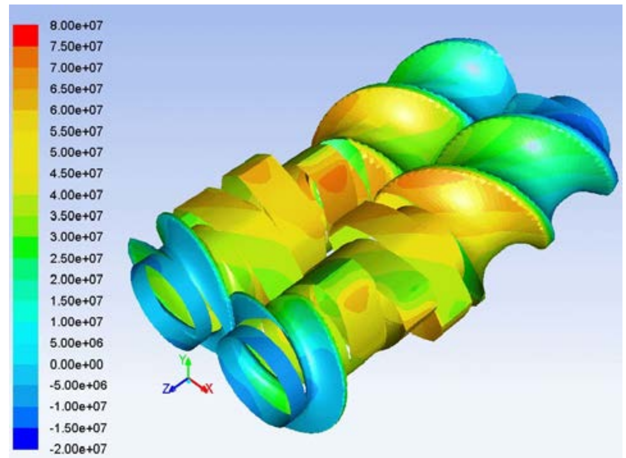


Figure 4: FEM simulation of screw element sequence

For 3 D modeling commercial and non-commercial programs are available, e.g. CFX, Fluent, OpenFoam, Star CCM, Fidap, Polyflow, and XimeX. They are mainly used to simulate local process conditions, even down to specific areas within an individual screw element.

## Simulation: 1D vs. 3D

The easiest way to describe the difference between 1D and 3D simulation is as follows: 1D provides a birds-eye view of the process, but can't zoom in on local details, while 3D can provide very detailed information of the immediate surroundings, but not what is happening in the neighborhood.

Bierdel and Lechner [1] provided some excellent graphics to illustrate this difference. Figure 5 shows a sample screw sequence, a series of conveying elements followed by a restrictive element.

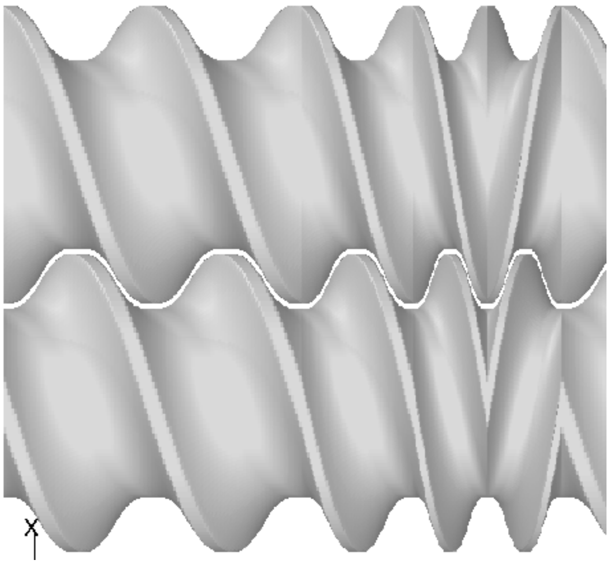

Figure 5: Screw configuration sequence.

Based on the screw configuration in Figure 5, Figure 6 depicts the overall pressure drop across the restrictive element as simulated by a 1D program. On the other hand, Figure 7 shows the 3D simulation that provides localized details of the pressure drop. As before, red orange indicates high pressure.

