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Dynamic Modelling and Simulation of Liquid Food Process Lines

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UNIVERSITY

Department of Food Technology, Engineering and Nutrition
Faculty of Engineering, LTH
Lund University, Sweden
2007

Akademisk avhandling för avläggande av teknologie doktorsexamen vid tekniska fakulteten vid Lunds universitet kommer att offentligens försvaras på engelska tisdagen den 12 juni 2007, kl. 13.00 i hörsal B, Kemicentrum, Getingevägen 60, Lund.

Fakultetsopponent: Professor César de Prada Moraga, Department of Systems Engineering and Automatic Control, University of Valladolid, Facultad de Ciencias, Valladolid, Spain

Academic thesis which, by due permission of the Faculty of Engineering at Lund University, will be publicly defended on Tuesday 12th of June 2007 at 13:00 in Lecture Hall B at the Center of Chemistry and Chemical Engineering, Lund, for the degree of Doctor of Philosophy in Engineering.

Faculty opponent: Professor César de Prada Moraga, Department of Systems Engineering and Automatic Control, University of Valladolid, Facultad de Ciencias, Valladolid, Spain

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Tomas Skoglund

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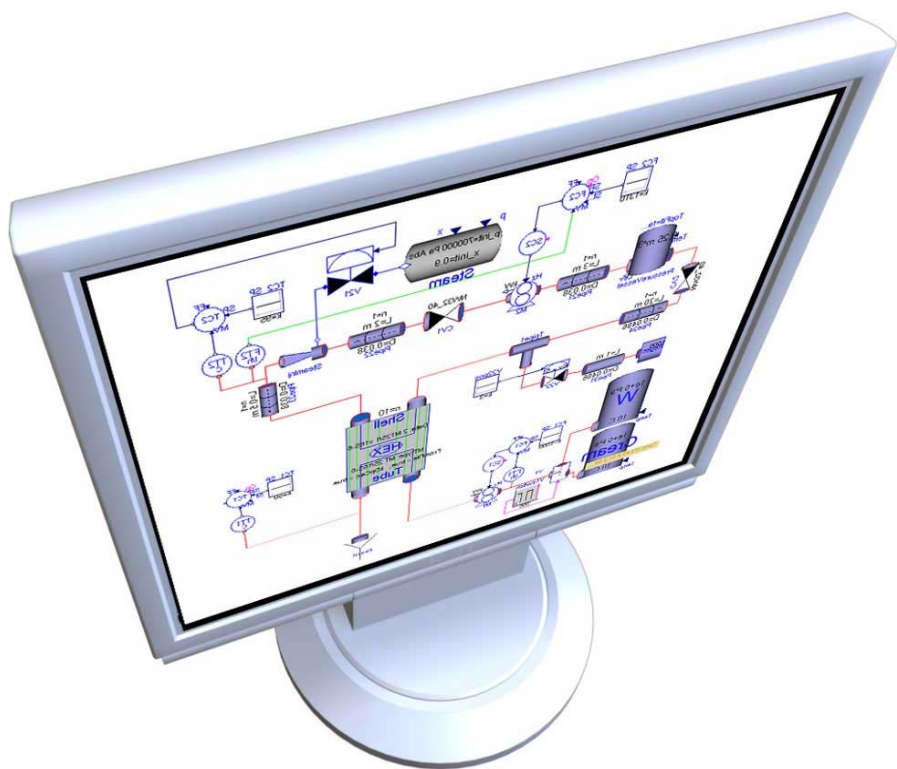
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To
Cecilia
Jannika ◦ Kristofer ◦ Gabriella

My heart leaps up when I behold
A rainbow in the sky:
So was it when my life began,
So is it now I am a man,
So be it when I shall grow old
Or let me die!
The child is father of the man:
And I could wish my days to be
Bound each to each by natural piety.

William Wordsworth (1770-1850)



ABSTRACT

In the present work a dynamic model library of components for process lines was developed. The analysis addressed characteristic aspects of liquid food process lines, and new models were developed for fluid transitions, dispersion, mixing zones and first-order chemical reactions in pipes and heat exchangers. The computational efficiency and accuracy of the models were analysed. It was demonstrated that classical models of fluid propagation in process lines could be combined with modern numerical methods to obtain computationally efficient dynamic models for the simulation of dispersed convective flow, with and without chemical reactions.

In particular it was demonstrated that a transport delay model was well suited for the simulation of thermal transients due to fluid transitions in heat exchangers. It was shown that the model could be extended to account for dispersion with a method that, although classical in approach, enables a certain freedom in the choice of degree of discretization depending on the demand for accuracy vs. computational speed. Further extension of the model with first-order chemical reactions to account for microbial deactivation was demonstrated.

The usefulness of the dispersed-convection model to predict the extent of mixing zones and the amount of product rejects in continuous processing was demonstrated. The relevance concerning product traceability is discussed and the concept “fuzzy traceability” introduced.

Keywords: Dynamic model, Dynamic simulation, Process lines, Fluid property transition, Heat exchanger, Dispersion, Liquid food, Microbial deactivation, Traceability, Fuzzy traceability

Populärvetenskaplig sammanfattning

Produktion av flytande livsmedel som exempelvis mjölk, juice och tomatketchup äger rum i komplexa produktionslinjer där råvaran flödar genom anläggningen samtidigt som den undergår olika steg av behandling. Exempel på behandling är gräddseparering, homogenisering och värmebehandling av mjölk. Ett annat exempel är rekombinering av apelsinjuice genom vattenutspädning av juicekoncentrat som har skeppats från Brasilien över Atlanten till Europa.

Processlinjer för livsmedel skiljer sig på ett antal viktiga punkter från processlinjer inom annan industri, exempelvis kemisk industri. Utmärkande för produktion av flytande livsmedel är:

- Frekventa starter och stopp
- Frekventa produktbyten
- Värmebehandling
- Hygieniska krav
- Mikrobiell aktivitet
- Regelbunden rengöring och disk

Detta leder till speciella aspekter som måste beaktas såväl vid konstruktion som vid drift av processlinjerna. Exempelvis uppstår vid varje start av ett värmebehandlingssystem (t.ex. en mjölkpastör) en blandning mellan vatten och produkt eftersom systemet försteriliseras med vatten. Produktens fysikaliska egenskaper skiljer sig ofta från vattnets ganska mycket. Vid startförloppet kan detta leda till oönskade effekter som t.ex. temperatursvängningar. Denna typ av variationer i tiden kan inte förutsägas med statiska dimensioneringsberäkningar. För detta fordras såkallad simulering eller, för tydlighetens skull, dynamisk simulering.

Hittills har dynamisk simulering inte varit vanligt förekommande inom mejerinäringen eller annan industri för produktion av flytande livsmedel. Detta gäller även tillverkningsindustrin för produktionsutrustning till dessa industrier. Förklaringen till detta hänger ihop med tekniska möjligheter och kostnader. Med teknikutvecklingen såväl avseende hårdvara som mjukvara har möjligheterna ökat medan kostnaderna sjunkit. En annan återhållande faktor har varit brist på systematisering i form av återanvändbar programkod för tillämpnings-

området. I detta arbete har därför ett dynamiskt modellbibliotek skapats för att möjliggöra regelbunden dynamisk simulering till en rimlig kostnad.

Vid framtagningen av modellbiblioteket har ovan nämnda typiska aspekter för produktion av flytande livsmedel beaktats. En ny värmeväxlarmodell för att effektivt kunna simulera den termiska effekten av ett byte av vätska (vatten—produkt eller produkt—produkt) har sålunda utvecklats. Även effektiva modeller för simulering av blandningszoner och mikrobiell avdödning (i t.ex. en mjölkpastör) har utvecklats. Genom matematisk analys och simuleringar har visats att modellerna är beräkningseffektiva jämfört med mer traditionella modeller.

Genom att kunna simulera de blandningszoner som uppstår vid flygande produktbyte eller byte av råvarutank, uppstår en möjlighet att ha bra kontroll på sammansättningen i kundförpackningarna vid dessa byten. Detta leder till möjligheter att använda dynamisk simulering integrerat i spårbarhetssystem. Sådan simulering erbjuder en bas för välgrundade beslut rörande indragning eller återkallande av produkt. Frågan diskuteras i termer av ”fuzzy spårbarhet”.

LIST OF PAPERS

This thesis is based on the following papers, which will be referred to in the text by their Roman numerals. The papers are appended at the end of the thesis.

- I. Skoglund, T., Årzén, K-E. and Dejmek, P. **(2006)**
Dynamic object-oriented heat-exchanger models for simulation of fluid property transitions
International Journal of Heat and Mass Transfer, 49, pp. 2291-2303
- II. Skoglund, T. and Dejmek, P. **(2007)**
A dynamic object-oriented model for efficient simulation of fluid dispersion in turbulent flow with varying fluid properties
Chemical Engineering Science, 62, pp. 2168-2178
- III. Skoglund, T. and Dejmek, P. **(2007)**
A dynamic object-oriented model for efficient simulation of microbial reduction in dispersed turbulent flow
Submitted to journal
- IV. Skoglund, T. and Dejmek, P. **(2007)**
Fuzzy traceability - A process simulation derived extension of the traceability concept in continuous food processing
Submitted to journal

The author's contributions to the papers

- I The author performed the system analysis, designed the models, carried out the simulations and wrote the manuscript.
- II The author performed the system analysis, designed the models, carried out the simulations and wrote the manuscript.
- III The author performed the system analysis, designed the models, carried out the simulations and wrote the manuscript.
- IV The author performed the simulations and wrote the major part of the manuscript.

Related publications:

- A. Skoglund, T. **(2003)**
Simulation of Liquid Food Processes in Modelica
Proceedings of the 3rd International Modelica Conference 2003, 51-58. Linköping, Sweden, November 3-4, 2003, Organized by the Modelica Association and Linköping University, Sweden. Available at www.modelica.org.
- B. Skoglund, T. **(2003)**
Modelling and Simulation of Liquid Food Processes
AfoT 2003, II International Workshop on Information Technologies and Computing Techniques for the Agro-Food Sector, Barcelona, Spain, November 27-28, 2003, Monograph CIMNE No-86.
- C. Skoglund, T. and Dejmek P. **(2006)**
A model library for dynamic simulation of liquid food process lines
Proceedings of FOODSIM 2006, 5-12, Naples, Italy, June 15-17, 2006, Organized by EUROSIS.

Preface

Very early in life, curiosity knocked on the door of my mind. Having let it in, we soon became close friends. So many things were intriguing, and revealing the secret of even the smallest mystery was exciting; like revealing the magician's tricks. Nature offered so many things to be explored. I was amazed ... and I was amused.

My fascination with science became part of my identity, but there are many roads in life, leading to an infinite number of fascinating places, not only in the academic world.

