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A dynamic object-oriented model for efficient simulation of fluid dispersion in turbulent flow with varying fluid properties

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Abstract

Dispersion coefficients for turbulent flow are commonly available, but the common models are not easily implemented for fast computation of dispersion in time-dependent large flow systems.

Criteria were developed to aid in the choice of parameters for a model combining plug flow with the N-continuously-stirred-tanks model to obtain the best agreement with the pure axial-dispersed plug-flow model, while simultaneously being computationally efficient. Solution accuracy and computational savings were demonstrated for a realistic food industry example. The proposed model includes a method of structuring the discretization to handle the simulation of pressure drop and momentum balance simultaneously with simulation of dispersion.

The criteria were derived from the analysis of Laplace transforms. It was also shown that the proposed model predicts the response to a step change in concentration in agreement with the exact solution of the axial-dispersed plug-flow model.

The model was written in the object-oriented language Modelica as an object in a library structure which is being developed to simulate complex liquid food process lines and their control systems.

Keywords: Dispersion, Residence time distribution, Fluid property transition, Dynamic model, Dynamic simulation, Liquid food

Article outline

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1. Introduction

Dynamic simulation of chemical process lines has not yet reached others than specialists and still has the potential for further development. Overviews of the current status have been given by Åström et al. (1998) and Cox et al. (2006). Cox et al. also present a vision of the many benefits of using dynamic simulation by those other than experts. We share this vision of applications within the field of liquid food processing and we are engaged in developing a library of such dynamic models (Skoglund, 2003; Skoglund and Dejmek, 2006; Skoglund et al., 2006).

Over the years, many tools and languages have been presented for dynamic simulation. Marquardt (1996) gives an overview of the trends and concludes that a common paradigm is the complete decoupling of model representation and its application. We have chosen the language Modelica (Modelica Association; Tiller, 2001) in the Dymola environment (Dynasim AB in Lund, Sweden). The purpose is to enable a non-specialist to quickly and easily configure liquid food process-line models for dynamic simulation. The Modelica language is non-causal, object-oriented, and suitable for physical modelling while fulfilling the requirement for a modern tool. Many Modelica models and libraries for dynamic simulation of thermo-fluid systems are currently being developed (e.g. Elmqvist et al., 2003; Tummescheit, 2002; Casella et al., 2006).

Time is always valuable in development and engineering. In large models, when simulation time easily becomes minutes and hours, time saving is a very strong impetus. The models we are developing are aimed at dynamic simulation of complex production lines for fluids that are mixtures of components (e.g. water, carbohydrates and fat) and include tanks, pipes, heat exchangers pumps, flash vessels, filling machines, sensors, PID controllers, logical sequences, etc. The dynamic simulations must cover flow rates, pressures, temperatures, concentrations and levels, and in our opinion such complex systems can not be practically simulated by means of detailed

CFD models with full time-space resolution. Our primary approximation is to consider only one space coordinate, that along the fluid channel. Therefore, to simulate large liquid food processing systems, e.g. complete milk pasteurizers, efficient dynamic models are required to avoid long computation times that cause long waiting times in development and engineering work. The need for computational speed becomes even more pronounced in real-time (in-line) simulations. Such simulations are performed to enable realistic communication with control systems and the operators' interface to ensure realistic mimicking of the dynamic behaviour of a full production line. Real-time simulations are becoming more common in other branches for various purposes, e.g. system verification and operator training (e.g. Bäckman & Edwall, 2005). Simulations of this kind will obviously impose heavy computational demands. Methods using suitable approximations are therefore required.

In the liquid food industry, production lines have sequences for start-up and shut-down. In the start-up case, water is run through the fluid channels in the plant followed by the food product, and in the shut-down case, the procedure is reversed, i.e. the product is flushed out by water. Direct product changeover, where one product is directly followed by another, is also employed. What these procedures have in common is that they are all concerned with transient changeover of fluid composition. These transients in composition cause zones of mixed fluids, i.e. material that cannot be used as consumable products and therefore represent production losses. These losses constitute not only losses of raw material, but also loss of production time and utilities, such as water and electricity, required to flush the mixing zone through the plant. Furthermore, the mixed zones contribute to the environmental load, since all the material cannot be reprocessed, and some is discharged to the sewage disposal system. The mixing of fluids also affects other operations as the fluids propagate along a flow channel, e.g. the heat transfer in a heat exchanger, Skoglund et al. (2006).

There is much in the literature about dispersion phenomena, particularly concerning the residence time distribution (RTD). Many models have been developed to describe fluid flow through pipes, with and without packing material. A great deal of work has also been carried out on developing methodologies for converting experimental data into model parameters. Overviews of the work in this area have been presented by Levenspiel and Bischoff (1963) and later in the comprehensive work of Wen and Fan (1975).

In his pioneering work Taylor (1953; 1954a; 1954b) derived conditions under which the flow can be approximated by axial-dispersed plug flow (ADPF), which is commonly applied in chemical engineering. Later authors discussed cases in which ADPF is a satisfactory approximation, e.g. Levenspiel and Smith (1957) and Serpemen and Deckwer (1974). In liquid food applications these conditions (high Reynolds number and long pipes) are often fulfilled. Furthermore, many experiments have been carried out to investigate how the dispersion coefficient depends on the channel geometry, the fluid and the flow rate. Such data are widely available, e.g. Fig. 5-15 in Wen and Fan (1975).

Another commonly used model is the N-continuously-stirred-tanks (N-CST) model. The popularity of this model is due to its mathematically simple structure compared with the ADPF model. Wen & Fan (1975) have derived the relationship between N in the N-CST model and the Péclet number, Pe, in the ADPF model. In cases of moderate dispersion, typical in food industry processes, this leads to large values of N, which in turn leads to a considerable computational demand when simulating large systems. Another model often described in the literature is the

combination of plug flow and one continuously stirred tank (PFCST), e.g. Levenspiel and Bischoff (1963).

To be able to handle the above mentioned transitions, during which the dispersion coefficient varies, the model parameters must adapt dynamically. This will lead to computational difficulties with a model like N-CST, which requires the value of the number of tanks, *N*, to vary with the value of the dispersion coefficient. Another important aspect is the need to dynamically handle pressure drop and momentum balance as the fluid properties change.