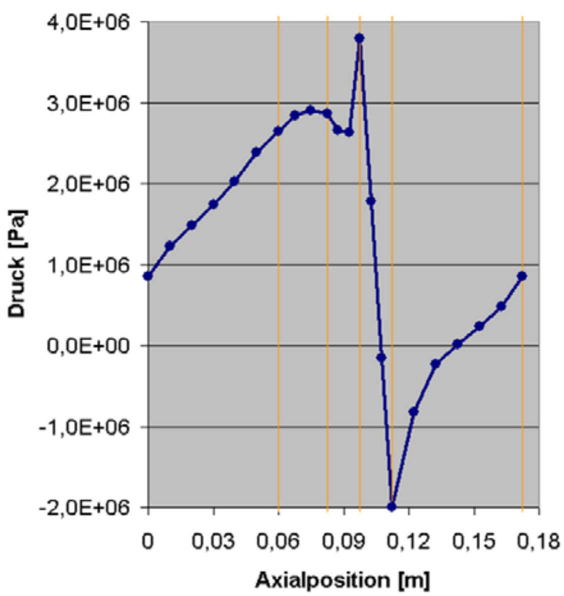


Figure 6: Pressure drop value across restrictive elements

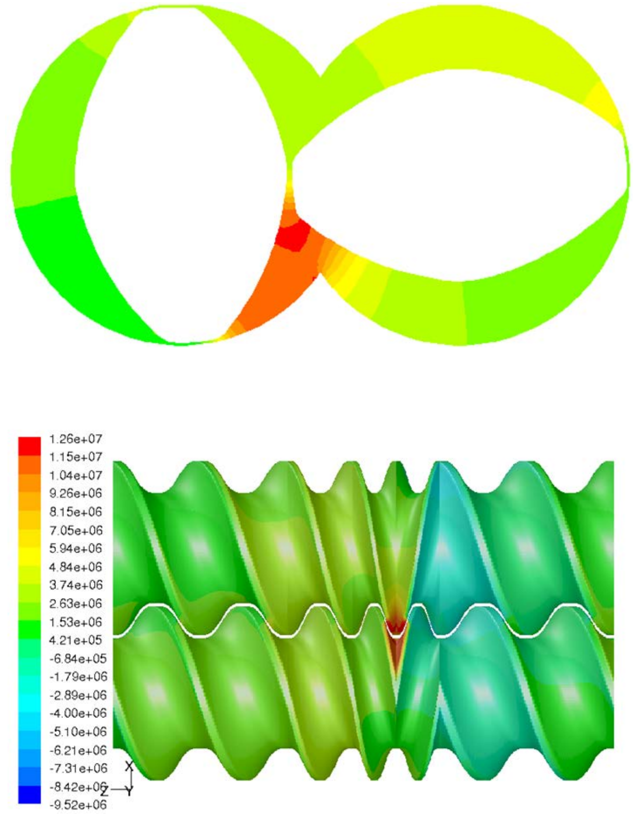


Figure 7: Pressure drop details at restrictive element.

## Simulation: Feed Intake Zone

Powder conveying capacity of an extruder depends on the properties of raw materials, the screw design and process conditions. Even if one has good characterization of the raw materials such as solid density, particle size distribution, porosity, etc., feed intake behavior cannot be calculated sufficiently without data from a lab trial or production run.

The equation in Figure 8 shows that the feed intake and conveying rate inside of the process section are a function of many variables and therefore subject to fluctuation. For example, Figure 9 illustrates the change in bulk density for a powder/granule feed stock in a lab size extruder between the feed intake section to the melting zone. The change depends on the process conditions (such as speed) and geometric data (screw pitch) of the given machine system.

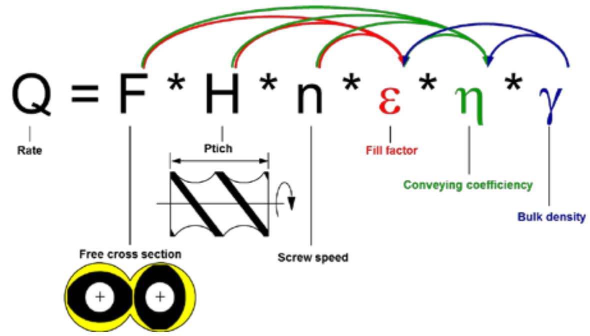


Figure 8: Conveying capacity for solids

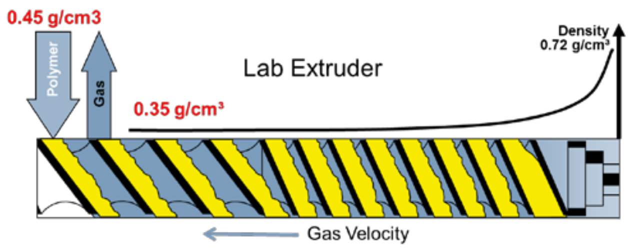


Figure 9: Powder feedstock conveying in lab compounder.