After many years of service at Tetra Pak, when I considered a proposition of new tasks, the opportunity to pursue a PhD project made the assignment significantly more attractive. After some time in my new position, I had a short conversation with Professor Petr Dejmek at Lund University, in which I presented some very early, somewhat vague ideas. After further discussions we defined a project. I was happy, and a little surprised that it wasn't more complicated to agree upon the framework of the project. The formal discussions took longer, and were more complicated, but eventually an agreement was signed, and having been granted the privilege I was determined to do my best for all three parties involved: Tetra Pak, Lund University and myself.

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Papers I - IV

1. Introduction

Computers have been available to almost everyone in their professional work or private life for many years. Nevertheless applications are still growing in new areas. This is due to increasing ability to deliver more computing power for less money due to the development of both hardware and software (Åström et al., 1998; Cox et al., 2006). Cox et al. presented a vision of the many benefits of using dynamic simulation by those other than experts. For example they say “*Imagine being able to build a high-fidelity, dynamic model of a process in just a few weeks, with the resulting model running 50 times real time on your laptop*”. The visions expressed in their article are shared in the present work concerning the development of a dynamic model library for the simulation of liquid food process lines.

Moreover, and in accord with the visions of Cox et al., it would be valuable if simulations could be run in real time, as this enables simulation with a link to the control system (programmable logic controller, PLC). This kind of hardware-in-the-loop (HWIL) system, i.e. PLC hardware connected to the process simulator, would extend the possibilities of dynamic simulation. Realistic simulation of the plant operation would be possible, increasing the chances of finding and correcting not only process design errors, but also errors in the PLC code or simply mismatches between the two. Furthermore, pre-tuning of parameters would be possible, enabling faster start-up of the plant. Operator training under realistic conditions would also be possible. However, the computational efficiency of the dynamic models is a limiting factor as the numerical solver has to solve the system of equations in a time always equal or less than the time taken for the real operation. Bäckman and Edwall (2005) have recently described a case in which HWIL simulation (HILS) was used in a paper mill for control logic validation and operator training. The results of the present work form the basis for further enhancement of the model library for HILS of liquid food process lines.

Dynamic simulation using computers has been applied for many decades to analyse and predict system dynamics in order to reduce or

avoid expensive experiments, to test dangerous or destructive processes, and in the development of fail-safe systems. Today object-oriented dynamic modelling tools are common (Wozny and Jeromin, 1991; Mattsson et al., 1994; Åström et al., 1998; Mattsson et al., 1998; Tiller, 2001; Tummescheit, 2002; Elmqvist et al., 2003; Modelica). Schneider and Marquardt (2002) have given a broad overview of information technology in which the technology need for chemical engineering and mathematical modelling is presented in a wider perspective. Marquardt (1996) presented an overview of the trends and concluded that a common paradigm is the complete decoupling of model representation and its application. This enables the construction of dynamic model libraries and, in the words of Marquardt, will provide “*model-based process engineering technology on the desktops of a much larger group of engineers*” than today. That was in 1996, and today it is on its way to becoming true. Examples of this are the model libraries for thermo-hydraulic applications presented by Eborn (2001) and Casella et al. (2006).

Some examples of industrial sectors within which dynamic simulation has been applied extensively over a long period are the automotive, robotics, aeronautical, space and chemical industries. The food industry has also adopted computer modelling for simulations of static behaviour and later also dynamic behaviour. Wang and Sun (2003) have presented a review of the field regarding heating and cooling. Computational fluid dynamics (CFD) is, for example, well established within food processing technology, where it has been used to analyse many processes. Norton and Sun (2006) reviewed the field and concluded that “*CFD will continue to provide explanations ... leading to better equipment design and process control for the food industry*”. However, dynamic simulation of liquid food process *lines* has not yet been practised on a broad scale. De Prada et al. (2003) described the simulation of sugar factories for operator training. In the present work liquid food process lines were simulated and due to the complexity of the problem, full CFD analysis was not deemed a practical approach. Therefore, the approximation of using only the spatial coordinate along the fluid propagation was used. This was motivated by earlier research,

e.g. Taylor (1954), Levenspiel and Smith (1957), Levenspiel and Bischoff (1963), Serpemen and Deckwer (1974), Roetzel and Balzereit (2000) and Eborn (2001).

Compared with other process industries, liquid food processes are characterised by frequent start-up and shut-down, product change “on the fly”, hygienic demands, fouling, cleaning between batches, microbial activity, and fluids with properties strongly dependent on composition and temperature (particularly viscosity and other rheological properties). For example, in dairies many different types of milk are often produced and pasteurized during a day. Before the milk is pumped into the production line, the equipment must be sanitized or pre-sterilized with hot water. The process line is then prepared for production by stabilizing the flow rates and temperatures required for production. The milk is then introduced, forcing the water out of the system, and production can then commence. The next type of milk can then be introduced on the fly, or production may be terminated by flushing out the milk with water. When production is completed the system is cleaned by pumping heated cleaning agents through the system, concluding with final flushing with water. Furthermore, there are legal demands on producers to keep records of the raw materials used in their products. This is called traceability.

Therefore, aspects that should be considered in dynamic modelling and simulation include start-up and shut-down transients, mixing zones, variability and propagation of fluid properties, microbial deactivation in pasteurizers, product–product contamination and traceability. Consequently, the dynamic modelling aspects addressed in the present work were:

- thermal dynamics in heat exchangers during fluid transitions,
- dispersion in production lines,
- chemical reactions (inactivation of microorganisms and quality degradation) during non-isothermal conditions with dispersion and varying flow, and
- mixed products and traceability.

Heat exchangers are common in many industries and much work has been devoted to various analyses. For example, static behaviour has been

analysed by Gut and Pinto (2003), Malinowski and Bielski (2004), and Sahoo and Roetzel (2002). Various dynamic aspects have been studied for example by Romie (1984, 1985, 1999), Tan and Spinner (1991), Roetzel and Xuan (1992), Xuan and Roetzel (1993a, 1993b), Lakshmanan and Potter (1994), Sharifi et al. (1995), Roetzel and Das (1995), Roetzel and Balzereit (2000), Abdelghani-Idrissi et al. (2001), Yin and Jensen (2003) and Luo et al. (2003). A good review of the field of heat-exchanger dynamics has also been given by Roetzel and Xuan (1999). Since heat treatment is one of the most common methods of preserving food, heat exchangers are ubiquitous also in the liquid food process industry.

The frequent occurring mixing zones, due to dispersion, caused by the many transitions of fluids, give rise to many problems. Dispersion is a classical chemical engineering topic and was studied by Taylor in his pioneering work (1953, 1954a, 1954b). Many models have since been developed to describe fluid flow through pipes, with and without packing material. An example of a model of dispersed flow, often described in the literature, is the combination of plug flow and a continuously stirred tank (PFCST), e.g. Levenspiel and Bischoff (1963). The flow in typical liquid food process lines is turbulent with high Reynolds numbers. Levenspiel and Smith (1957) and Serpemen and Deckwer (1974) showed that these cases are well described by the axial-dispersed plug flow (ADPF) model. Frequency analysis based on Laplace transforms is a suitable method of analysing the dynamics of dispersion models (e.g. Hopkins et al., 1969), as it accounts for arbitrary signal responses more generally than the more commonly used method of comparing moments of residence time distributions (RTDs), as in the work of Bischoff and Levenspiel (1962a, 1962b). Overviews of the work of dispersed flow were presented by Levenspiel and Bischoff (1963) and Wen and Fan (1975).

Inactivation of microorganisms and quality degradation of food is commonly described by first-order chemical reactions (e.g. Kessler, 2002; Walstra et al., 1999; Burton, 1988). In liquid food applications thermal treatment is performed through a heating – holding – cooling process, either batch-wise or continuously. In the continuous process the fluid is pumped through a system of heat exchangers and pipes. The flow causes mixing, i.e. dispersion. In other words, the system is a chemical

reactor with dispersed flow and, in heat exchangers, under non-isothermal conditions too. Most studies of chemical reactions in heat exchangers deal with steady-state conditions (e.g. Hawthorne et al., 1968; Phillips et al., 1997). Regarding dynamic simulation, Galle et al. (2001) studied gas flows and Haugwitz (2005), liquids.

Safe food is important to human health, and large-scale food production in a global market poses a potential threat to society due to the potential large-scale health consequences of unsafe food reaching retailers and consumers. Furthermore, food producers want to protect their brands. To ensure minimal effects on health (and brands), traceability systems are well motivated. In fact traceability is usually required by law, e.g. EU Regulation 2002. Traceability, in terms of chain traceability and internal traceability, have been described by Moe (1998). One of the cornerstones in traceability systems is the definition of a batch. Kim et al. (1999) defined a traceable resource unit (TRU) as a unit with unique characteristics. However, when dealing with continuous processing, as is often the case with liquid foods, defining a TRU is difficult. One reason is that many zones of mixed batches may occur due to mixing of raw material (source TRUs) when one fluid is used to expel another from the system during a production change on the fly. Dynamic simulation, by means of dispersion models, constitutes a means of better controlling these mixing zones.

2. Objectives

The vision of being able to predict and tune actual plant performance before building the plant drove momentum into this project. The desire is to be able to evaluate and validate numerous criteria regarding plant performance by means of a “living” drawing board containing dynamic models of process components. Being able to predict the plant’s performance already at design and train operators before the control room is built would prove invaluable. Another mental image of the future is the possibility of running a “virtual” plant in parallel with the real plant as a means of plant diagnostics.

With these visions in mind the project was concerned with characteristics related to liquid food process lines, concluding the following specific objectives.

1. To analyse and create a basic dynamic model library suitable for the simulation of typical dynamics of liquid food process lines.
2. To analyse and create dynamic models of heat exchangers for efficient simulation of the transition of fluids with different properties.
3. To analyse and create dynamic models of fluid channels for efficient simulation of mixing phases at fluid transitions.
4. To analyse and create dynamic models for the efficient simulation of first-order chemical reactions in a tubular reactor under both isothermal and non-isothermal conditions.

3. Process dynamics and simulation

When designing a production line for processing of liquid food, for example, a milk pasteurizer, production parameters such as capacity, fluid properties and temperatures are used to calculate and select type and size of components, for example, pumps, pipes and heat exchangers. The engineer can then be sure that the system will meet the static demands defined by the production parameters. However, dynamic phenomena, such as variations in *control loops* (e.g. Fig. 3 below) or transients during *transitions* (e.g. Fig. 4 below) between different production states (including start-up, flushing, shut-down, etc.) are not analysed. This is often the reason for unexpected dynamic problems occurring in the real production line, for example, oscillations in control loops, pressure shocks or serious disturbances during a state transition. There is thus a need for dynamic simulation to predict system (process and control) dynamics. Furthermore, dynamic simulation allows operators to be trained and controllers can be tuned beforehand, enabling swift plant start-up.