This paper proposes a model that is an approximation of axial-dispersed plug flow. It combines mathematical simplicity and satisfactory accuracy with low computational demand. The model also allows for dynamic changes in the dispersion coefficient for concentration simulations, as well as for simulation of pressure drop and momentum balance. This makes it suitable for the simulation of large systems with dynamic variations in fluid properties and dispersion coefficient. The model was developed in a modern object-oriented modelling language. Based on this model, simulations of the fluid changeover from water to cream were performed to analyse the fluid dispersion and the transient behaviour.

In the evaluation, frequency response analysis was carried out using the transfer function based on the Laplace transform. This method was used as it handles arbitrary signal responses more generally than the more commonly used method of comparing moments of concentration distributions as in e.g. Bischoff and Levenspiel (1962a; 1962b). The Laplace transform and the transfer function have also been used by other authors to compare different models, e.g. Hopkins et al. (1969).

2. The proposed computationally efficient dispersion model

For turbulent flow in pipes, the axial-dispersed plug-flow (ADPF) model can be employed (Taylor, 1954a; Levenspiel, and Smith, 1957; Serpemen and Deckwer, 1974). With no source term and no chemical reaction the mass balance is given by Eq. (1).

$$\frac{\partial C(x,t)}{\partial t} + v\frac{\partial C(x,t)}{\partial x} - D\frac{\partial^2 C(x,t)}{\partial x^2} = 0 \qquad \textbf{(1)}$$

It is appropriate to carry out further analysis in the frequency domain by Laplace transformation.

2.1 Laplace transform and transfer function of the axial-dispersed plug-flow model

The Laplace transform of Eq. (1) is given by:

$$s\boldsymbol{C}(x,s) + v\frac{\partial \boldsymbol{C}(x,s)}{\partial x} - D\frac{\partial^2 \boldsymbol{C}(x,s)}{\partial x^2} = 0 \qquad \textbf{(2)}$$

For a semi-infinite long pipe where the exit concentration is studied at $x = L$, this equation represents a system with the transfer function:

$$\boldsymbol{G}_{ADPF}(s) = e^{\frac{vL}{2D}} e^{-\frac{vL}{2D}\sqrt{1+\frac{4D}{v^2}s}} \qquad \textbf{(3)}$$

which expressed with the dimensionless variables $s^* = \tau s$ and $Pe = vL/D$ becomes:

$$\boldsymbol{G}_{ADPF}(s^*) = e^{\frac{Pe}{2}} e^{-\frac{Pe}{2}\sqrt{1+\frac{4}{Pe}s^*}} \quad \textbf{(4)}$$

It is well known that this can be represented approximately by an N-continuously-stirred-tanks (N-CST) model. Wen and Fan (1975), p. 121, have derived the condition for a good approximation.

$$N_{N-CST} = \frac{vL}{2D} = \frac{Pe}{2} \quad \textbf{(5)}$$

This equation shows that a large Péclet number requires a large number of tanks, N. This means that cases with plug flow, corresponding to no dispersion (D=0), require an infinite number of tanks. The convergence to plug flow as $N \to \infty$ is well known and has been demonstrated previously (Skoglund et al., 2006). As shown in the same article the "numerical dispersion", due to limited discretization of a heat exchanger, can be avoided by employing a model containing dynamic transport delay. Similarly, we are now seeking more efficient ways to handle axial-dispersed plug flow than using the N-CST model with large values of N.

2.2 Frequency analysis

To be able to handle both large and small values of Pe the new approach employs a combination of a pipe with plug flow (transport delay) and N identical continuously stirred tanks in series (PFNCST). This is illustrated in Fig. 1. For N=1 this model coincides with the well-known simpler combined model using a plug-flow part followed by a single stirred tank (e.g. Levenspiel and Bischoff, 1963).

In the following we will derive a relationship between the model parameters (τ_0, τ_N and N) and the system parameters (τ and Pe) that minimizes the difference between the solutions of Eq. (1) and the proposed PFNCST model. The procedure adopted is to make a Taylor expansion of Eq. (3) and compare the first terms with the corresponding Taylor expansion of the transfer function of the proposed PFNCST model. The model error is further analysed with frequency-response analysis.

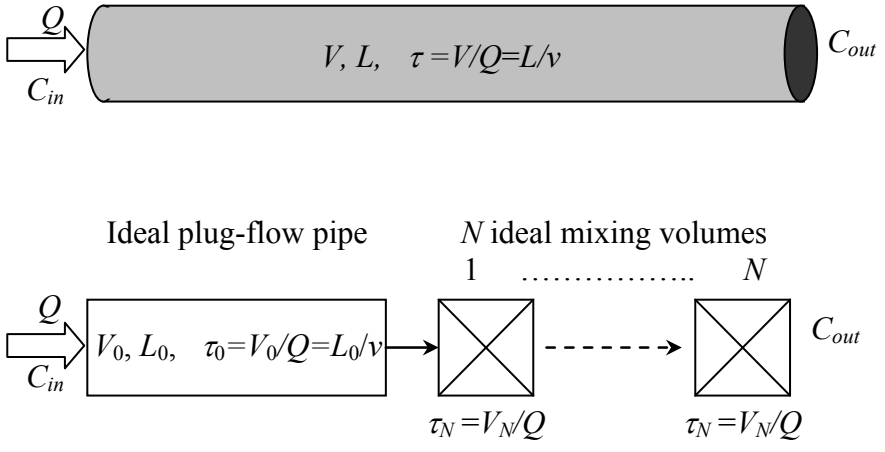

Fig. 1. A pipe and the corresponding proposed model, where $V = V_0 + NV_N$.

The mass balance of the proposed PFNCST model with a transport delay τ_0 and N ideal mixed tanks can be expressed as follows.