In general, for pellets feed intake limitations do not have to be considered. For powders the feed intake may become critical if the medium particle size d50 falls below 150 µm. The feed intake depends strongly also on the screw configuration including the design of the melting zone. A screw pitch in the feeding area of 1.7 D to 2.0 D is recommended as well as feed intake zone minimum length of 4 D.

Use of neural networks was investigated as a way to model solids conveying better [2]. The technology has shown good results if the system is "trained". This means that actual process data has to be incorporated as an informational foundation and can then be used to simulate the process. This technique can be used to verify the scale-up from a lab test to a larger machine.

Figure 10 shows results from a ZSK 40 test where PP powder and 30% talc are fed into the main feed at Barrel 1. Simulation 1 which used a "trained" system, i.e. based on real process data input from a lab trial, shows very good results. These results are well aligned with the actual data compared to the trial data. Without real process data, the blue line shows definitely a large deviation from the reality.

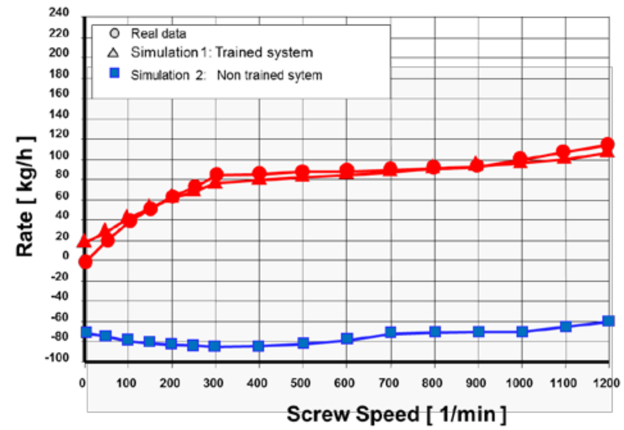


Figure 10: Simulation of Feed Intake

## Simulation: Melting and Homogenization of Polymers

As shown in Figure 11, polymer entering the melting zone undergoes a phase change from solid to the melt. Still today, this phase change has not been accurately calculated by simulation software. Therefore it is important that the development engineer knows basic material properties such as melting point, viscosity, and enthalpy curves. From this data, the minimum specific energy input required can be defined and based on this the melting zone can be designed.

At the end of the melting zone the polymer should be completely molten. This strongly depends on the screw design and the process conditions. Figure 12 shows the melt quality variation of a polyethylene having experienced varying process conditions. Polymer Sample 1 shows a complete molten product at the end of the melting zone whereas Sample 4 still contains unmolten polymer as the screw speed was too low.