3.1 Dynamic systems

The dynamics of a system is mathematically described by time-differential equations. There are ordinary differential equations (ODEs) in time. For example first-order chemical reactions, with the reaction constant k .

$$\frac{\partial C}{\partial t} = -kC \quad (1)$$

There are also partial differential equations (PDEs) where the dependency is related to more than one variable. For example, first-order chemical reactions in a diffusive (dispersive) convective flow, with the velocity vector \mathbf{v} and diffusion (dispersion) D .

$$\frac{\partial C}{\partial t} = -\nabla \cdot \mathbf{v}C + \nabla \cdot D\nabla C - kC \quad (2)$$

Solving this numerically (for example with CFD) in a general geometry requires substantial computation. Each space coordinate that can be neglected will reduce the need for computation considerably. In a typical

liquid food process line, it is possible to regard the concentration in a cross section of the fluid channel as being constant (e.g. Levenspiel and Smith, 1957; Serpemen and Deckwer, 1974). This leads to the one-dimensional form of Eq. (2). With constant scalar velocity, v , and diffusion (dispersion), D , it becomes:

$$\frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} + D \frac{\partial^2 C}{\partial x^2} - kC \quad (3)$$

In models for static calculations the time differential terms are set to zero, whereas in dynamic modelling and simulation they must be included.

3.1.1 Object orientation and model library

Modern modelling tools include solvers and enable the use of object orientation and graphical interfaces. In object-oriented programming (OOP) the code is structured in independent, but cooperating pieces (objects) with a given task of data processing. An object can receive and send messages from and to other objects. Thus, the final code can be seen as a collection of cooperating objects rather than a collection of functions or a list of instructions, as in traditional programming. The advantages with OOP are its greater flexibility and maintainability. It utilizes modularity and inheritance, and enables code generation that is easier to understand, which is particularly important in large-scale programming.

When OOP is combined with a graphical interface, the objects are often displayed as icons that can be graphically connected to create the communication links between the objects. This facilitates code generation even more, and enables programming by non-programmers through a procedure more like graphical configuration. See Fig. 2.

Åström et al. (1998) have described the evolution of modelling tools and given some examples. The tool that was used in the present work was Dymola, based on the language Modelica (Tiller, 2001). The Modelica language is an object-oriented language, which allows convenient, component-oriented modelling of complex systems described by differential and algebraic equations (see below). A Modelica-based tool, like Dymola, provides a user environment for editing, compilation – including symbolic manipulation and sorting of the equations – and simulation. The user interface of the library created in this work is shown

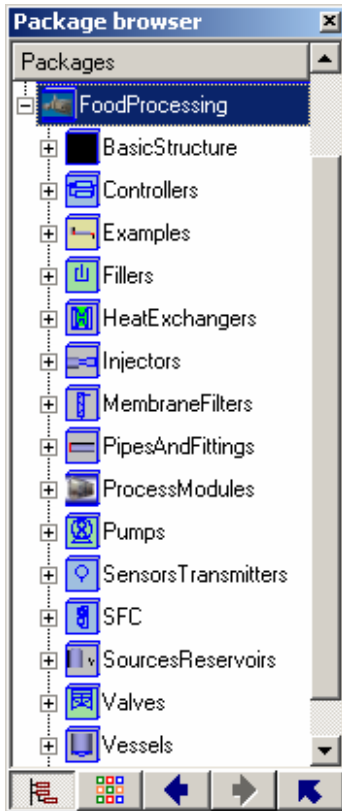


Fig. 1. User interface of the dynamic model library for applications to liquid food process lines.

in Fig. 1. Fig. 2 shows how a valve is “dragged” from the sub-library “Valves” into the diagram layer of a process line model. In this example, the total program code of the process line, i.e. the process line model, is created by collecting and connecting the objects that represent the components in the process line.

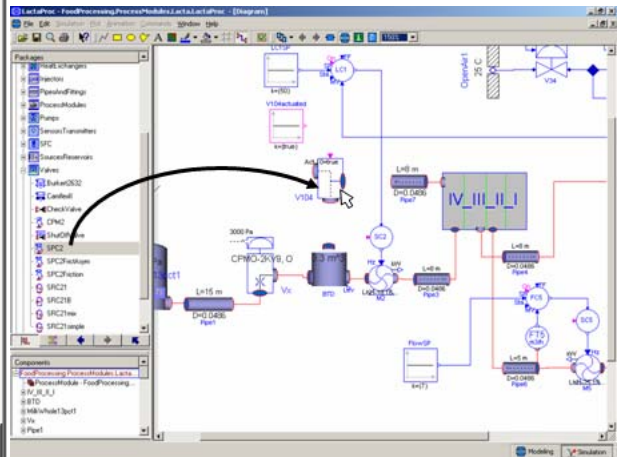


Fig. 2. Dragging and dropping a valve from the library into the diagram layer of a process line model.

3.2 Dynamics in liquid food process lines

As already mentioned, there are different types of dynamics in a process line. The two major types of dynamics in a liquid food process line are described below.

- *Dynamics under quasi-stationary conditions* due to disturbances or other unavoidable variations. This type of dynamic is often regulated via control loops to maintain predefined values of, for example
 - flow rate,
 - temperature and
 - concentration.

See also section 3.2.1 “Variables of interest” below. These variables relate to conservation laws, for example mass conservation, energy (thermal) conservation, volume conservation (incompressibility) and momentum conservation. (This is described in *Related publications A, B and C.*) An example is given in Fig. 3, which shows the results of simulating an in-line juice blending system with a closed control loop for the sugar concentration. The figure shows the sugar concentration

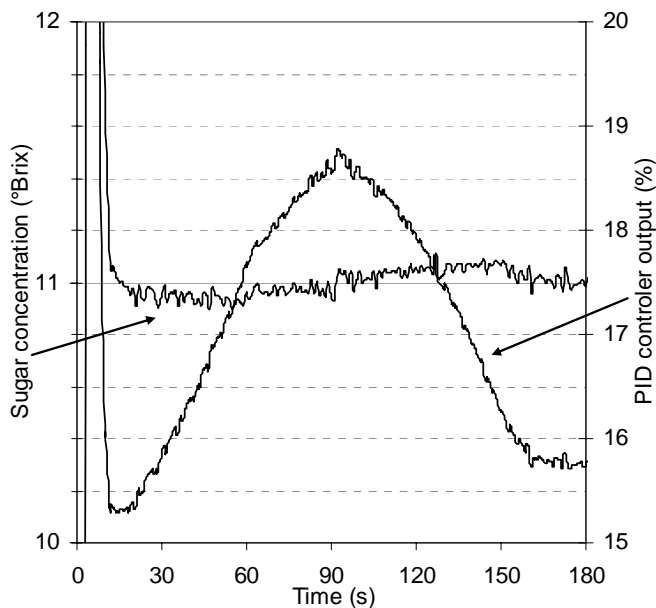


Fig. 3. Controller output and concentration around the set point in a simulated continuous juice blending line.

and the controller output to the juice concentrate pump during the first 3 minutes after the initial start-up. The throughput of water varies and the proportional, integrating and derivative (PID) controller manages

to keep the blended juice close to the set point of 11 °Brix. The noisy appearance of the curves is caused by the simulated inaccuracy of the Brix sensor.

- *Dynamics due to transitions between different states*, for example, transition in a milk pasteurizer from pre-sterilization with water to production conditions. More generally, there may be transitions in the process due to:
 - start-up or shut-down of production,
 - opening or closing of valves,
 - starting or stopping of pumps,
 - change of product (fluid) source or
 - changes in set points for control loops.

In Fig. 3, the transient of the start-up is visible during the first 15 seconds. Another transient is shown in Fig. 4. The figure shows the thermal effect when the product (cream) enters a heat exchanger after water during a start-up sequence in a pasteurizer (at constant flow rates and inlet temperatures of product and hot water as heating medium).

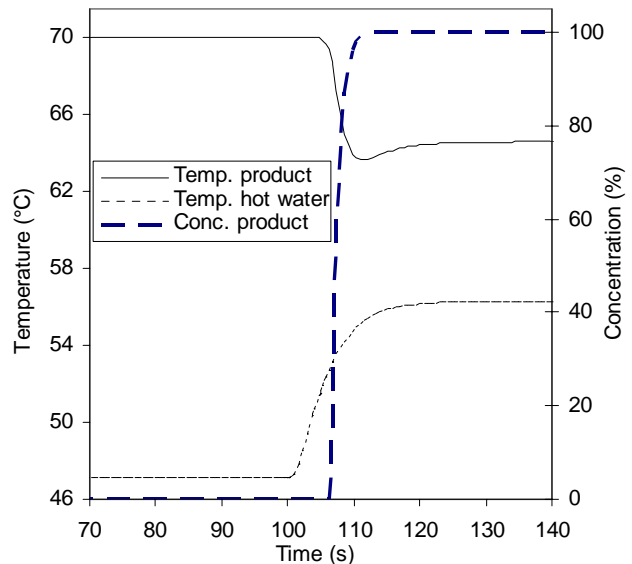


Fig. 4. Simulated fluid transition in a heat exchanger. Data were obtained at heat exchanger exits at constant flow rates and inlet temperatures.

This means that models for dynamic simulation of liquid food process lines should be capable of handling arbitrary variations in time of the above mentioned parameters and variables. Hence, a set of ODEs is required to describe the system. Moreover, a set of algebraic equations (AEs) is required to describe empirical engineering design correlations,

e.g. the fanning friction factor or convective heat transfer coefficient. The combined set of differential and algebraic equations (DAE) describes the whole system. To this logics are added, describing discrete events that cause changes in equations, representing various changes in the process, e.g., starting a pump or closing a valve.

Furthermore physical properties vary along the flow direction, while variations across the flow direction can usually be neglected. This means there is a need for PDEs to describe the system, despite the fact that only one space coordinate is considered. This implies axial discretization of the models. Methods commonly used to compute PDEs are the finite element method (FEM), e.g. Casella and Schavio (2003), the finite difference method (FDM), e.g. Heath (2002), and the finite volume method (FVM), e.g. Elmqvist et al. (2003). In the present work the discretization was performed in the form of finite volumes, also denoted control volumes, for which the balance equations were formulated.

3.2.1 Variables of interest

The analysis of the processes, phenomena and variables that are of interest forms the basis for the implementation of a dynamic model library. A major part of liquid food processing is concerned with heating, cooling, separation, mixing and buffering by means of pumps, valves heat exchangers, vessels and pipes, etc. Sometimes, compressed air and boiling are involved. Consequently, the transfer of mass and heat are important, and are described by conservation equations formulated dynamically. Furthermore, the dynamics of flow (acceleration and retardation) implies momentum conservation. Besides these extensional variables (mass, thermal energy and momentum), there are related intensive variables of interest, for example, density, mass flow rate, temperature and pressure. Other interesting related variables are volume, volumetric flow rate, level in tanks and concentration of the food components, e.g. fat, carbohydrates and protein.

4. Fluid transitions

During state transitions in a production line, one fluid is often “pushed” through the system by another. This means that dynamic simulation requires dynamic component models that can simulate such transitions effectively. Difficulty arises as the changes are often rapid due to opening and closing of valves. Since the dispersion term is usually small compared with the convective term in Eq. (3) (assuming no chemical reactions), this leads to considerable computation due to the need of high degree of discretization to reflect the rapid changes.