For $\forall\ i \in [1, N]$: $V_N \frac{\partial C_i}{\partial t} + QC_i - QC_{i-1} = 0$ **(6)**

where

$C_{i=0}(t) = C_{in}(t - \tau_0)$ **(7)**

and represents the delay in the ideal plug-flow pipe.
The combined transfer function of this is

$$\boldsymbol{G}_{PFNCST}(s) = \frac{e^{-\tau_0 s}}{(1 + \tau_N s)^N} \quad \textbf{(8)}$$

where the time constant $\tau_N = V_N / Q$ has been introduced.
Compatibility requires that the volume considered in the model is the same as the total volume in the original pipe

$V = V_0 + NV_N$ **(9)**

With the average transport time $\tau = V/Q$ this gives

$N\tau_N = \tau - \tau_0$ **(10)**

Thus:

$$\boldsymbol{G}_{PFNCST}(s) = \frac{e^{-(\tau - N\tau_N)s}}{(1 + \tau_N s)^N} = \frac{e^{-\frac{L}{v}s} e^{N\tau_N s}}{(1 + \tau_N s)^N} \quad \textbf{(11)}$$

and when the dimensionless argument s^* is used the expression becomes:

$$\boldsymbol{G}_{PFNCST}(s^*) = \frac{e^{-s^*} e^{N\frac{\tau_N}{\tau}s^*}}{\left(1 + \frac{\tau_N}{\tau}s^*\right)^N} \quad \textbf{(12)}$$

To investigate the conditions under which Eq. (3) can be approximated by Eq. (11), we assume that:

$\left|\frac{4D}{v^2}s\right| << 1$ and $|N\tau_N s| << 1$ **(13)**

It should be noted that Eq. (13) is an assumption made to proceed in the analysis to find a relationship between model parameters. The frequency analysis, step response analysis and breakthrough analysis below confirm the validity of parameter values for the range of liquid food applications considered. The fulfilment of the first inequality is, however, confirmed by the fact that normally $D < 0.05$ m^2/s, $v > 1$ m/s and $|s| = |i\omega| = 2\pi f \lesssim 2\pi \bullet 0.2$ s^{-1}. The second inequality cannot be confirmed before we know the relationship between the model parameters, i.e. the result expressed in Eq. (20) and the required values of N given by the error analysis below. This means that the original equations can be approximated by Taylor expansions ignoring higher order terms. Taylor expansion of Eq. (3) gives:

$$\boldsymbol{G}_{ADPF}(s) = e^{\frac{vL}{2D}} e^{-\frac{vL}{2D}\sqrt{1+\frac{4D}{v^2}s}} =$$

$$= e^{\frac{vL}{2D}} e^{-\frac{vL}{2D}\left(1+\frac{4Ds/v^2}{2}-\frac{\left(4Ds/v^2\right)^2}{8}+\frac{\left(4Ds/v^2\right)^3}{16}-\frac{5\left(4Ds/v^2\right)^4}{128}+\ldots+\binom{1/2}{k}\left(4Ds/v^2\right)^k+\ldots\right)} \quad \textbf{(14)}$$

$$\Rightarrow$$

$$\boldsymbol{G}_{ADPF}(s) = e^{-\frac{L}{v}s} e^{\frac{LD}{v^3}s^2-\frac{2LD^2}{v^5}s^3+\ldots} \quad \textbf{(15)}$$

With further Taylor expansion of the second factor in this expression we obtain:

$$\boldsymbol{G}_{ADPF}(s) = e^{-\frac{L}{v}s}\left(1+\frac{LD}{v^3}s^2-\frac{2LD^2}{v^5}s^3+\ldots\right) \quad \textbf{(16)}$$

Similarly, we perform a Taylor expansion of Eq. (11).

$$\boldsymbol{G}_{PFNCST}(s) = e^{-\frac{L}{v}s}\left(1+N\tau_N s+\frac{\left(N\tau_N s\right)^2}{2!}+\frac{\left(N\tau_N s\right)^3}{3!}+\ldots.\right)\cdot$$
$$\cdot\left(1-N\tau_N s+\frac{N(N+1)}{2!}\left(\tau_N s\right)^2-\frac{N(N+1)(N+2)}{3!}\left(\tau_N s\right)^3+\ldots\right) \quad \textbf{(17)}$$

By multiplying the parentheses and collecting the lower-order terms we obtain:

$$\boldsymbol{G}_{PFNCST}(s) = e^{-\frac{L}{v}s}\left(1+\frac{\left(N\tau_N s\right)^2}{2N}-\frac{\left(N\tau_N s\right)^3}{3N^2}+\ldots\right) \quad \textbf{(18)}$$

Assuming the conditions defined by Eq. (13), we regard higher order terms as being negligible. Then Eqs. (16) and (18) become equivalent if:

$$\frac{LD}{v^3} = \frac{\left(N\tau_N\right)^2}{2N} = \frac{N{\tau_N}^2}{2} \quad \textbf{(19)}$$

or

$$\tau_N = \sqrt{\frac{2LD}{Nv^3}} = \sqrt{\frac{2\tau^2}{NPe}} = \tau\sqrt{\frac{2}{NPe}} \quad \textbf{(20)}$$

This, together with Eq. (10), is the essence of the analysis that describes the relationship between the system parameters (τ and Pe) and the model parameters (τ_0, τ_N and N). These relationships determine which values of τ_0 and τ_N should be used for any chosen value of N.

Inserting Eq. (20) in Eq. (12) gives

$$\boldsymbol{G}_{PFNCST}(s^*) = \frac{e^{-\left(1-\sqrt{\frac{2N}{Pe}}\right)s^*}}{\left(1+\sqrt{\frac{2}{NPe}}s^*\right)^N} \quad \textbf{(21)}$$

It is interesting to observe what happens if N is chosen according to Eq. (5). Using Eq. (20) this gives $N\tau_N = \tau$. From Eq. (10) we then conclude that $\tau_0 = 0$. This means no plug-flow part, only N continuously stirred tanks. In other words, the new model converges to the N-CST model as N approaches $Pe/2$.

