beyond the obvious

# Process modelling and simulation

## How to improve speed and flexibility in R&D and factory optimisation

# Contents

INTRODUCTION

# How to create an accurate cost-benefit analysis of your investment?

In many industries, new equipment and factories require multi-million-dollar investments. When the stakes are high, there is no room for human error. The planning and cost estimates have to be accurate.

Building a factory just to discover that the operation is economically or technically unsatisfactory is not feasible. But how do you get accurate cost-benefit data on the project in advance?

The answer lies in modelling and simulation. By creating accurate models of industrial processes and running simulations with the models to study the effects of different scenarios on the process, you can quickly validate your investments before making the final investment decisions.

In this guide, we'll reveal how modelling and simulation are used in industrial research and development, project proposal and delivery as well as production optimisation processes, and what their key benefits for each process are. We'll also cover how to choose a suitable partner for your modelling and simulation needs.

**What are process modelling and process simulation?**

**Modelling** means the construction of an accurate mathematical representation of a system or process.

**Simulation** calculates how changes in the modelled process affect the process performance. When you know the exact properties of a system, simulation helps you predict the impact of any changes. Simulation is used for the design, development, analysis, and optimisation of unit operations or processes.

There are several types of models:

- **Dynamic models** capture the time dependency of a system. Dynamics exist at different scales in the processes, ranging from molecular level to piping and equipment, and even to plant level. All the levels require different computational approaches, such as computational fluid dynamics (CFD). The target of dynamic models is often to acquire process transient understanding. For example, what kinds of gradual changes occur in process tank levels when making a specific change in operating conditions.
- **Steady-state models** concentrate solely on the outcomes of a process instead of the dynamic changes during a specific period of time. For example, how does installing a water filter in a production line affect the water balances in the whole plant?

Plant-wide simulations often utilise dynamic modelling for operations-related questions that require accuracy, whereas steady-state modelling is used for scenario analyses that require computational efficiency. In this guide, we'll mainly concentrate on steady-state models, which provide fast estimates and are suitable for most industrial processes.

# Top reasons to use modelling and simulation

There are several benefits of using modelling and simulation creatively in industrial decision-making processes. The most significant ones are:

**Speed:** Modelling and simulation allow you to calculate changes to complex systems in a matter of seconds.

**Resources:** Simulation results can guide an industrial process to significantly increase its efficiency by reducing excessive material and energy consumption.

**Flexibility:** Alternative choices can be safely tested before making an investment.

**Predictability:** Covering the whole lifecycle of a factory or piece of equipment from the R&D phase to factory optimisation supports data-driven decision making.

## How are modelling and simulation used in industry?

Modelling and simulation are ever-present in industrial operations. Industrial processes are always looking to optimise their production in some way, for example by reducing emissions or the use of resources. Simulation is a cost-efficient way to examine the benefits of potential updates.

How are modelling and simulation used during plant life cycle?

- In the **R&D phase**, models and simulations complement the data provided by experimental work. The result is a holistic representation of the system, compared to individual test results that can only give data on the attributes that were measured in a physical lab test.
- In the **project investment proposal phase**, fast simulation-based estimates support service providers in making realistic proposals and budgets for industrial projects.
- In the **project delivery phase**, accurate models of individual pieces of equipment and the overall process pave the way for a digital twin – a complete model of the delivered system.
- In the production optimisation phase, modelling and simulation provide a safe way to validate competing solutions.

## Who uses modelling and simulation services?

- **Engineering consultancy businesses** that want to concentrate on the core aspects of a project, such as management, automation, piping, dimensioning or general coordination.
- **Production facilities** that aim to optimise their processes or need to meet environmental regulations.
- **Equipment manufacturers** that need to analyse or improve the solution they offer or develop.
- **Non-profit organisations** looking for innovative ways to make their region, field or cause more attractive.

# Modelling and simulation in research and development

The research and development (R&D) phase is the domain of new innovations. Equipment manufacturers and industrial plants are constantly looking for new solutions to optimise their production or reduce their emissions. But how do you find the projects with the most potential?

Existing research and laboratory tests play a major role in creating new solutions that revolutionise industries. However, the R&D process greatly benefits from having a partner with expertise in both research and modelling.

### Why do we need modelling and simulation in R&D?

By calculating material and energy balances and production costs, simulation can help define if a product or solution is worth continuing the development efforts or just a waste of money. This is a vital part of ensuring that only the most profitable solutions go into production.

