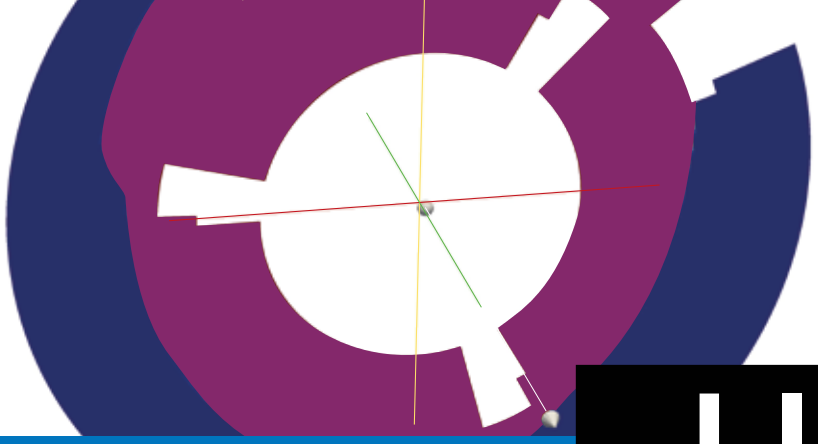


LIST

Kneading - Mixing - Drying

Reliable scaling of production plants using process simulation

How we can assist you with this challenge.

Case Study | May 2020

Case Study

From our technology centre

How can complex processes with highly viscous liquids be simulated?

Processes involving the handling of highly viscous liquids pose major challenges for our customers. The research on the specific behaviour of these substances is still quite scant in conventional process technology. As a result, there are significant risks in implementing such processes.

LIST can support you with this. After focusing our efforts on the mixing and kneading of highly viscous substances for many years, we are now specialists in this area.
We have found that simulating the kneading process is often helpful, even necessary, in order to improve an existing process or to calculate the requirements for a new process.
To achieve this, it must first be possible to describe the process in mathematical models. As a pioneer in this field, we have been developing our own models for multi-phase mixing processes for some time now.

In developing this process, we are able to continuously improve our product range and adapt it to the needs of our customers. It goes without saying that our kneaders should correspond to your processes and not the other way around.
We test demanding kneading processes for our customers at our technical centre in Arisdorf near Basel (Switzerland). This helps us collate data which we then use to develop new models. We reference literature and databases to compile data on general substances or complement them with empirical research from our laboratory.

> The pilot tests typically provide data on evaporation rates, heat exchange coefficients or reaction rates.

> The data drawn from literature and databases consist of specific enthalpy, density or evaporation enthalpy of solvents or thermodynamic balances.

A lot of our customers want to increase their production output and, in order to achieve this, they need larger kneading reactors. To determine exactly what size they need, we test kneaders of different sizes. We then use the data from these tests to simulate the process for a new kneader and carry out a scale-up.

This is only possible if we have gained sufficient data in the experiment to be able to establish reliable mass and energy balance equations. The model can be used more specifically to calculate how the volume of the kneader affects its output.

“ Our kneaders should correspond to your requirements in the best way possible, not the other way around.”

Karsten Güdemann CEO LIST Technology, chartered engineer

Test kneader in our laboratory and scale-up magnified to thousands of times

LIST Technology *Test Center*

Scale-up or simulation of the process?

If a process can be easily calculated with an analytical, mathematical transformation, this would be defined as a scale-up, not a simulation of the process.
A scale-up can be calculated with simple programs such as MS Excel. By contrast, complex mathematical or numerical tools are required to calculate the simulation of the process.