The question is how accurate the new model is. This question is vital since the analysis is based on the assumptions in Eq. (13). Before we assess the accuracy we evaluate the second inequality of Eq. (13). By using Eq. (20) it can be expressed as $\tau\sqrt{\frac{2N}{Pe}}\omega << 1$. According to Eq. (5) the N-CST model requires $N = Pe/2$ and our demand is that the proposed model requires that N is far less. This means that $\sqrt{\frac{2N}{Pe}} << 1$ which gives $\tau\sqrt{\frac{2N}{Pe}}\omega << \tau\omega$, and since $\tau\omega$ mostly < 1 the condition is fulfilled.

To assess the accuracy (for $N << Pe/2$), we determined the error in the model regarding amplitude and phase. Eqs. (4) and (21) are used to plot these errors. Figs. 2a and 2b show curves for the relative error in amplitude, $|\boldsymbol{G}_{PFNCST}(i\omega^*) / \boldsymbol{G}_{ADPF}(i\omega^*)| - 1$, and the error in phase shift, $\arg(\boldsymbol{G}_{PFNCST}(i\omega^*)) - \arg(\boldsymbol{G}_{ADPF}(i\omega^*))$. It can be seen that both errors are small over a wide range of ω^* and Pe, even for moderate values of N.

To better illustrate the relevance for typical cases, Figs. 3a and 3b show the corresponding errors plotted as a function of the dispersion coefficient, D, for $L = 20$ m, $v = 2$ m/s and $\omega = 2$ rad/s.

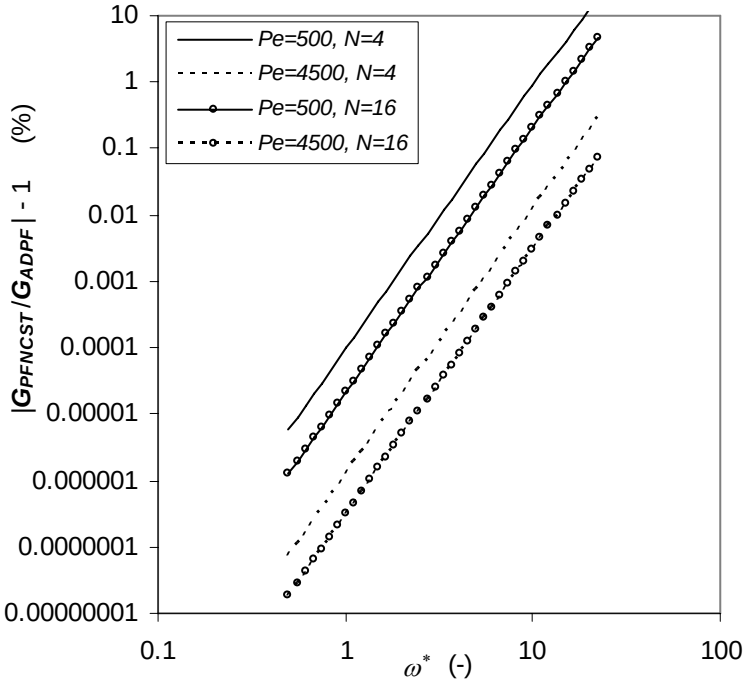

Fig. 2a. Accuracy of the proposed model for different degrees of dispersion and different choices of number of stirred tanks, *N*. The accuracy is displayed as the error in terms of the relative amplitude quotient $|\boldsymbol{G}_{PFNCST}(i\omega^*) / \boldsymbol{G}_{ADPF}(i\omega^*)| - 1$ for two values of the Péclet number, each for two values of *N*.

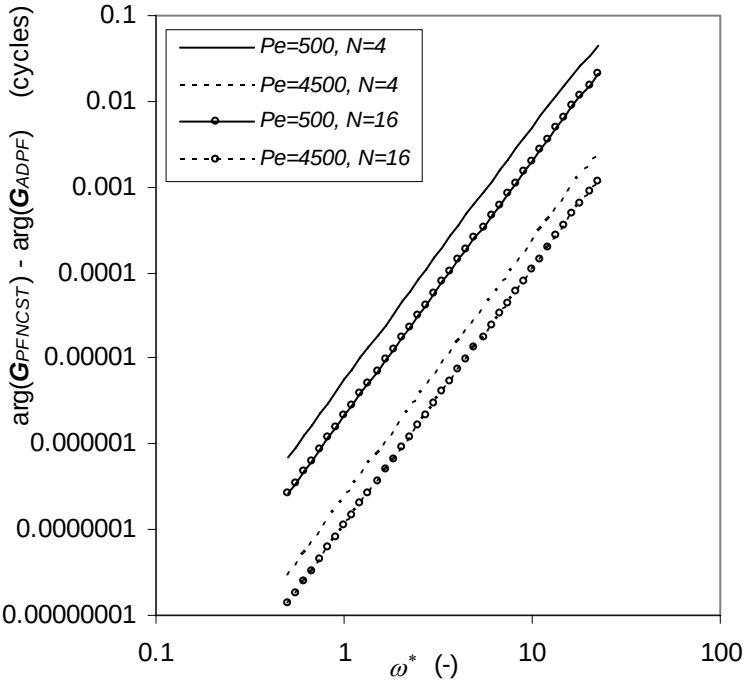

Fig. 2b. Accuracy of the proposed model for different degrees of dispersion and different choices of number of stirred tanks, *N*. The accuracy is displayed as the error in terms of the phase-shift difference $\arg(\boldsymbol{G}_{PFNCST}(i\omega^*)) - \arg(\boldsymbol{G}_{ADPF}(i\omega^*))$ for two values of the Péclet number, each for two values of *N*. (Note that the phase-shift difference is expressed in cycles instead of radians.)