In R&D, a large amount of data is created through laboratory tests. However, the laboratory work itself can only give answers to individual, strictly refined questions. Simulation can widen the horizon.

Simulation supports process engineering by filling in the gaps when upscaling from a lab environment to a real plant. No one has the complete process in their lab, which means that everything can't be tested. In a lab, you'll conduct a test in a flask, but the end-product is usually an industrial-scale solution.

*“The costs of R&D get higher the further the process goes. This is why having accurate information from the beginning is vital.”*

**Eemeli Hytönen**
Technology Manager, VTT

### The R&D process

Research and development projects usually start with a business having a need or a problem that requires a new innovation.

**Idea and concept**: Existing research provides a framework for a new concept, which is then validated and refined with modelling and simulation. The result is a rough draft, which already includes a simulation of the mass and energy balances of the draft concepts and a rough estimate of their cost-benefit ratios.

**Laboratory phase**: Laboratory experiments provide further proof of the concept’s potential. The laboratory phase provides accurate data of the individual parts of the concept. These individual pieces of information can then be utilised in making a more detailed cost and performance analysis.

**Pilot phase**: All the individual data gathered from research, laboratory tests and simulation are combined to support the design process and running long-term experiments in a pilot-scale system. The pilot phase also includes the creation of a careful, simulation-based techno-economic analysis of the competing options and the selection of the most promising one. Thorough simulations are needed, as the demonstration phase already requires substantial investments.

**Demonstration phase**: The first industrial-scale, commercial product or solution is created. The models and simulations of the previous phases can be used to assess how the upscaled solution performs.

**Commercialisation**: When the new solution is up and running, a combination of sensors and simulation can be used to optimise its performance. At this point, the focus of simulation shifts from R&D to process optimisation, a topic we’ll discuss later in this guide.

REFERENCE CASE

# Idea generation & lab phase in protein ingredient production

VTT participated in an EU project that aimed at developing protein ingredient production concepts from food processing side streams. In the project, VTT used a funnel approach to enable the utilisation of powerful engineering tools and methods already during the experimental product and process R&D phases. The steps in this early-stage process engineering funnel were:

### 1. Idea generation

The objective was to list all ideas in the defined context and to define the experimental strategy without prioritisation. We listed 70 different concepts for the isolation and concentration of protein. Then we identified the proper experimental and mathematical procedures and measurement units to get comparable data for technical and economic analyses.

### 2. Lab phase

Experimental lab trials for the whole concept or a part of it were performed altogether for 40 concepts based on the identified procedures. The objective was to perform a technical check for the ideas in lab conditions to validate their potential to achieve the overall objective. The technically viable concepts were passed to the next step.

### 3. Light techno-economic assessment (TEA)

A light TEA was conducted for eight concepts. Experimental data and factorial process engineering estimation routines were used to get preliminary overall mass and energy balances and an estimate of the production costs for the product. This step yielded a ranking of the concepts based on production cost estimates. Only the four most promising alternatives were retained after this step.

### 4. Pre-feasibility process design

The four most promising overall concepts were selected for a more detailed pre-feasibility process design analysis and their mass and energy balances were modelled with the Balas® steady-state simulation software. The goal of this step was to conduct more rigorous mass and energy balance calculations by replacing the shortcuts used in step 3 with values based on modelling and simulation. As a result, we got an analysis of the techno-economic feasibility of the most potential concepts.

This funnel approach supported the technology development and brought case-specific aspects systematically into early-stage R&D. The four-step funnel refined the concept ideas into viable process concepts, prioritised them and expedited the process of upscaling the technically and economically promising ones.

# Modelling and simulation in project proposal and delivery

If research and development was the phase of new innovations, the project proposal and delivery phase is all about providing the perfect solution for satisfying the needs of the customer.

**Why do we need modelling and simulation in the project proposal and delivery phase?**

When a request for proposal regarding a new solution, production line or plant is sent out, the proposal creation process has to be careful but lightning fast. You have to calculate the mass and energy balances of the upcoming project, make cost estimates and an implementation plan to create a plausible proposal in a matter of days, or even hours. This requires vast experience and expertise in modelling and simulation.

Even when dealing with existing solutions, the number of variables with their individual properties is often so great that advanced modelling and simulation are required to accurately validate solution performance.