4.1 Fluid transitions in heat exchangers

During start-up or shut-down of a pasteurizer, fluid transition will take place. The main component in a pasteurizer is a heat exchanger, which means that a dynamic heat-exchanger model is required. Casella and Schavio (2003) described how a heat exchanger was modelled with FEM. In the present application, a model is required that can effectively handle transitions.

In this work the method was based on FVM and adapted to fluid transitions. *Paper I* describes this adaptation. The heat transfer was modelled in a standard way, but the fluid propagation, physically described by Eq. (3) with $k = 0$ (and a small value of D), makes the model more complicated when accounting for the propagation of fluid during a sudden change in properties. The dynamic model was validated by Kauhanen (2004).

As the principle of the present work was to transform known physical mechanisms into computationally less demanding forms, the new model introduced in *Paper I* was motivated by the finding of Xuan and Roetzel (1993b), namely that the diffusive and dispersive heat capacity flow is negligible in a typical liquid food process line compared with the convective heat capacity flow, i.e. when the Péclet number, Pe , is greater than 55. Thus the assumption was that a plug-flow model would be sufficient and that the dispersion could be neglected. That means that Eq. (3) can be simplified to the pure convective form, Eq. (4).

$$\frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} \quad (4)$$

This represents uniform propagation of the fluid, i.e. plug flow. Solving this equation traditionally would require a high degree of discretization (and large equation systems) to simulate the rapid changes that are typical in liquid food process lines, e.g. when activating a change-over valve to change fluid. To avoid the problem of solving Eq. (4), a dynamic transport-delay function was introduced. The mathematical construct of this plug-flow model replacing Eq. (4), is expressed in Eq. (5), which states that the composition at the fluid channel exit appears delayed by the time τ .

$$\hat{C}_{out}(t) = \tilde{\hat{C}}_{in}(t) = \hat{C}_{in}(t - \tau) \quad (5)$$

The delay, τ , is considered dynamically, i.e. it adapts to varying velocity according to Eq. (6).

$$\tau = \tau(v(t)): L = \int_0^{\tau} v(t) dt \quad (6)$$

The modelling tool was utilized to implement this velocity-dependent transport delay through the fluid channels.

The change of fluid composition affects the fluid properties density, ρ , thermal conductivity, λ , specific heat capacity, c_p , and viscosity, μ (or consistency, K , and flow behaviour index, n), e.g.

$$\mu_{out} = \mu(\hat{C}_{out}, T_{out}) = \mu(\tilde{\hat{C}}_{in}, T_{out}) \quad (7)$$

The heat-exchanger model presented in *Paper I* was based on this property propagation model of the fluid in the channels. The transport-delay model was discretized, see Fig. 5, and in *Paper I* it was demonstrated that the model was more computationally efficient, by a factor of approximately ten, than a more typical control volume model. The reason is that the new model requires less discretization for a specific level of accuracy, and the reason for this is that the transport delay handling of fluid properties requires no discretization to capture quick changes (e.g. a step), whereas a standard method requires high discretization. Fig. 4 shows the simulated thermal effect of a fluid transition from water to cream.



Fig. 5. A heat-exchanger control volume including two channels with 2 inlets and 2 outlets (solid arrows). The thermal interface (metal) is illustrated by the diagonally striped area, and the transport delays are illustrated by long dashed arrows.

5. Dispersed flow

When fluids, e.g. water or milk, propagate in a process line, mixing takes place although the convective part of the mass transfer mechanism dominates over the dispersion (turbulent diffusion), which, simplified expressed, means that v is large compared with D . See Eq. (3) (with $k = 0$). Expressed more correctly, the Péclet number, $Pe = vL/D$, is high. The Péclet number varies in a process line depending on the geometry, velocity and fluid properties. According to Wen and Fan (1975, p. 146), it was experimentally found that for turbulent flow in pipes the dispersion coefficient depends on the Reynolds number as in Eq. (8).

$$\frac{D}{Lv} = \frac{1}{Pe} = \frac{d}{L} \left(3.0 \cdot 10^7 Re^{-2.1} + 1.35 Re^{-0.125} \right) \quad (8)$$

This means that Péclet numbers for flow in pipes in liquid food process lines are typically, but not limited to, 100-4000. By setting $k = 0$ and rewriting Eq. (3) in a dimensionless form we arrive at:

$$\frac{\partial C}{\partial \tilde{t}} = -\frac{\partial C}{\partial \tilde{x}} + \frac{1}{Pe} \frac{\partial^2 C}{\partial \tilde{x}^2} \quad (9)$$

As mentioned above, the *thermal* effect of dispersion in heat exchangers is normally negligible. However, to be able to simulate and predict mixing phases during fluid transitions in a process line, the dispersion cannot be ignored. Levenspiel and Smith (1957) and Serpemen and Deckwer (1974) showed that flow with high Reynolds number, typical for liquid food process lines, is well described by the axial-dispersed plug flow (ADPF) model, which means that Eq. (9) is applicable. Fig. 6 illustrates the ADPF model when a concentration pulse propagates along a pipe.

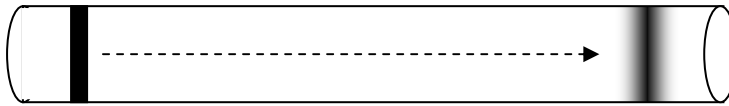


Fig. 6. Propagation of a concentration pulse in a pipe with axial-dispersed plug flow.

A classical model of ADPF describes the fluid channel as a combination of continuously stirred (=ideally mixed) tanks. A model with N continuously stirred tanks (N-CST) in series became popular. Wen & Fan (1975) derived the relationship between N in the N-CST model and the Péclet number, Pe , in the ADPF model.

$$N_{N-CST} = \frac{vL}{2D} = \frac{Pe}{2} \quad (10)$$

With the values of Pe given above, this implies large values of N , which means considerable computing. The difference between this method and modern methods (FDM, FEM or FVM) is that the classical method transforms the physical reality into another, similar, physical reality, whereas the modern methods transforms the mathematical description of the physical reality into computable algebraic forms by approximating the differential equations, i.e. replacing the infinitesimal steps (in e.g. time or space) by small finite steps. The accuracy of the outcome will then depend on how small the steps are. Consequently, the accuracy can be increased but more computation will be required. However, in the classical model the accuracy cannot be improved by increasing the value of N since it is part of the physical model, and must fulfil Eq. (10).

In *Paper II* a new model, based on a combination of a classical and a modern approach, was analysed. The idea was to transform the physical mechanism expressed in Eq. (9) into a similar form, which, depending on the degree of discretization, yields gradually increasing accuracy, but always higher accuracy than the corresponding modern standard method.

Eq. (9) has one extra term for dispersion, compared with the convective Eq. (4), and since Eq. (4) was replaced by the mathematical construct in Eq. (5) it was assumed that Eq. (5) could be extended with a corresponding dispersive term. Hence, the dispersive term $D \cdot \partial^2 C / \partial x^2$ in Eq. (3), representing mixing, was replaced by N ideal mixed volumes V_N , mathematically expressed by the mass balance for each volume:

$$V_N \frac{\partial C_{out}}{\partial t} = QC_{in} - QC_{out} \quad (11)$$

Hence, the model proposed in *Paper II*, PFNCST (plug flow with N continuously stirred tanks), is based on the idea of dividing the fluid channel into an *array*, where each element is composed of a plug flow model and an ideally mixed volume (tank). See Fig. 7.

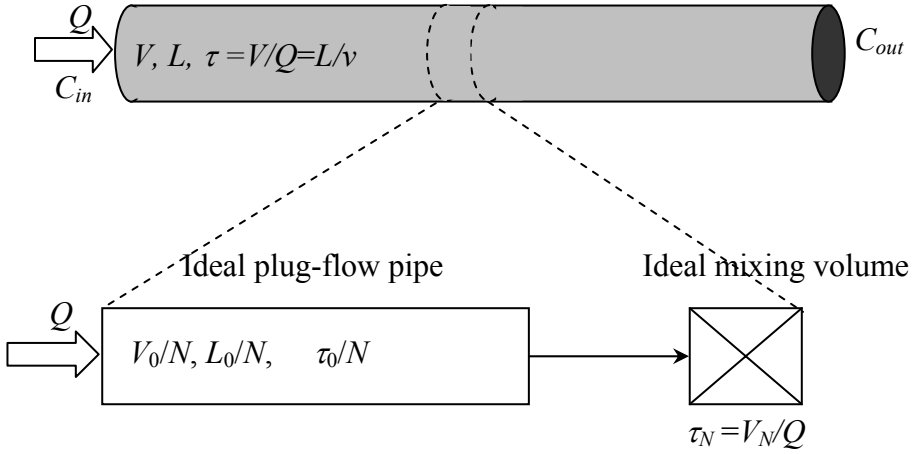


Fig. 7. Pipe with one of N control volumes in the PFNCST model described in *Paper II*

The only parameter in Eq. (9), Pe , will correspond to one parameter in the model, i.e. the relationship between the volume of the plug flow part and the volume of the mixing volume. For conservation reasons the total volume must be constant. Hence, the model is a one-parameter model combined with the discretization number N , which affects the accuracy. Analysis produced the relationship in Eq. (12).

$$V_N = V \sqrt{\frac{2}{NPe}} \text{ or in terms of residence times } \tau_N = \tau \sqrt{\frac{2}{NPe}} \quad (12)$$

The procedure used to analyse classical models has often been the method of comparing *moments* (variance, skewness, etc.) of residence time distributions (RTDs) of a pulse input (e.g. Bischoff and Levenspiel, 1962a, 1962b). The Laplace transform and transfer-function analysis have also been applied by other authors to compare different models, e.g. Hopkins et al. (1969) in their analysis of the RTD. However, their analysis did not take full advantage by analysing both aspects of dynamic systems – phase shift and amplitude – which can be carried out by means of frequency analysis. In *Paper II* both aspects were analysed based on the relationship in Eq. (12). The advantage of an analysis taking both aspects into account is that the accuracy of the model for an arbitrary input, i.e. concentration variations, will be given by its frequency

spectrum. The model proposed in *Paper II* (PFNCST) is intended for dynamic simulations of complete process lines, and therefore large variations in input values must be accounted for by the model. Therefore this was also taken into account in the analysis.

To further evaluate the model, complementary analyses were carried out for an ideal case, similar to typical cases in the food industry, i.e. step responses. Thus both the rate of change, $\partial C/\partial t$, and break-through time of a step response were analysed. Good agreement was found with exact solutions. A particularly interesting result of the model was that the rate of change of a step response at time $\tau = L/v$ quickly converges to the “exact” solution.

5.1 Mixing zones

The operation of liquid food process lines implies frequent changes of fluids, which leads to many zones with mixed products. This causes losses of raw material, thermal energy, electric energy and production time, in other words, substantial production costs and environmental load. It is therefore important to design production lines that cause a minimum of mixing, i.e. as few and as small mixing zones as possible. To enable optimal scheduling of the production, it is important to be able to predict the sizes of the possible mixing zones in a plant.