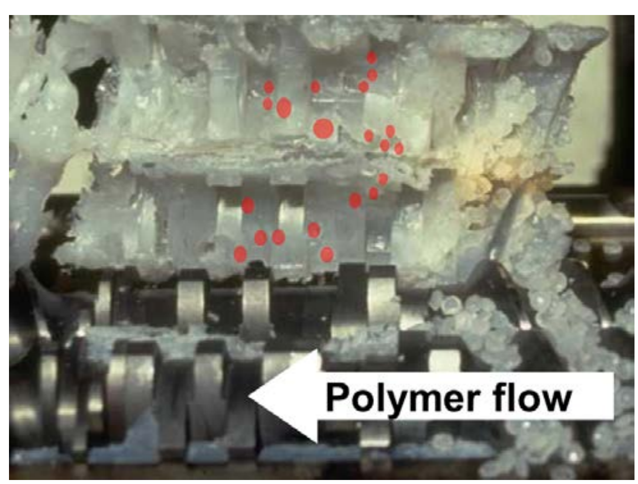


Figure 11: Melting zone showing transformation of polymer


Figure 12: Melting performance

An example of the difficulty a simulation program can have to accurately predict the melting section performance of the twin-screw compounding process, as well as the misleading information that can be provided is shown in Figure 13 a-d. The basis for this inaccuracy can be two-fold. First, the algorithm for polymer melting may be inadequate. The various calculations based on the influence of extruder operating conditions and material parameters may not have the correct balance. In addition to the model algorithm, the correct input data is critical. While it is relatively easy to provide extruder operating data, quality material data is less readily available. For example, the initial particle size of the polymer will have an influence on melting. Figure 10 depicts the melting for pellets, but many compounding lines, especially for polyolefins, process powder which flows significantly different from pellets. One can measure solids flow, heat transfer, coefficient of friction etc. in the lab, but under actual dynamic conditions, there are innumerable uncontrollable influences such as fluidization that impact actual heat transfer, coefficient of friction, etc.

The Figure 13 sequence depicts a comparison between data derived for melting HDPE based on a simulation and an actual ZSK 92 run. The percent melting of HDPE on the ZSK 92, as well as the melt temperature are almost identical between the lab extruder run versus simulation software. However, the calculated specific energy is much higher compared to the trial and does not fit with respect to the HDPE enthalpy curve. A simulated specific energy of 0.283 kWh/kg would lead to a melt temperature of almost 400°C whereas the trial as well as the simulation shows a melt temperature of 216°C and 222°C, respectively. Additionally, the model shows that the material is approximately 50% melted at the end of the first kneading block section, but is then fully melted by screw conveying elements prior to entering the second kneading block section. The actual test data indicated some unmelt remained at discharge from the extruder.

In this example a reality check of comparing predicted temperature versus specific energy against the enthalpy curve would identify that the melt temperature and the specific energy don't agree and that one or potentially both are incorrect. Without experimental data as an anchor point it is, in most cases, difficult to know which one is closest to being correct.