After delivery, the model can act as a digital twin of the new plant or manufacturing line. The twin can be used for future performance and optimisation projects.

## Proposal

In the proposal phase, the key is to arrive at a cost estimate that is not perfect but accurate enough. The fast offer creation processes require robust models that create representations of the key process equipment and systems of the required solution. Using steady-state models that have been developed earlier and the model libraries of simulation software, you can calculate the mass and energy balances in a few hours.

At this stage, there's no time for highly detailed modelling of individual pieces of equipment. That's why you need a modern simulation software that includes a high-quality, up-to-date standard model library, and expertise in developing models.

## Project delivery

When the project begins, you need to analyse the relationship between the complete system and its individual parts. Equipment manufac-

turers provide basic information about their products, but they can't know how the product affects the performance of each delicate and complex production system. The initial offer model needs to be refined to a more sophisticated steady-state model that recognises the properties of the individual parts in the system.

Plants and production lines have to be updated and optimised regularly. When that time comes, a digital twin can help you optimise the production.

A digital twin is a complete model of an industrial system, a plant for example. As the whole operation exists as a digital model, you can run your own simulations and analyse the effects of optimisation projects.

Complying with environmental regulations is a constant topic in industry. A digital twin can provide reliable information on the changes you need to make to achieve the targets of new regulation.

Many businesses choose to merely react to regulation. However, getting a digital twin with your factory delivery and proactively responding to the regulations is often the more cost-efficient option. You no longer have to pay for expensive modelling and simulation for every single optimisation project. You can focus on the holistic optimisation of your factory.

**A hypothetical project proposal:**

Modelling is only one part of proposal preparation but it's vital for getting the balance right between trying to win the project and ensuring it's also profitable. Here's how the process could hypothetically go:

1. A customer sends specifications of a production line renewal to potential implementation project providers, who are asked to submit a proposal for the work.
2. For the project proposal, the company models the target process based on the given specifications. Existing simulation models are utilised and fitted to the specifications.
3. The simulation results are used for main equipment dimensioning and preliminary piping information that form the basis of the investment cost estimates for the process renewal.
4. A few alternative scenarios that reach the required specifications are created to give the customer confidence in the solution and the possibility to influence the final renewal strategy. The cost information is used in preparing the final proposal.