This leads to higher demands on the manufacturers of production equipment. They must design production lines with small mixing zones and give corresponding performance guarantees. This, in turn, requires accurate simulation of mixing zones in complete production lines.

The dispersion model proposed in *Paper II* was implemented in component models, and a model of a real milk sterilization line¹ was configured. See Figs. 8 & 9. The system was simulated for product filling after start-up with water and vice versa, i.e. product emptying with water during shut-down. The capacity was 7000 l/h. The same sequences were also performed in experiments where the concentration of product² was

¹ The modelled milk sterilizer is a commercial product, Tetra Therm[®] Aseptic Flex, designed and manufactured by Tetra Pak Processing Systems, Lund, Sweden.

² A dilute salt solution was used as the “product”.

measured. Figs. 10 & 11 show the results. The simulated and actual losses of raw material (milk fit to drink, 0.5 % - 97.5%) were as follows.

- Filling
 - average of two experiments: 79 litres
 - simulation: 66 litres
- Emptying
 - average of two experiments: 24 litres
 - simulation: 22 litres
- Total
 - average of two experiments: 103 litres
 - simulation: 88 litres

If we had considered the production of two products with water flush between them, then the total product losses would have been twice as high. Performing a product change on the fly may reduce the product loss if the product-product contamination is more acceptable than water dilution. The disadvantage of this could be diffusing batch identities. See section 5.3 on traceability.

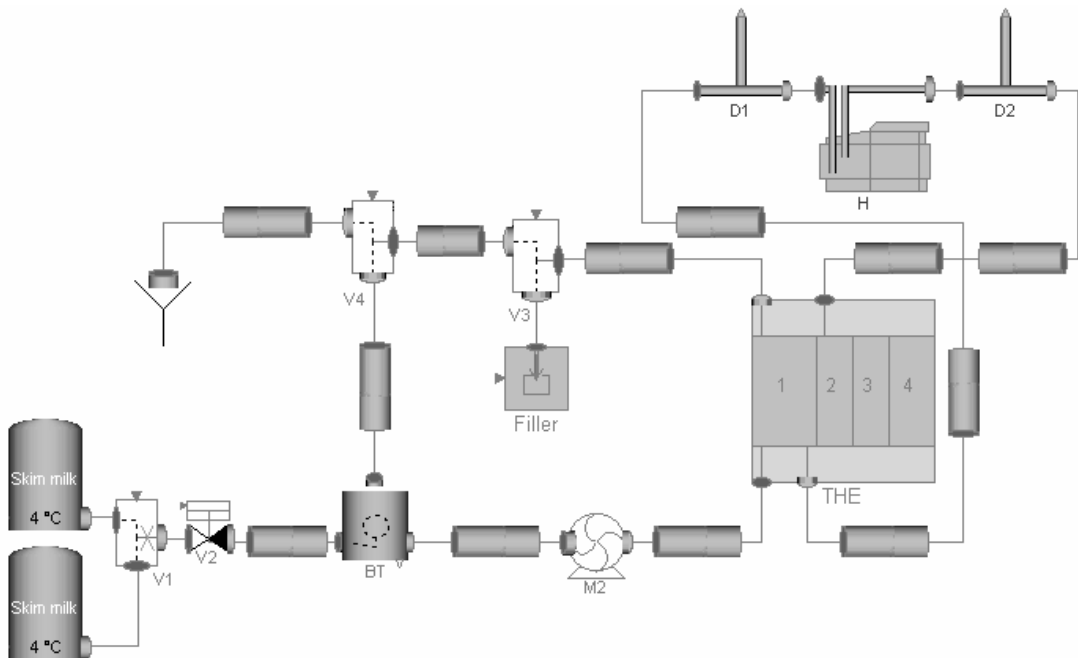


Fig. 8. Flow chart of a real milk sterilization line with the following major components: two source tanks (“Skim milk”), a balance tank (BT), a tubular heat exchanger system (THE, see Fig. 9), a homogenizer (H) with two pressure dampers (D1 and D2) and a packaging machine (Filler).

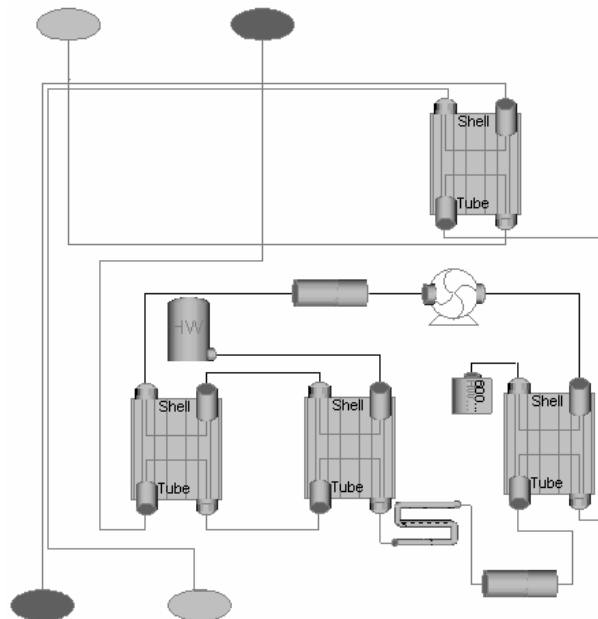


Fig. 9. Flow chart of details in the tubular heat exchanger system, THE, in Fig. 8.

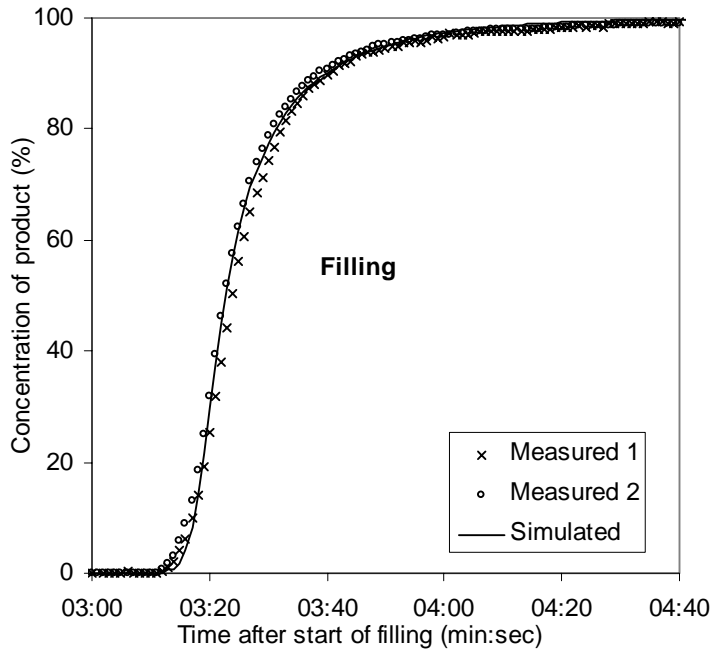


Fig. 10. Concentration of product at V3 in Fig. 8 around 4 minutes after the start of the filling process.

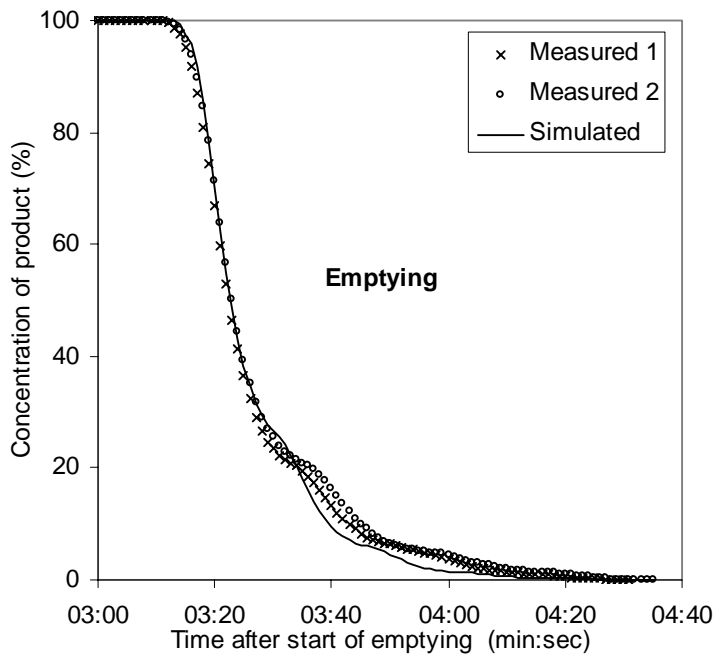


Fig. 11. Concentration of product at V3 in Fig. 8 around 4 minutes after the start of the emptying process.

5.2 Chemical reactions

A large proportion of liquid food production involves processing to deactivate microorganisms by heating of the product. During this process the quality of the product is also affected. Much work has been done on describing these processes. A comprehensive survey of the field has been published in IDF Bulletin No. 392 (2004). This bulletin contains many articles, for example the review article by Valdramidis et al. (2004). A widely used model of the processes is the first-order chemical reaction model (e.g. Kessler, 2002; Walstra et al., 1999; Burton, 1988). The model parameters for first-order chemical reactions are the reaction constant, k_0 , and activation energy, E_a . Within the field of deactivating microorganisms, these parameters are commonly replaced by the decimal reduction time, D_r , and the temperature increase for decimal reduction, z_r , both related to a reference temperature, T_r . The formal mathematical relationships between the model parameters for a strictly first-order chemical reaction are given in Eqs. (13) and (14).

$$E_a = \ln(10)RT_r^2 \left(\frac{1}{z_r} + \frac{1}{T_r} \right) \quad (13)$$

$$k_0 = \frac{\ln(10)e^{\frac{E_a}{RT_r}}}{D_r} \quad (14)$$

The complex situation in a whole pasteurization or sterilization line makes it difficult to calculate the total effect in non-isothermal dispersed flow, particularly for dynamic changes during transitions in the production, e.g. a change in capacity, or a change of fluid when many variables are changed or disturbed simultaneously, for example, viscosity, flow rate, temperature and dispersion. In these cases, dynamic simulation helps predict and understand the deactivation of microorganisms and quality change. Measurements may seem a good alternative, but apart from the cost of experiments, it is very difficult to measure microorganism content during the rapid changes that take place in many continuous heat-treatment processes. Moreover, in many cases, e.g. sterilization lines, the target for the reduction of microorganisms is a factor of 10^{12} , which makes it extremely difficult or costly to measure.

Since the first-order chemical reaction model is so widely spread, and with reaction parameters available, this model was implemented as an extension to the dispersion model proposed in *Paper II*. This is described in *Paper III*, which presents analyses of the model with first-order chemical reactions during:

- axial-dispersed plug flow,
- non-isothermal conditions and
- variable flow.