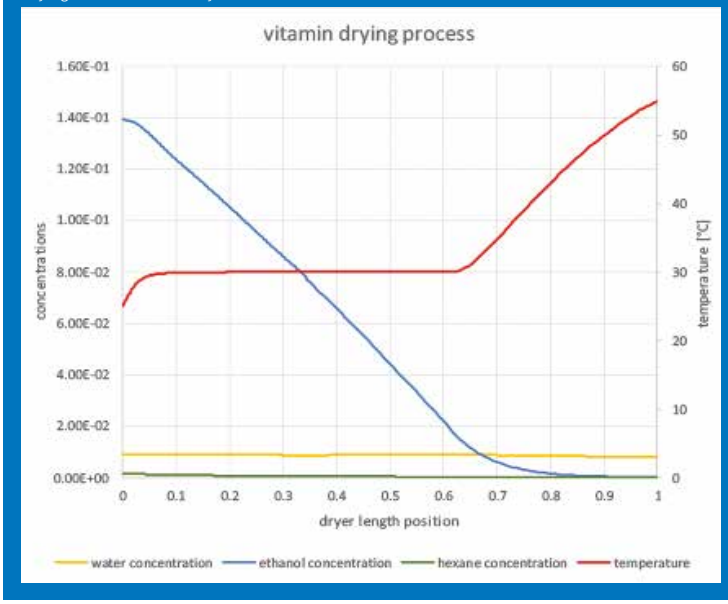
It is therefore customary to describe mass and energy balances with a system of differential equations, and numerical integration is required to solve this system of equations. Properties such as thermodynamic equilibrium are only implicit, i.e. not analytical, so we need to use iterative solvers.

> We use Mathcad software for these calculations, as it has its own functional methods for numerical integration.

> However, for some unknown reason, this software is only able to deal with numerical iterations to a limited extent.

We have therefore developed our own procedures based on the secant method.

Drying rate curve of a crystalline vitamin



Two examples of applications for process simulation

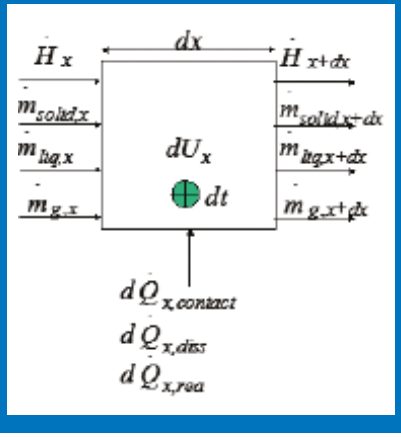
Degas and dry solutions

In order to extract plastic from a polymer solution, the gas must first be removed from the solution.
The concentration of the plastic increases continuously until all the solvent has evaporated in the kneading process.
We can simulate and predict these kinds of drying processes:

It describes the individual components of the solution, e.g. a solvent and its polymer content, in their liquid and gaseous state.
Since the process in the kneader is continuous, the time factor is not relevant for this calculation. The conditions of the material flow, which we enter in the kneader, are also known and constant. Using integration, we can now calculate how much solvent has already evaporated and where over the length of the machine. The material flows of the phases are entered into the equilibrium condition at the phase boundary and the dissipation of the mechanical energy of the stirrer and contact heat are entered into the energy equation.
This differential then provides the temperature level of the product at each point along the reactor, which in turn influences the equilibrium and transfer of the substance.
We can calculate how all parameters are retroactively influenced using iterative processes. We have developed particularly efficient computational models to deal with these extremely complex processes.

When the heat transmission determines the process

You can pinpoint the conditions in which a mixture of substances begins to cook when the cooking point is reached. You then apply this to the energy equation.
This is very useful if you do not want a liquid to evaporate completely – for example, when producing solvents, as they are a recyclable material. However, this method does not work if there are several volatile components.
We have therefore developed a combined approach to better understand and describe the drying processes, because these kinds of processes are often determined in sections by heat as well as mass transfer.



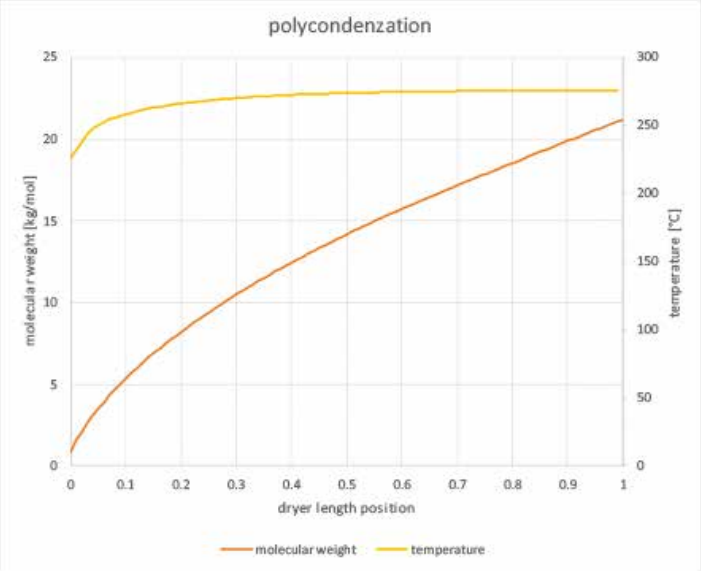
Differential thermal balance on a section of the reactor