# Modelling and simulation in production optimisation

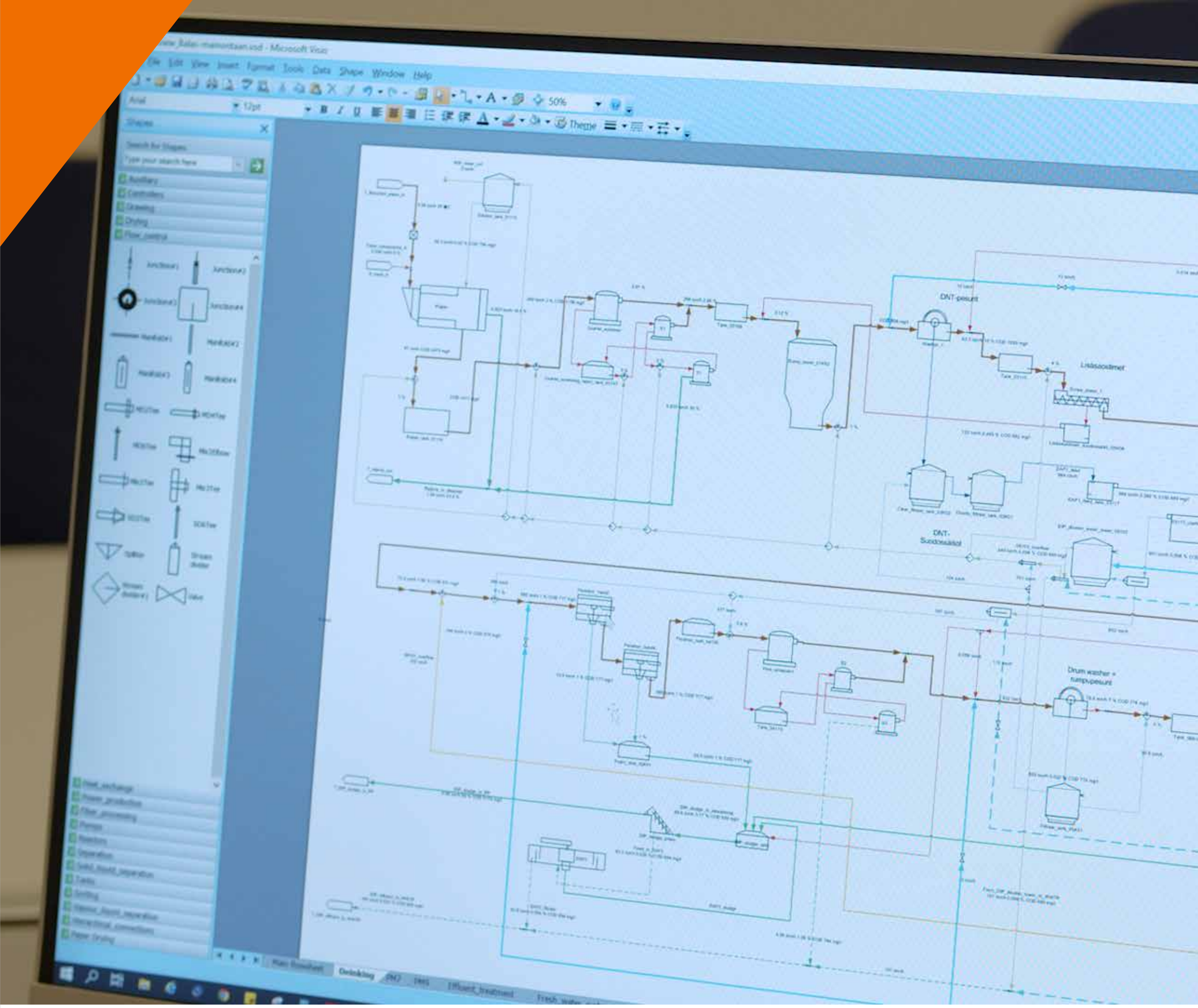
Production optimisation means updating existing production lines and plants to yield better results.

Even a plant using cutting-edge technologies requires constant optimisation to remain cost-competitive. There are factories that have been operational for decades, but the equipment and production lines have been updated and optimised various times.

Changing regulations, new materials and technologies and global trends demand flexibility from the process industry. Often a more profitable alternative for shutting down operational and efficient factories is using the side streams of the current production lines or adopting new technology to enable the production of completely new products.

*"Identifying and implementing the low-hanging optimisation fruits of the existing process before investing in brand new technologies or solutions is fundamental and cost-efficient."*

**Lotta Sorsamäki**
Research Scientist, VTT




### Why do we need modelling and simulation in the production phase?

Modelling and simulation can support factory modifications by providing a cost-efficient and risk-free means to experiment on new methods and technologies without the need for heavy investments.

Let's say a printing paper machine is on the verge of shutdown because of low profitability but converting it from traditional water forming technology to foam forming technology and from printing paper to foam-formed, wood-based EPS substitute could give the machine a new lifeline. By simulating the effects of the modified process, the paper mill could calculate the cost-benefit ratio of the new operation fast and cost-efficiently.

Along with pure production optimisation, environmental regulations are often the reason old factories need to update their production lines. Even though there are numerous sensors in the factory that provide data on the operation, everything can't be measured. Also, the sensors only provide data of the current status of the system, not on the effects of the proposed changes. Modelling and simulation are needed to validate new investments before final decisions are made.

## The optimisation process

Optimisation processes start with an organisation or a company presenting a need or a problem. The customer and the scope of the project define whether a generic simulation model suffices or if the problem at hand requires a more specific solution.

Often a generic simulation model is useful for large company groups or organisations that aim to analyse general trends or a new technological direction. The generic models can then be developed into individual projects that cover the needs of a specific company, factory or production line.

A plant optimisation project requires creating a reference model of the starting point. When the reference model is ready, you can actually start analysing how the required changes could be achieved and what kinds of effects the specific changes to the system have.

As was the case with R&D, also production optimisation requires combining experimental results and separate performance data with sophisticated simulation methods. An operational factory is normally equipped with hundreds of sensors that provide significant amounts of data on the current process.

As you can never measure every single aspect of a factory operation, the sensor data alone doesn't enable high-quality optimisation. Combining the sensor data and physics-based simulation models can reveal the low-hanging fruits with minimum investment and maximum effect.