To translate the tabulated reaction data used in the simulations (Kessler, 2002; Walstra et al., 1999; Burton 1988), Eqs. (13) and (14) were used. To improve calculations in the model for *non-isothermal* processes, the mean temperature in the discretized finite volumes was replaced by the approximation in Eq. (15) based on an evaluation of Eq. (1) during a linear temperature change, with a temperature dependency of k , according to the Arrhenius equation. (The definitions of the symbols used can be found in the Notation at the end of this thesis.)

$$\ln\left(\frac{C_{in}}{C_{out}}\right) = \int_0^\tau k_0 e^{-\frac{E_a}{RT_{in}\left(1+\frac{\dot{T}t}{T_{in}}\right)}} dt \approx \int_0^\tau k_0 e^{-\frac{E_a}{RT_{in}}\left(1-\frac{\dot{T}t}{T_{in}}\right)} dt = \tau k_0 e^{-\frac{E_a}{RT_{in}}} e^{\frac{E_a \Delta T}{RT_{in}^2} - 1} \quad (15)$$

This equation was evaluated and used in the model. The model exhibited good computational efficiency. Fig. 12 shows how the simulation of the logarithmic reduction, $\log(C_{in}/C_{out})$ converges to the same value for a traditional model and the model proposed in this work. The corresponding computation time (CPU time) shows that the proposed model requires approximately one tenth of the CPU time required for the traditional model.

Furthermore to efficiently account for *variable flow* in pipes, i.e. tubular reactors, the true residence time, τ , was calculated using the modelling tool in a similar way as for the concentration and the fluid properties in Eqs. (5) and (7). In this way, a dynamic residence time was calculated accurately according to Eq. (16) independently of the level of discretization.

$$\tau(t) = t - \bar{t}_{in} \quad (16)$$

Thus, simulations of first-order chemical reactions in pipes with plug flow are correct for varying flow without any discretization (*Paper III*).

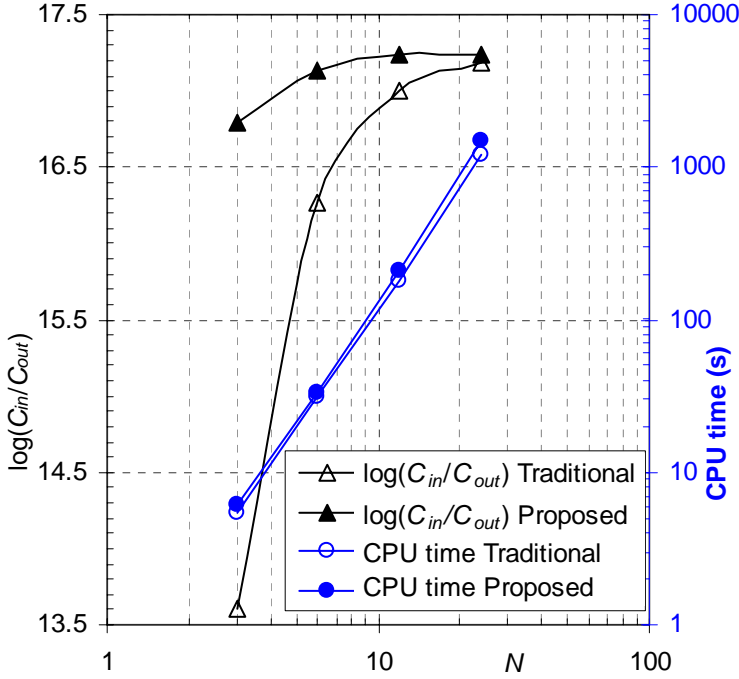


Fig. 12. Convergence of computed logarithmic reduction, $\log(C_{in}/C_{out})$, and corresponding computation time, CPU time.

5.3 Traceability in continuous processing

Traceability systems are normally designed for distinct batch production where the content of a final product is well defined. In all current traceability systems the definition of a batch is fundamental. Kim et al. (1999) define a traceable resource unit (TRU) as a unit with unique characteristics that no other unit can have, from a traceability point of view, in a batch process. However, as Moe (1998) states, when dealing with continuous processing, defining a TRU is difficult. The practice of changing production with as few costly cleaning cycles (or water flushing) as possible between batches leads to production with changeover on the in fly, which creates mixing zones where one batch,

based on certain raw materials and production parameters, is gradually replaced by another, with a different composition and different production parameters. The implication of this kind of production, from a traceability point of view, is that a withdrawal or recall of a final product must cover more than one batch, unless the producer has good knowledge of the mixing zones. In *Paper IV*, the benefit of being able to simulate the mixing zones was analysed and discussed in terms of “*fuzzy traceability*” due to the non-distinct batch identities in a continuous production line. Fig. 13 shows the simulated mixed content in the consumer packages in a realistic UHT milk production line, illustrated previously in Figs. 8 and 9. The mixing zone was caused by a production changeover on the fly.

Data from such simulations can be used to calculate cost consequences based on criteria for product contamination. The data shown in Fig. 13 were combined with such criteria and production costs to calculate the cost of product withdrawal. The results are shown in Fig. 14. Changes in production parameters can be studied to evaluate the effect on the mixing zones. This is illustrated in *Paper IV*.

Figs. 13 and 14 demonstrate that applying dynamic simulation in traceability systems can improve production management in terms of better process information. This will lead to better handling of rejects or withdrawals, reducing production costs and improving consumer faith in products.

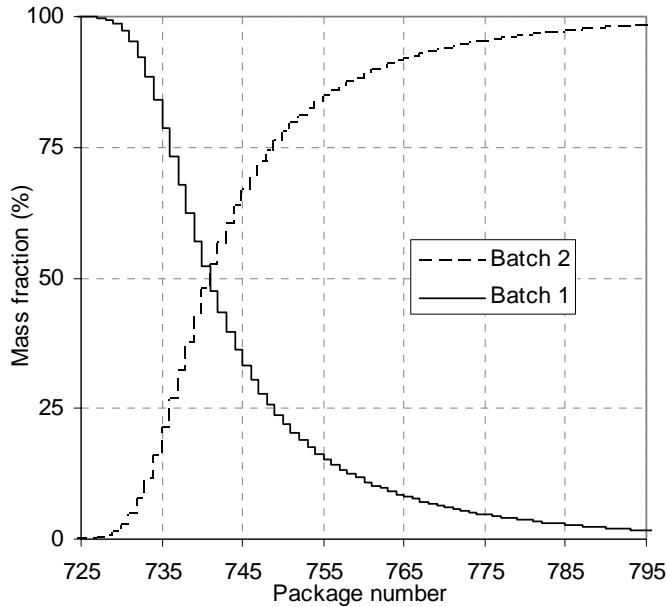


Fig. 13. Content in consumer packages of a product with the same specification, but based on different batches. The mixing zone is caused by changeover on the fly.

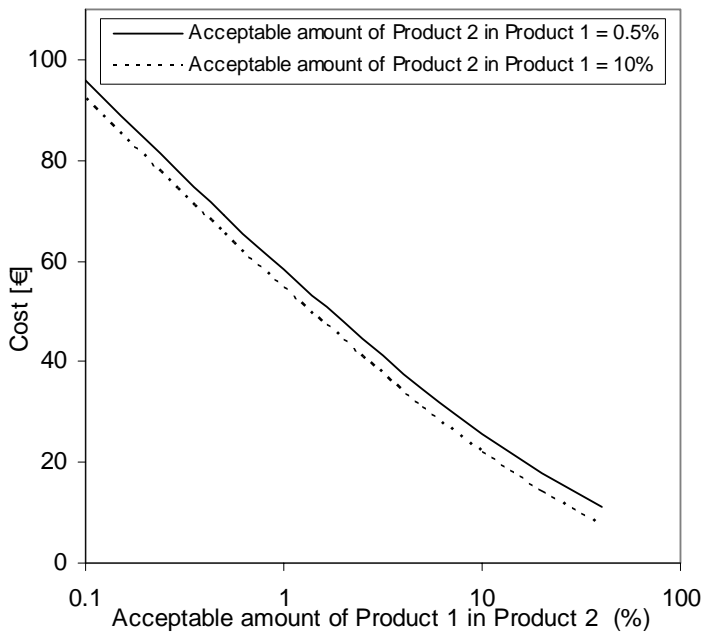


Fig. 14. Cost of withdrawal depending on the acceptable contamination level, calculated from data shown in Fig. 13. The cost was assumed to be 0.5 € per litre final product.

6. Conclusions

A dynamic model library with novel models was developed using a modern object-oriented language (Modelica). The models were adapted for the simulation of liquid food process lines.

It was demonstrated that a transport delay model was well suited for the simulation of convective fluid propagation. It was also demonstrated that classical models of fluid propagation in process lines could be combined with modern numerical methods to obtain computationally efficient dynamic models for the simulation of dispersed convective flow, with and without chemical reactions. The main results are summarized below.

The physics of convection:

$$\frac{\partial C}{\partial t} + v \frac{\partial C}{\partial x} = 0 \quad (17)$$

Classic transformation into an infinite number of volumes (tanks):

$$\text{For } \forall i \in [1, N]: \frac{V}{N} \frac{\partial C_i}{\partial t} + QC_i - QC_{i-1} = 0 \quad (18)$$

and $N \rightarrow \infty$

Model in this thesis:

$$\hat{C}_{out}(t) = \hat{\tilde{C}}_{in}(t) = \hat{C}_{in}(t - \tau) \quad (19)$$

$$\text{where } \tau = \tau(v(t)): L = \int_0^\tau v(t) dt \quad (\text{dynamic transport delay}) \quad (20)$$

The physics of axially dispersed plug flow:

$$\frac{\partial C}{\partial t} + v \frac{\partial C}{\partial x} - D \frac{\partial^2 C}{\partial x^2} = 0 \quad (21)$$

Classic transformation into “N continuously stirred tanks”: (N-CST model):

$$\text{For } \forall i \in [1, N]: \frac{V}{N} \frac{\partial C_i}{\partial t} + QC_i - QC_{i-1} = 0 \quad (22)$$

where

$$N = \frac{vL}{2D} = \frac{Pe}{2} \quad (23)$$

Combined model in this thesis:

$$\text{For } \forall i \in [1, N]: V_N \frac{\partial C_i}{\partial t} + QC_i - QC_{i-1} = 0 \text{ (dispersion part)} \quad (24)$$

where

$$C_{i=0}(t) = C_{in}(t - \tau_0) \quad (\text{plug flow}) \quad (25)$$

$$\text{where } \tau_0 = \tau_0(v(t)): L_0 = \int_0^{\tau_0} v(t) dt \quad (\text{dynamic transport delay}) \quad (26)$$

$$V = V_0 + NV_N \quad (\text{volume conservation}) \quad (27)$$

$$V_N = V \sqrt{\frac{2}{NPe}} \quad (\text{from Paper II}) \quad (28)$$

N can be chosen freely to balance the speed and accuracy of the simulations as in modern numerical methods, but *N* must be $\leq Pe/2$.