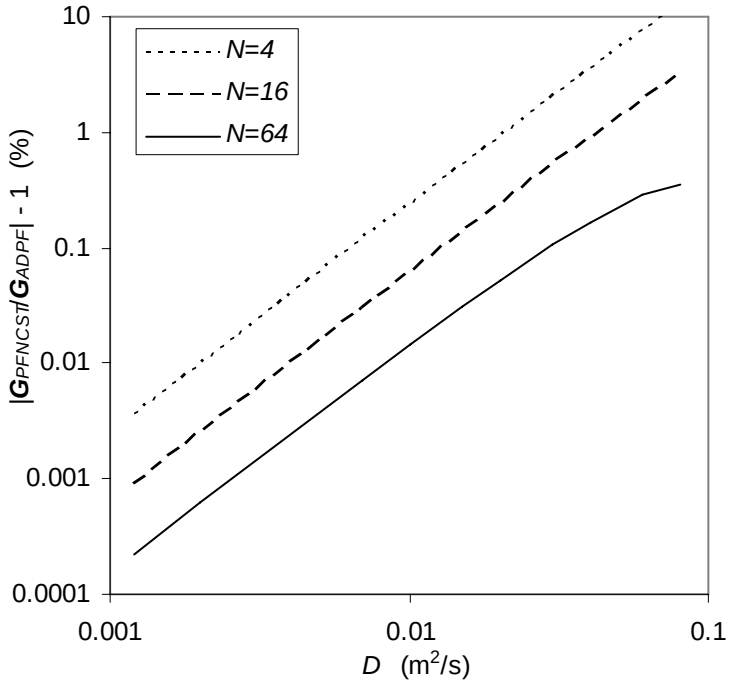

Fig. 3a. Accuracy of the proposed model for different choices of number of stirred tanks, *N*. The accuracy is displayed as the error in terms of the relative amplitude quotient $|\boldsymbol{G}_{PFNCST}/\boldsymbol{G}_{ADPF}| - 1$ as a function of the dispersion coefficient, for three values of *N* (*L*=20 m, *v*=2 m/s, ω=2 rad/s).

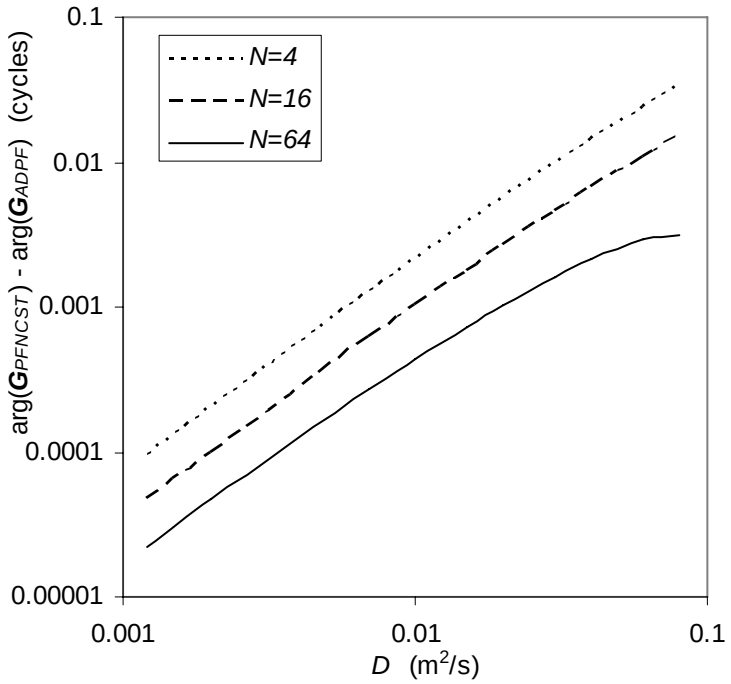

Fig. 3b. Accuracy of the proposed model for different choices of number of stirred tanks, *N*. The accuracy is displayed as the error in terms of the phase-shift difference $\arg(\boldsymbol{G}_{PFNCST}) - \arg(\boldsymbol{G}_{ADPF})$ as a function of the dispersion coefficient, for three values of *N* (*L*=20 m, *v*=2 m/s, ω=2 rad/s).

2.3 Step-response analysis

Since step responses are of particular interest when analysing mixing zones and product losses in a liquid food plant, an alternative and complementary analysis has also been carried out. In this section we will prove that the derived result above also predicts a step response with good accuracy. More precisely, we will study the change of the concentration at the outlet, at the time *L/v* after an inlet concentration step. We will show that the rate of change in concentration, calculated with the proposed PFNCST model, gives a result deviating only slightly from that calculated by the ADPF model even for moderate values of *N*.

We start by stating that the rate of change in concentration at time *L/v* after a step input is the same for both the axial-dispersed plug-flow model, Eq. (3), and the new model, Eq. (11).

The response at the output to a step input with the magnitude C_{step} to the system described by $\boldsymbol{G}_{ADPF}$, Eq. (3) is:

$$\frac{1}{C_{step}} C_{out}(\xi) = \frac{1}{2}\left[1 - erf(\xi)\right] \tag{22}$$

where

$$\xi = \frac{L - vt}{\sqrt{4Dt}} = \frac{\sqrt{Pe}}{2} \frac{\left(1 - t^*\right)}{\sqrt{t^*}} \tag{23}$$

and

$$erf(\xi) = \frac{2}{\sqrt{\pi}} \int_0^{\xi} e^{-x^2} dx \tag{24}$$

The rate of change in the output concentration is then:

$$\frac{1}{C_{step}} \frac{\partial C_{out}}{\partial t} = \frac{1}{C_{in}} \frac{\partial C_{out}}{\partial \xi} \frac{\partial \xi}{\partial t} = \frac{L + vt}{4\sqrt{\pi D t^3}} e^{-\frac{(L-vt)^2}{4Dt}} \tag{25}$$

The rate of change at time $t = L/v = \tau = \tau_0 + N\tau_N$ is then given by:

$$\frac{1}{C_{step}} \frac{\partial C_{out}}{\partial t}\bigg|_{t=\frac{L}{v}} = \frac{1}{2\sqrt{\pi}} \sqrt{\frac{v^3}{DL}} = \frac{1}{2\sqrt{\pi}} \frac{\sqrt{Pe}}{\tau} \tag{26}$$

For the new model we first identify the inverse Laplace transform of $\boldsymbol{G}_{PFNCST}$, Eq. (8)

$$G_{PFNCST}(t) = \frac{(t - \tau_0)^{N-1} e^{-\frac{t-\tau_0}{\tau_N}}}{(N-1)!\,\tau_N^N} \tag{27}$$

The Laplace transform of the exit concentration as a result of a step input with the magnitude C_{step} is $C_{step} \frac{1}{s} \boldsymbol{G}_{PFNCST}(s)$