Other processes that we were able to successfully simulate:

Complex reaction processes and other types of processes

- Polycondensation: This is a special type of polymerisation that leads to the formation of a volatile by-product when chains are formed, which must be removed by evaporation, creating, for example, polyamide PA66, a polymer used to make nylon stockings and many other products.
- We have successfully simulated the vacuum crystallization of a polymer additive based on the CSTR cascade, a model for processes with step-by-step back mixing.
- The mechanically dissipated output of the stirrer can be described based on the viscosity of the substance and the fill level in the reactor chamber.
- The fill level profile can be calculated over the length of the kneading reactor.

As our valued customers, we would like you to benefit from the results from these simulations.



Course of the molecular weight and temperature during polycondensation of polyamide

The planning of a system

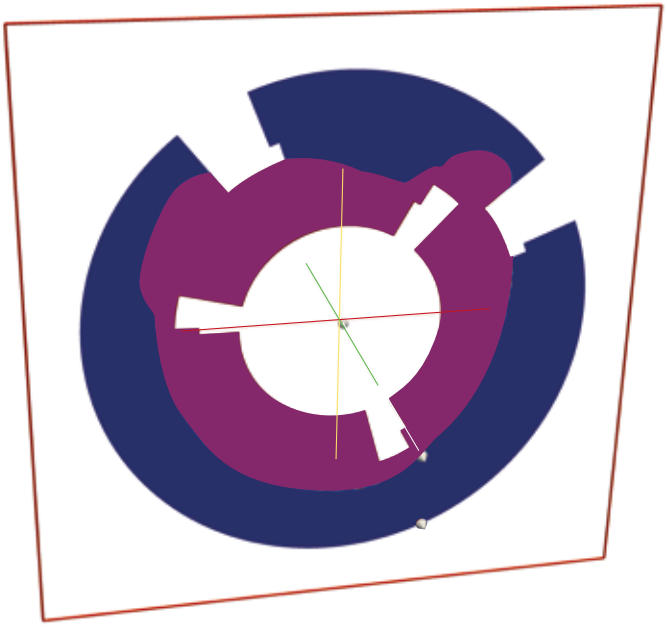
If you want to optimize a process, the challenge lies not so much in improving individual devices but rather in correctly combining devices and process conditions. We calculate these processes using the commercial software ChemCAD. This software offers a lot of standard operations that can be adapted to suit your needs.

> By way of example: For polymer solutions, we have applied a pre-concentration through flash evaporation and combined this with the kneading process. In this way, we are able to greatly increase the efficiency of the kneading process.

Computational Fluid Dynamics

Numerical Fluid Mechanics or Computational Fluid Dynamics (CFD) allow us to fully describe flow conditions in the kneading reactor. In highly complex mixing chambers such as those in our kneaders, unitary process steps cannot be described with simple Reynolds-Average Navier-Stokes (RANS) equations. Since there is no commercial software suitable for highly viscous mixtures of substances, we already began specifically researching Computational Fluid Dynamics many years ago.

In 2018, we were able to adapt the first iterative solver for high-viscosity systems in the OpenFOAM software. We further developed this solver to be able to work out the flow conditions in kneaders. This enables us to better understand various unitary process components such as the mixing ratio, mechanical dissipation and heat transfer.



Sectional view of a single-shaft reactor: purple = solid phase of the substance, blue = gaseous phase.

Give us a call.

LIST has gained extensive know-how in the field of process simulation. Our intention is to be able to improve our calculations for kneading process and combinations of kneading processes with standard operations.

If you have any questions about individual areas of process simulation, **please feel free to contact us.**

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