The physics of axially dispersed plug flow with first-order chemical reactions:

$$\frac{\partial C}{\partial t} + v \frac{\partial C}{\partial x} - D \frac{\partial^2 C}{\partial x^2} + kC = 0 \quad (29)$$

Model in this thesis:

Based on the combined axial dispersion model above with the following added:

Concentration factor in each control volume:

$$e^{-\frac{Pe}{2N} \left(\sqrt{1 + \frac{2\tau_{0N}k}{Pe}} - 1 \right)} \quad (\text{from Paper III}) \quad (30)$$

Approximation in non-isothermal flow conditions:

$$\ln \left(\frac{C_{out}}{C_{in}} \right) = -\tau k(\max(T_{out}, T_{in})) \frac{1 - e^{-\frac{E_a |\Delta T|}{R \max(T_{out}, T_{in})^2}}}{\frac{E_a |\Delta T|}{R \max(T_{out}, T_{in})^2}} \quad (\text{from Paper III}) \quad (31)$$

with $k(T)$ according to the Arrhenius equation.

Modelling of chemical reactions during *arbitrary flow variations* by using the true hold-up time through the transport-delayed time.

$$\tau(t) = t - \tilde{t}_{in} \quad (\text{from Paper III}) \quad (32)$$

In particular it was demonstrated that:

- The convection model exhibited good computational performance for thermal transients in heat exchangers during fluid transitions (*Paper I*).
- The dispersion model exhibited good computational performance in simulating axially dispersed plug flow, typical for liquid food applications (*Paper II*). The model also showed good

- performance as regards step response (rate of change and break through time).
- The extended dispersion model including first-order chemical reactions showed good performance in non-isothermal and non-constant flow, typical for liquid food applications (*Paper III*).

Furthermore, it was illustrated how the dispersion model could be utilized for the simulation of mixing zones in production lines to enhance production management in terms of better process information concerning traceability, “*fuzzy traceability*”, for improved handling of rejects or withdrawals (*Paper IV*).

Specifically, it can be concluded that combining classical and modern modelling methods provides opportunities for efficient dynamic simulation. More generally, the overall conclusion is that dynamic phenomena present in liquid food production lines, can be simulated by means of dynamic modelling using a modern, object-oriented modelling tool.

This work thus provides benefits for the liquid food processing industry. Some of the benefits are the possibility of better predicting and understanding the phenomena and problems in a production line. Thus, by means of dynamic simulation, performance can be improved and problems can be resolved.

Furthermore, the computationally efficient models presented in this thesis offer other potential benefits as it may enable real-time simulation. This leads to a number of possibilities. For example, real-time simulation, with a link to the control system, can be employed for realistic operator training and to improve process design and PLC programs. Real-time simulation can also be used for process diagnosis as it enables simulation in parallel with the real process to detect process deviations.

7. Future outlook

This thesis signifies the end of a PhD project, and a small contribution to the broad topic of dynamic simulation of liquid food process lines. Hopefully, many of the visions of Cox et al. (2006) will be realised within the coming decade. However, there are still many hurdles to be overcome. Below are some suggestions for future research.

- Models adapted for more complex fluids than power-law fluids, for example, Herschel-Bulkley fluids, are needed.
- Models are required for fluids containing particles or other multi-phase systems.
- There is a need for better generic knowledge of the relations between rheological properties and composition and temperature.
- Models of rheological properties in more complex fluids, e.g. those containing starch and fibres, are required.
- There is a need for feasible models for the dynamic simulation of mixing zones in laminar flow in complex process lines.
- There is a need for models that can simulate the dispersion in plate heat exchangers based on the flow patterns (e.g. maldistribution) rather than a lumped dispersion included in a single dispersion coefficient.
- Adaptations should be made for real-time simulation aiming at HILS.
- More validation of models is needed.
- More models for fouling are needed. Some are available, but there is much left to be done, particularly regarding mineral fouling of milk.
- Models for cleaning are required, i.e. the removal of fouling. Some work has been done, but a great deal remains.

With the development of modelling tools, including solvers, future process and control engineers in the food industry will no longer have to rely on “a heuristic understanding of plant dynamics when making key decisions affecting plant operability,” in the words of Cox et al. (2006).

Notation

Latin letters

C	Volumetric concentration, kg m^{-3}
\hat{C}	Concentration component vector (in the present case a 5-element vector of water, carbohydrates, protein, fat and ash), kg m^{-3}
\vec{C}	C at channel exit delayed by transport through the channel, i.e. $\vec{C}(t) = C(t - \tau)$, kg m^{-3}
$\vec{\hat{C}}$	\hat{C} at channel exit delayed by transport through the channel, i.e. $\vec{\hat{C}}(t) = \hat{C}(t - \tau)$, kg m^{-3}
c_p	Specific heat capacity, $\text{J kg}^{-1} \text{K}^{-1}$
D	Dispersion or diffusivity, $\text{m}^2 \text{s}^{-1}$
D_r	Microbial decimal reduction time at the reference temperature T_r , s
d	Diameter or hydraulic diameter, m
E_a	Energy of activation in the Arrhenius equation, $k = k_0 e^{\frac{E_a}{RT}}$, J mol^{-1}
K	Consistency of fluid defined by $\sigma = K \dot{\gamma}^n$, Pa s^n
k	Chemical reaction constant, depending on the temperature according to the Arrhenius equation, $k = k_0 e^{\frac{E_a}{RT}}$, s^{-1}
k_0	Chemical reaction constant, s^{-1}
L	Length of flow channel, m
L_0	Total length of plug flow components in the PFNCST model, m
N	Discretization number in models (i.e. grid size = L/N) or number of continuously stirred tanks in the N-CST dispersion model, -
n	Flow behaviour index of fluid, defined by $\sigma = K \dot{\gamma}^n$, -
Pe	Péclet number, defined by vL/D (the ratio of convective flow rate to dispersive flow rate), -
Q	Volumetric flow rate, $\text{m}^3 \text{s}^{-1}$
R	Universal gas constant, $8.31451 \text{ J mol}^{-1} \text{K}^{-1}$
Re	Reynolds number, defined by $Re = \rho v d / \mu$, -

Notation

T	Absolute temperature, K
T_r	Reference temperature for microbial reduction kinetics, K
\dot{T}	Rate of temperature change, K s ⁻¹ or °C s ⁻¹
t	Time, s
\bar{t}	t delayed by virtual transport through the channel, i.e. $\bar{t}(t) = t(t - \tau)$, s
\tilde{t}	Dimensionless time, defined by $\tilde{t} = t / \tau$, -
V	Volume, m ³
V_0	Total volume of plug flow components in the PFNCST model, m ³
V_N	Volume of one of the N ideally mixed volumes (continuously stirred tanks) in the PFNCST mode, m ³
v	Velocity or mean velocity over a channel cross-sectional area, m s ⁻¹
x	Axial spatial coordinate (along the fluid channel), m
\tilde{x}	Dimensionless axial spatial coordinate (along the fluid channel) defined by $\tilde{x} = x / L$, -
z_r	The microbial decimal reduction temperature increase, °C or K

Greek letters

ΔX	Change in X
$\dot{\gamma}$	Shear rate, s ⁻¹
λ	Thermal conductivity, Wm ⁻¹ K ⁻¹
μ	Dynamic viscosity, defined by $\mu = \sigma / \dot{\gamma}$, Pa s
ρ	Density, kg m ⁻³
σ	Shear stress, Pa
τ	Average transport time (residence time) for a fluid through a channel, V/Q or L/v , s More generally, including dynamic delay, i.e. varying velocities: $\tau = \tau(v(t)) : L = \int_0^\tau v(t) dt$
τ_0	Total transport time (residence time) for a fluid through all the plug flow components in the PFNCST model, $L_0/v = V_0/Q$, s

More generally, including dynamic delay, i.e. varying velocities:

$$\tau_0 = \tau_0(v(t)) : L_0 = \int_0^{\tau_0} v(t) dt$$

τ_N Average transport time (residence time) for a fluid through one of the N continuously stirred tanks in the PFNCST model, V_N/Q , s

τ_{0N} Transport time (residence time) for a fluid through one if the N plug flow parts in the PFNCST model, $L_0/(Nv) = V_0/(NQ)$, s
More generally, including dynamic delay, i.e. varying velocities:

$$\tau_{0N} = \tau_{0N}(v(t)) : \frac{L_0}{N} = \int_0^{\tau_{0N}} v(t) dt$$

Subscripts

in Channel inlet
out Channel outlet

Other symbols

A Laplace transform of A

∇ Gradient vector operator $\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)$

∇^2 Scalar operator $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

X Vector X

\vec{X} X delayed by transport through a channel, i.e. $\vec{X}(t) = X(t - \tau)$,
e.g. $X_{out}(t) = \vec{X}_{in}(t) = X_{in}(t - \tau)$

Acronyms

ADPF	Axial-dispersed plug flow
AE	Algebraic equation
CFD	Computational fluid dynamics
DAE	Differential algebraic equation (combination of ODEs and AEs)
FDM	Finite difference method
FEM	Finite element method
FVM	Finite volume method
HILS	HWIL simulation
HWIL	Hardware-in-the-loop
N-CST	N continuously stirred tanks
ODE	Ordinary differential equation
OOP	Object oriented programming
PDE	Partial differential equation
PFCST	Plug flow combined with 1 continuously stirred tank
PFNCST	Plug flow combined with N continuously stirred tanks
PID	Proportional integrating controller
PLC	Programmable logic controller
RTD	Residence time distribution
TRU	Traceable resource unit

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References

- Abdelghani-Idrissi, M.A., Bagui, F., Estel, L. (2001) Analytical and experimental response time to flow rate step along a counter flow double pipe heat exchanger. *International Journal of Heat and Mass Transfer*, 44, pp. 3721-3730.
- Åström, K. J., Elmqvist, H., Mattsson, S. E. (1998) Evolution of Continous-time Modeling and Simulation. *The 12th Simulation Multiconference, ESM'98*, June 16-19, 1998, Manchester, UK.
- Bäckman, J., Edvall, M. (2005) Using Modelica and Control Systems for Real-time Simulations in the Pulp. *Proceedings of the 4th International Modelica Conference*, March 7-8, 2005, pp. 579-583, Hamburg University of Technology (TUHH), Germany. Organized by the Modelica Association and TUHH. (<http://www.modelica.org>)
- Bischoff, K. B., Levenspiel, O. (1962a) Fluid Dispersion-Generalization and Comparison of Mathematical Models - I. Generalization of Models. *Chemical Engineering Science*, 17, pp. 245-255.
- Bischoff, K. B., Levenspiel, O. (1962b) Fluid Dispersion-Generalization and Comparison Of Mathematical Models - II. Comparison of Models. *Chemical Engineering Science*, 17, pp. 257-264.
- Burton, H. (1988) Ultra-High-Temperature Processing of Milk and Milk Products, *Elsevier Applied Science*, London (1988) ISBN 1-85166-170-0.
- Casella, F., Schiavo, F. (2003) Modelling and Simulation of Heat Exchangers in Modelica with Finite Element Methods. *Proceedings of the 3rd International Modelica Conference*, Linköping, Sweden, November 3-4, 2003, pp. 343-352, Organized by Modelica Association and Linköping University, Sweden. (<http://www.modelica.org>)
- Casella, F., Otter, M., Proelss, K., Richter, C., Tummescheit, H. (2006) The Modelica Fluid and Media library for modelling of incompressible and compressible thermo-fluid pipe networks. *Proceedings of the 5th International Modelica Conference*, Vienna, Austria, September 4-5, 2006, pp. 631-640, Organized by Modelica Association and Arsenal Research, Austria. (<http://www.modelica.org>)