The inverse Laplace transform of this, Råde & Westergren (2001) p 326, gives the exit concentration.

$$\frac{1}{C_{step}} C_{out}(t) = Laplace^{-1}\left(\frac{1}{s} \boldsymbol{G}_{PFNCST}(s)\right) = \int_{0-}^{t} G_{PFNCST}(\tau) d\tau \tag{28}$$

This means that the rate of change in concentration is

$$\frac{1}{C_{step}}\frac{\partial C_{out}}{\partial t} = G_{PFNCST}(t) = \frac{(t-\tau_0)^{N-1} e^{-\frac{t-\tau_0}{\tau_N}}}{(N-1)!\tau_N^N} \quad \textbf{(29)}$$

The rate of change at time $t = L/v = \tau = \tau_0 + N\tau_N$ is thus:

$$\left.\frac{1}{C_{step}}\frac{\partial C_{out}}{\partial t}\right|_{t=\tau_0+N\tau_N} = \frac{\left(\frac{N}{e}\right)^N}{N!\tau_N} \quad \textbf{(30)}$$

Requiring equality of the rates of change in Eqs. (26) and (30) gives:

$$\frac{1}{2\sqrt{\pi}}\sqrt{\frac{v^3}{DL}} = \frac{\left(\frac{N}{e}\right)^N}{N!\tau_N} \Rightarrow \tau_N = \frac{2\sqrt{\pi}}{N!}\left(\frac{N}{e}\right)^N\sqrt{\frac{DL}{v^3}} \quad \textbf{(31)}$$

To simplify this we use Stirling's formula:

$$N! = \sqrt{2\pi}N^{N+1/2}e^{-N}(1+\varepsilon_N) \quad \textbf{(32)}$$

where $\varepsilon_N \to 0$ as $N \to \infty$.

Inserted into Eq. (31) this leads to:

$$\tau_N = \sqrt{\frac{2LD}{Nv^3}}\frac{1}{1+\varepsilon_N} \to \sqrt{\frac{2LD}{Nv^3}} \text{ as } N \to \infty \quad \textbf{(33)}$$

This is exactly the same result as that given by the Taylor expansion of the Laplace transforms, Eq. (20). It is also worth noting that the error in Stirling's formula is 8.4 % for N=1 and only 2.8 % already for N=3. In other words, in terms of change rate of the concentration at the time L/v, the PFNCST model provides a good approximation of the response to step changes in input concentrations even for small values of N.

2.4 Comparison of the proposed model with the exact solution of a pulse and breakthrough

Fig. 4 shows an example where the PFNCST model is compared with the exact solution of Eq. (1). The diagram shows the response of a unit pulse input with a duration of t_p=0.25 τ. The model solution was plotted for different values of N. The plot shows good agreement between the model and the exact solution, even for moderate values of N.

A common practical view of fill-up or purging processes is that there is a point in time at which the flushing fluid first reaches the exit of the channel. According to the ADPF and N-CST models, no such point exists in a strict mathematical meaning. However, since $C(\xi)$ is very small for reasonable values of ξ ($C(\xi)<10^{-5}$ for $\xi>3$ in Eq. (22)), corresponding to a period of time during which the concentration in practice is negligible, not to say impossible to measure, it is relevant to define a practical breakthrough point. To analyse how well the new model reproduces breakthrough times, such calculations were carried out. Fig. 5 shows the initial rise in concentration at a step response for a typical case (Pe=10000, v=1.5 m/s and L=20 m) calculated exactly and with the new PFNCST model with different values of N. The

diagram shows the breakthrough times for X_b=0.2 %, a value clearly below practical limits of detection. The error in this breakthrough time was calculated for a range of values of *Pe* and *N* and the results are shown in Fig. 6. The figure shows that the new model gives a good prediction of the breakthrough for typical cases and at reasonable values of *N*.

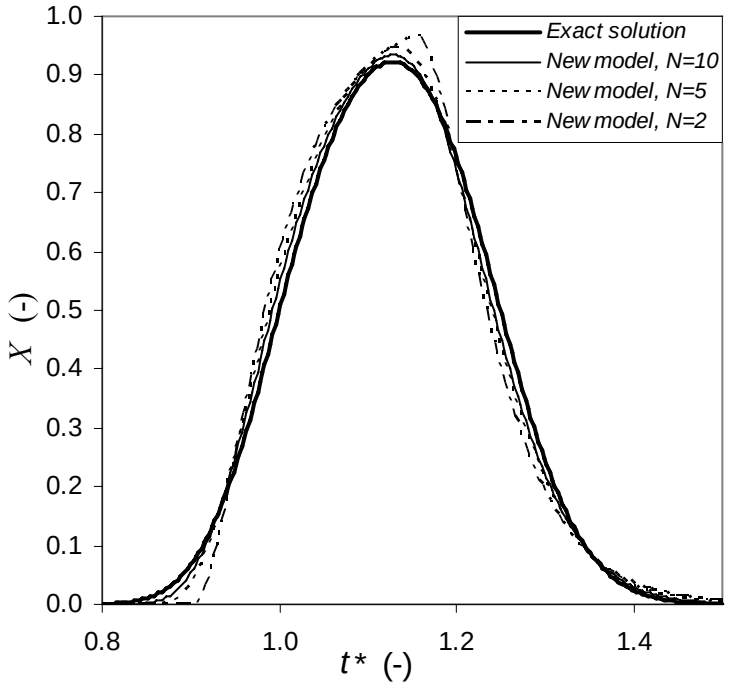

Fig. 4. Response to a pulse change in concentration for three values of *N*. The pulse-duration is t_p^*=0.25, *Pe*=400, *L*=20 m and v = 1 m/s (D = 0.05 m^2/s)