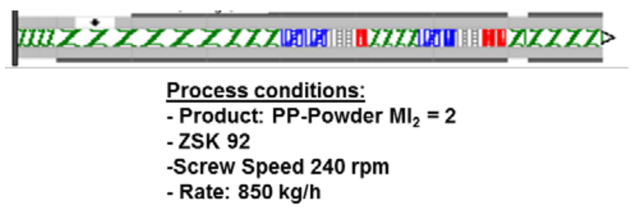


Figure 13a: Example screw configuration

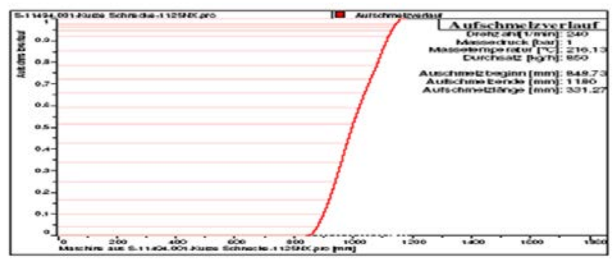


Figure 13b: Simulation of melting

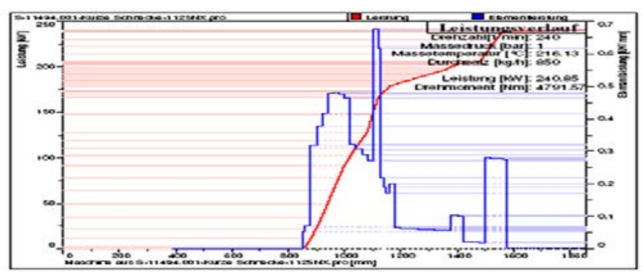


Figure 13c: Simulation of melt temp and power consumption

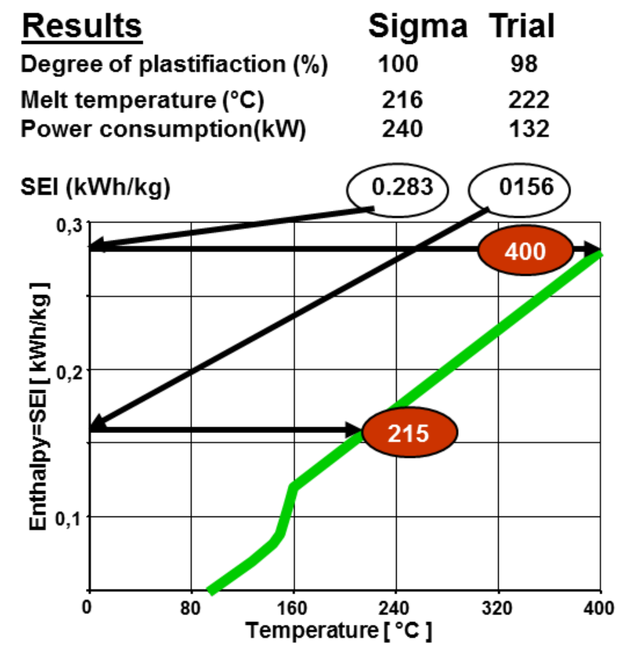


Figure 13d: Comparison of results, simulation vs. data.

## Simulation: Pressure Buildup Zone

Once the polymer has been melted and mixed, simulations can perform very well if appropriate as well as accurate data is provided. Figure 14 illustrates the sub-programs that comprise ZSKalc simulation software and provide the required input parameters. These are used in consort to calculate the process:

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- Exco for the screw configuration
- Propfit for the material data
- Rebex for the discharge pressure
- Geometry data of the machine

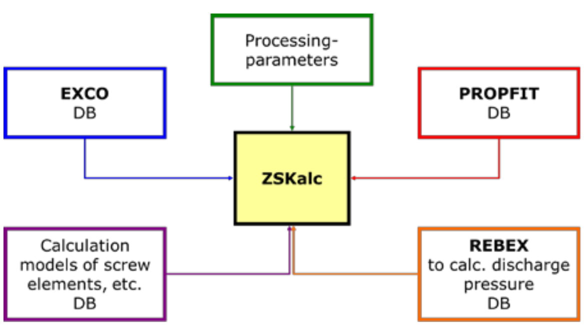


Figure 14: Coperion data structure for ZSK calculations

As an example for beneficial program utilization, back-up length and the temperature increase in the process section can be simulated very precisely if well-defined material properties are provided. This simulation software allows one to calculate the optimum screw pitch for the pressure built-up which will minimize the back-up length and the specific energy input.

Figure 15 depicts the calculation of different parameters using ZSKalc for scale up to a ZSK 380 running 46 tonnes/hr. of melt fed LDPE.

Red – Material Temperature
Blue – Barrel Temperature
Black – Pressure
Pink – Specific Mechanical Energy
Colored Circles & Square – Run data

As can been seen from the results in Figure 10, the predicted melt temperature, discharge pressure and specific mechanical energy are virtually spot on.

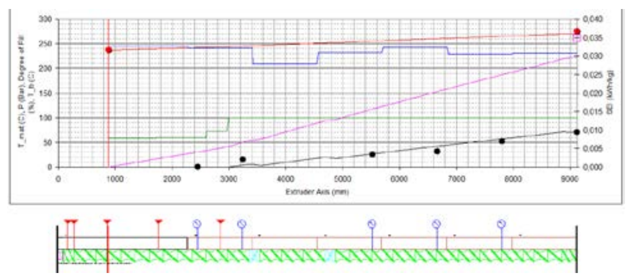

Figure 15: Simulation with ZSKalc

## 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 process characteristic trends, e.g. the influence of screw speed on the specific energy input. The screw configuration in the pressure build-up zone can be designed more effectively.

## References

1. M. Bierdel, F. Lechner, Scale-up mit Simulationsprogrammen: Vergleigh von Simultion mit Realitaet, VDI Tagung 2013
2. U. Feuerlein, Verbesserung von Compoundiermaschinen durch Prognose der Einzugsgrenzen ueber Analytische Pulverkennwerte, Diplomarbeit – Berufsakademie Stuttgart, 2004