- Cox, R.K., Smith, J.F., Dimitratos Y. **(2006)** Can simulation technology enable a paradigm shift in process control? Modeling for the rest of us. *Computers & Chemical Engineering*, 30, pp. 1542-1552.
- De Prada, C., Merino, A., Pelayo, F., Acebes, F., Alves, R. **(2003)** A simulator of Sugar Factories for Operator Training, *AfoT 2003, II International Workshop on Information Technologies and Computing Techniques for the Agro-Food Sector*, Barcelona, Spain, November 27-28, 2003, Monograph CIMNE No-86.
- Eborn, J. **(2001)** On Model Libraries for Thermo-hydraulic Applications, *PhD thesis ISRN LUTFD2/TFRT - - 1061 - - SE, Department of Automatic Control, Lund Institute of Technology*, Lund, Sweden.
- Elmqvist, H., Tummescheit, H., Otter, M. **(2003)** Object-Oriented Modeling of Thermo-Fluid Systems. *Proceedings of the 3rd International Modelica Conference*, Linköping, Sweden, November 3-4, 2003, pp. 269-286, Organized by Modelica Association and Linköping University, Sweden (<http://www.modelica.org>).
- EU Regulation (EC) 178/2002 articles 14-20 **(2002)**
- Galle, M., Agar, D. W. Watzenberger, O. **(2001)** Thermal N₂O decomposition in regenerative heat exchanger reactors. *Chemical Engineering Science*, 56, pp. 1587-1595.
- Gut, J.A.W., Pinto, J.M. **(2003)** Modeling of plate heat exchangers with generalized configurations. *International Journal of Heat and Mass Transfer*, 46, pp. 2571-2585.
- Heath, M. T. **(2002)** Scientific computing : an introductory survey. *McGraw-Hill, cop*, New York, USA.
- Haugwitz, S. **(2005)** Modeling and control of the open plate reactor. *Licentiate thesis. Department of Automatic Control, Lund Institute of Technology*, Lund, Sweden.
- Hopkins, M. J., Sheppard, A. J., Eisenklam P. **(1969)** The use of transfer functions in evaluating residence time distribution curves. *Chemical Engineering Science*, 24, pp. 1131-1137.
- IDF Bulletin N° 392 **(2004)** Food Safety Objective (FSO) & Performance Objective (PO). *Bulletin of the International Dairy Federation* N° 392/2004.

- Hawthorn, R. D., Ackerman, G. H., Nixon, A.C., **(1968)** A mathematical model of a packed-bed heat-exchanger reactor for dehydrogenation of methylcyclohexane - comparison of predictions with experimental results. *Aiche Journal*, 14, pp. 69-76.
- Kauhanen, P. **(2004)** Verifying the dynamic model of a heat exchanger configuration. MSc thesis, *Department of Chemical Engineering, Faculty of Engineering LTH*, Lund, Sweden.
- Kessler, H.G. **(2002)** Food and Bio process Engineering. *Verlag A. Kessler*, München, Germany, ISBN 3-9802378-5-0.
- Kim, H.M., Fox, M.S. and Gruninger, M., **(1999)** An ontology of quality management – enabling quality problem identification and tracing. *BT Technology Journal*, 17, pp. 131-140.
- Lakshmanan, C.C., Potter, O.E. **(1994)** Dynamic simulation of a counter current heat exchanger modelling-start-up and frequency response. *Int. Commun. Heat Mass Transfer*, 21, pp. 421-434.
- Levenspiel, O., Bischoff, K. B. **(1963)** Patterns of flow in chemical process vessels. *Advances in Chemical Engineering*, 4, pp. 95-198.
- Levenspiel, O., Smith W. **(1957)** Notes on the Diffusion-Type Model for the Longitudinal Mixing of Fluids in Flow. *Chemical Engineering Science*, 6, pp. 227-233.
- Luo, X., Guan, X., Li, M., Roetzel, W. **(2003)** Dynamic behaviour of one-dimensional flow multistream heat exchangers and their networks. *International Journal of Heat and Mass Transfer*, 46, pp. 705-7153.
- Malinowski, L., Bielski, S. **(2004)** An analytical method for calculation of transient temperature field in the counter-flow heat exchangers. *International Communications in Heat and Mass Transfer*, 31, pp. 683-691.
- Marquardt, W. **(1996)** Trends in Computer-Aided Process Modeling. *Computers and Chemical Engineering*, 20, pp. 591-609.
- Mattsson, S. E., Elmqvist, H., Otter, M. **(1998)** Physical system modeling with Modelica. *Control Engineering Practice*, 6, pp. 501-510.
- Mattsson, S. E., Ericsson, M., Östberg, P. **(1994)** An Object-oriented model of a heat exchanger unit. *The Object-Oriented Modeling and*

- Simulation Conference at the European Simulation Multiconference*, Barcelona, Spain, June 1-3, 1994.
- Modelica, object oriented modelling language. *Modelica Association*, <http://www.modelica.org>.
- Moe, T. (1998) Perspectives on traceability in food manufacture. *Trends in Food Science and Technology*, 9, pp. 211-214.
- Norton, T., Sun, D-A. (2006) Computational fluid dynamics (CFD) – an effective and efficient design and analysis tool for the food industry: A review. *Trends in Food Science & Technology*, 17, pp. 600-620.
- Phillips, C. H., Lauschke, G. and Peerhossaini, H. (1997) Intensification of batch chemical processes by using integrated chemical reactor-heat exchangers. *Applied Thermal Engineering*, 17, pp. 809-824.
- Roetzel, W., Balzereit, F. (2000) Axial dispersion in shell-and-tube heat exchangers. *International Journal of Thermal Sciences*, 39, pp. 1028-1038.
- Roetzel, W., Das, S. K. (1995) Hyperbolic axial dispersion model: concept and its application to a plate heat exchanger. *International Journal of Heat and Mass Transfer*, 38, pp. 3065-3076.
- Roetzel, W., Xuan, Y. (1992) Transient-Response of Parallel and Counterflow Heat-Exchangers. *Journal of Heat Transfer-Transactions of the Asme*, 114, pp. 510-512.
- Roetzel, W., Xuan, Y. (1999) Dynamic Behaviour of Heat Exchangers. *WIT Press*, UK, ISBN 1853125067.
- Romie, F.E. (1984) Transient-Response of the Counterflow Heat-Exchanger. *Journal of Heat Transfer-Transactions of the Asme*, 106, pp. 620-626.
- Romie, F.E. (1985) Transient-Response of the Parallel-Flow Heat-Exchanger. *Journal of Heat Transfer-Transactions of the Asme*, 107, pp. 727-730.
- Romie, F.E. (1999) Response of counterflow heat exchangers to step changes of flow rates. *Journal of Heat Transfer-Transactions of the Asme*, 121, pp. 746-748.
- Sahoo, R. K., Roetzel, W. (2002) Hyperbolic axial dispersion model for heat exchangers. *International Journal of Heat and Mass Transfer*, 45, pp. 1261-1270.

- Schneider, R., Marquardt, W. (2002) Information technology support in the chemical process design life cycle. *Chemical Engineering Science*, 57, pp. 1763–1792.
- Serpemen, Y., Deckwer, W-D. (1974) Instationary Dispersed Plug Flow Model with Linear Rate Processes. *Ind. Eng. Chem. Fundam.*, 13, pp. 399–400.
- Sharifi, F., Narandji, M.R.G., Mehravaran, K. (1995) Dynamic Simulation of Plate Heat-Exchangers. *International Communications in Heat And Mass Transfer*, 22, pp. 213-225.
- Tan, N.K., Spinner, I.H. (1991) Approximate solution for transient response of a shell and tube heat exchanger. *Industrial & engineering chemistry research*, 30, pp. 1639-1646.
- Taylor, G. (1953) Dispersion of soluble matter in solvent flowing slowly through a tube. *Proceedings of the Royal Society of London Series A*, 219, pp. 186-203.
- Taylor, G. (1954a) The dispersion of matter in turbulent flow through a pipe. *Proceedings of the Royal Society of London Series A*, 223, pp. 446-468.
- Taylor, G. (1954b) Diffusion and Mass Transport in Tubes. *Proceedings of the Physical Society of London*, 67, pp. 857-869.
- Tiller, M. (2001) Introduction to Physical Modeling with Modelica. *Kluwer Academic Publishers*, Massachusetts, USA, ISBN 0-7923-7367-7.
- Tummescheit, H. (2002) Design and Implementation of Object-Oriented Model Libraries using Modelica, *PhD thesis ISRN LUTFD2/TFRT - - 1063 - - SE, Department of Automatic Control, Lund Institute of Technology*, Lund, Sweden.
- Valdramis, V.P., Geeraerd, A.H., Beraerts, K., Devlieghere, F., Debevere, J., and Van Impe, J.F. (2004) Accurate Modelling of Non-Loglinear survival Curves. *IDF Bulletin* N° 392.
- Walstra, P., Geurts, T. J., Noomen, A., Jellema, A. and van Boekel, M. A.J.S. (1999) Dairy Technology: principles of milk properties and processes, *Marcel Dekker*, New York, ISBN 0-8247-0228-X.

References

- Wang, L., Sun, D-W. (2003) Recent developments in numerical modelling of heating and cooling processes in the food industry – a review. *Trends in Food Science & Technology*, 14, pp. 408-423.
- Wen, C. Y., Fan, L. T. (1975) Models for Flow Systems ad Chemical Reactors. *Marcel Dekker*, New York, USA (1975) ISBN 0-8247-6346-7.
- Wozny, G., Jeromin, L. (1991) Dynamic Process Simulation in Industrial Practice. *Chemie Ingenieur Technik*, 63, pp. 313-326.
- Xuan, Y., Roetzel, W. (1993a) Dynamics of shell-and-tube heat exchangers to arbitrary temperature and step flow variations. *Aiche Journal*, 39, pp. 413-421.
- Xuan, Y., Roetzel, W. (1993b) Stationary and dynamic simulation of multipass shell and tube heat exchangers with the dispersion model for both fluids. *International Journal of Heat and Mass Transfer*, 36, pp. 4221-4231.
- Yin, J., Jensen, M. K. (2003) Analytic model for transient heat exchanger response. *International Journal of Heat and Mass Transfer*, 46, pp. 3255 – 3264.