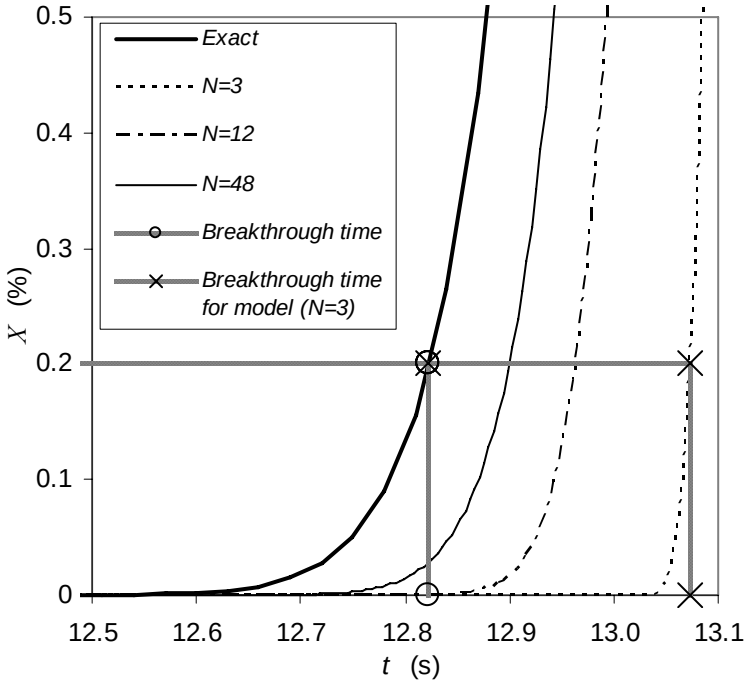

Fig. 5. Illustration of the initial breakthrough of a step response for Pe=10000, v=1.5 m/s and L=20 m. The breakthrough time is indicated for X_b=0.2 %.

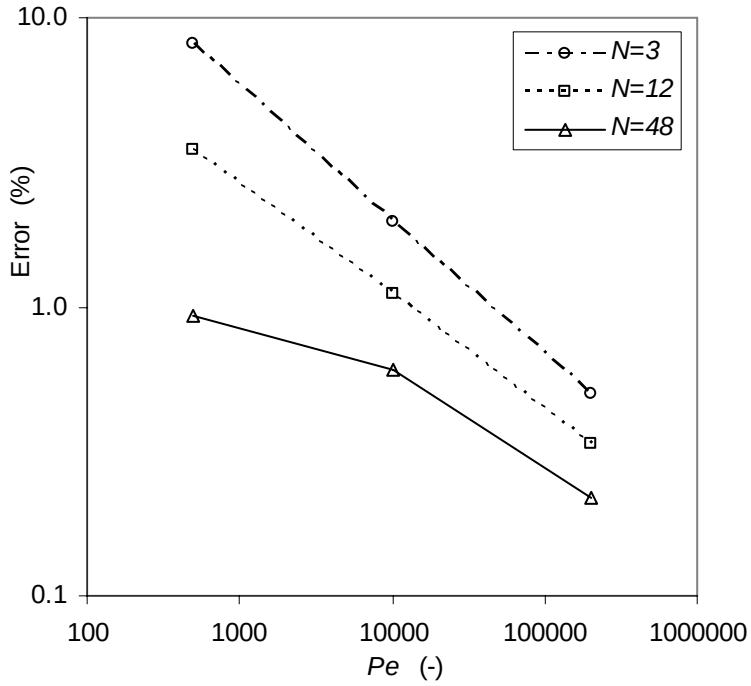

Fig. 6. The error in break-through time for X_b=0.2 % as a function of Pe for different values of N (v=1.5 m/s and L=20 m).

2.5 Pressure drop and momentum balance

Since pressure drop and momentum balance depend on fluid properties, propagation and dispersion also have effects on the pressure. To consider these effects adequately the model described by Eq. (8) and Fig. 1 can be reformulated as in Eq. (34), i.e. the same transfer function but now interpreted as N "control volumes" with a transport delay τ_0/N and one tank with the time constant τ_N.

$$\boldsymbol{G}_{PFNCST}(s) = \frac{e^{-\tau_0 s}}{(1+\tau_N s)^N} = \frac{e^{-N\frac{\tau_0}{N}s}}{(1+\tau_N s)^N} = \left(\frac{e^{-\frac{\tau_0}{N}s}}{1+\tau_N s}\right)^N \quad \textbf{(34)}$$

It is illustrated in Fig. 7. The advantage of this model structure is that the discretization includes the transport delay part with the dispersion. Since the plug-flow model includes equations for friction factors and momentum balance this structure improves the dynamic calculation of pressure changes as fluid properties propagate and disperse along the channel.

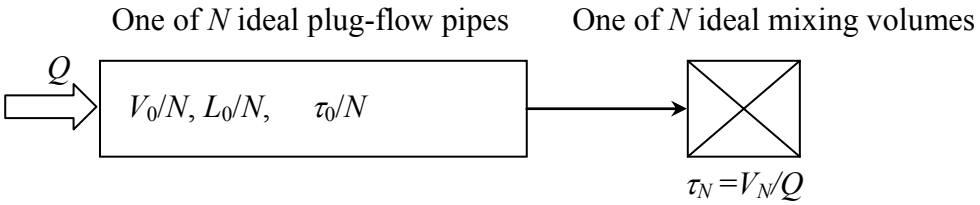

Fig. 7. One of N identical "control volumes" of the proposed model.

3. Model implementation and simulation

The new dispersion model for turbulent flow was implemented in the modelling language Modelica[1]. According to Eqs. (10) and (20) the model parameters, τ_0 and τ_N, depend on the Péclet number, *Pe*, which in turn depends on the Reynolds number, *Re* (Wen and Fan, 1975; Taylor, 1954a). Hence the model parameters depend on variables such as velocity and viscosity. Therefore, in a *dynamic* dispersion model, these parameters (τ_0 and τ_N) must be variables that change accordingly. Since $\tau_0 = L_0/v$ and $\tau_N = V_N/Q$, the most straightforward approach would be to vary L_0 and V_N respectively. This is, however, not desirable for the following reasons.

i. The models were constructed hierarchically, where the dispersion pipe model uses existing models for pipes and ideal mixing volumes that uses constant lengths and volumes respectively during a simulation.
ii. Variable lengths and volumes create problems concerning mass balance.
iii. Variable lengths and volumes were believed to cause computational problems.