When optimisation strategies are identified and modelled, they can be used to further refine the solutions using scenario simulations and mathematical optimisation. This shows if the solution can reach the expected targets and, if so, what the costs are.

REFERENCE CASE

# Tissue paper mill

VTT participated in an EU project that aimed at reducing the water consumption in pulp and paper industry. The paper mill chosen for the case study was old and spent four times more water than a modern paper mill. The target was to cut the water consumption down by 25 percent by performing process configuration changes and implementing water purification equipment. In the project, VTT used process modelling and simulation to evaluate the effects of the water reduction actions on the water consumption in the system.

1. To adhere to tightened regulations, the customer had completed specific modifications to their process to cut water consumption. Because sensor data showed lower improvements in the water consumption than expected, modelling and simulation were used to discover the maximum theoretical improvement of the water reduction actions.

2. VTT made a reference model of the process before any actions. The reference model was validated using sensor and measurement data. The simulation of the reference model showed the original water consumption that was targeted to decrease by 25 %.

3. The performed process configuration changes were added to the reference model and the simulation results were validated with new sensor and measurement data. The simulation results showed that a 22 % reduction in the water consumption should have been achieved.

4. The problem was narrowed down to process operation rather than the process itself. The production restrictions had caused a need for frequent shutdowns and start-ups, which increased washing water consumption. This dimmed the positive effects of the simultaneous water reduction actions.

5. In addition to the process configuration changes, the customer implemented a water purification filter to the process. The filter was included in the simulation model, and the model was validated with a third set of sensor and measurement data. The simulations showed that adding a water filter to the production line cuts the water usage by an additional 5 %.

6. A what-if model confirmed that adding several water filters would bring even more savings.

7. The chemical oxygen demand (COD) level in the process water was modelled in all cases to evaluate the effects of decreased water usage.

# What to consider in a modelling and simulation partnership

Industrial process modelling and simulation range from the molecular modelling level to plant-wide models and include everything in between.

Even though some modelling and simulation assignments are straightforward, most projects benefit from an interdisciplinary approach where research, laboratory work, modelling, simulation and sensor data work hand in hand. This is why you should consider the following aspects when looking for a modelling and simulation partner:

**Research**: Your partner should have a strong background in the latest trends and findings regarding both your field and modelling and simulation methods. This way the partner immediately understands your specific needs and can cater for them optimally. If your partner is a pioneer in the research and new innovations in your field, you're going to benefit from it.

**Laboratory**: Along with a strong knowledge of recent publications, it is beneficial if your partner can do laboratory work to validate the chemical processes. Pilot runs often require industrial chemists, scientists and a proper research infrastructure. This enables your partner to either work at their own laboratory or bring their equipment to your facility depending on the needs of the project.

**Software**: A state-of-the-art modelling and simulation software is essential for success. To save your time and resources, your partner should be able to provide generic models for a large variety of industrial processes.

**Experience**: Optimally, the partner should have vast experience of prior projects that are similar to yours. This ensures efficiency and reliability.

**Versatility**: Combining different methods is the key to a successful project. Data-driven, physics-based, computational fluid dynamics, steady-state – don't settle for one approach. Your partner should be able to combine experimental methods, laboratory research and straightforward simulations.

*“Hundreds of chemical elements interact in industrial processes and a single element or unexpected interaction can trigger the whole operation to fail. Combining steady-state and data-driven approaches, for example, is often needed to solve the problem.”*

**Eemeli Hytönen**
Technology Manager, VTT

# Why VTT?

Process modelling and simulation is a complex field with numerous variables that need to be considered for optimal results. VTT is a research centre that links pioneering research, strong substance matter expertise and the latest technology to support industrial businesses and organisations.

We understand your industrial context and have the modelling and simulation expertise to make an impact and support your strategic goals. What distinguishes us from most modelling and simulation partners, however, is that we also do groundbreaking research. We can simulate everything we research or vice versa. We use lab experiments, pilot-scale runs and sensor data to validate our simulations and give you an edge.

This enables us to participate in every phase of your industrial processes’ life cycle. We can support equipment manufacturers with challenging modelling tasks through our R&D process. We can optimise existing industrial systems or participate in delivering new factories and solutions by modelling and simulating.

If you have a modelling or simulation need that requires expertise and experience, don’t hesitate to contact us.

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