For these reasons the dynamic variations of τ_0 and τ_N were instead implemented as modulations of v and Q. It should, however, be noted that the simultaneous dynamic simulation of the pressure drop and momentum balance uses the true channel length, L, and velocity, v.

[1] Modelica was the program language. The tool was Dymola supplied by Dynasim AB.

In the present study a complete system of component models was set up to simulate a pipe during product changeover, where one fluid is followed by another. The system is illustrated in Fig. 8, and can be described as follows.

- A pipe 20 m long with a diameter 48.6 mm (standard type with an outer diameter of 51 mm).
- Two fluids at 10 °C; either water or cream (15 % fat or 30%), in two or three phases during the simulation:
  - Phase 1: Fluid 1
  - Phase 2: Fluid 2
  - Phase 3 (in some experiments): Fluid 1
- A flow rate of 10 000 l/h (controlled by a PID controller, stable during the fluid transitions)

In some simulations Fluid 1 = Fluid 2, i.e. the viscosity and density remain unchanged during the transitions, which means that the dispersion coefficient, *D*, also remains constant during the transition. See below and Eq. (35)

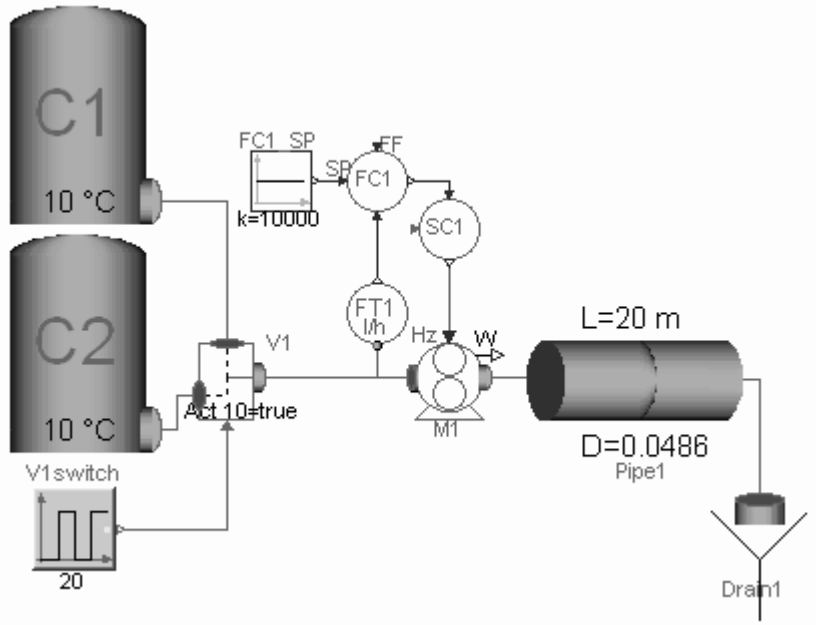

Fig. 8. The design of a theoretical experiment as a system of dynamic models, whereof one, denoted "Pipe1", is the new PFNCST model. Depending on the change-over valve, V1, the pipe is connected to either a source denoted "C1" or a source denoted "C2". The flow rate control loop includes a sensor (FT1), a PID controller (FC1), a flow set point (FC1_SP), an inverter (SC1) and a pump (M1).

4. Results

Simulations were carried out by numerically solving the system of model equations using the Dassl solver in Dynasim's Modelica-based program Dymola version, 5.3c. The following simulations were run with different values of the dispersion coefficient.

Phase 1 (0-30 s):	Start-up of the system with fluid 1 to allow flow to stabilise
Action 1 (at 30 s):	Changeover from fluid 1 to fluid 2 at the pipe inlet
Phase 2 (30-40 s):	Continue to allow the transient to stabilise
Action 2 (at 40 s):	Changeover from fluid 2 to fluid 1 at the pipe inlet
Phase 3 (40-50 s):	Continue to allow the transient to stabilise

The output response was studied in the interval 40-60 s where the subsequent concentration transition reaches the pipe outlet.

4.1 Simulation of product-to-product transition

The system was simulated during transition from one fluid to another with the same rheological properties, i.e. with the same Reynolds number. According to Wen and Fan (1975), p. 146, for turbulent flow the dispersion coefficient depends on the Reynolds number as in Eq. (35)

$$\frac{D}{Lv} = \frac{1}{Pe} = \frac{2R}{L}\left(3.0 \cdot 10^{7} Re^{-2.1} + 1.35 Re^{-0.125}\right) \quad \textbf{(35)}$$

For the set-up in Fig. 8 the values obtained were D=0.025 m^2/s (Pe=1183) for water and D=0.037 m^2/s (Pe=813) for cream (15% fat). During the transition from water to cream and vice versa intermediate values will occur (see below).

Figs. 9 and 10 show simulation results for cream-to-cream changeover with the new PFNCST model compared with the exact solution to Eq. (1) (ADPF model) with a step input. The figures also show the results of simulation where the pipe was replaced by an N-CST model.

4.2 Convergence − Simulations with varying values of N

The convergence rates of the N-CST model and the proposed PFNCST model were investigated by calculating the RMS[1] errors of the simulated results. The results are given in Fig. 11, which shows the required CPU time vs. the RMS error for simulations with different number of mixed tanks, N. The plot shows that, for a given level of accuracy, the N-CST model requires considerably more CPU time[2] (a factor 30-100) than the PFNCST model.

4.3 Simulations with varying dispersion

The dispersion may vary depending on flow rate, channel geometry and fluid properties. Hence, to further analyse how the dynamic dispersion model handles variations, simulations were performed for fluid transitions where the dispersion coefficient, D, varies according to Eq. (35). Simulations of transitions from water to cream (with 30 % fat; D=0.11 m^2/s, Pe=280) and vice versa were performed. The results were compared with the exact solution of step responses for water-water and cream-cream transitions. The results are given in Fig. 12, which clearly shows the ability of the new model to handle dynamic variation of the dispersion coefficient.

[1] Root-Mean-Square

[2] A standard PC was used: Dell Optiplex SX270 with Intel® Pentium® 4 CPU 3.2 GHz, 1.0 GB RAM

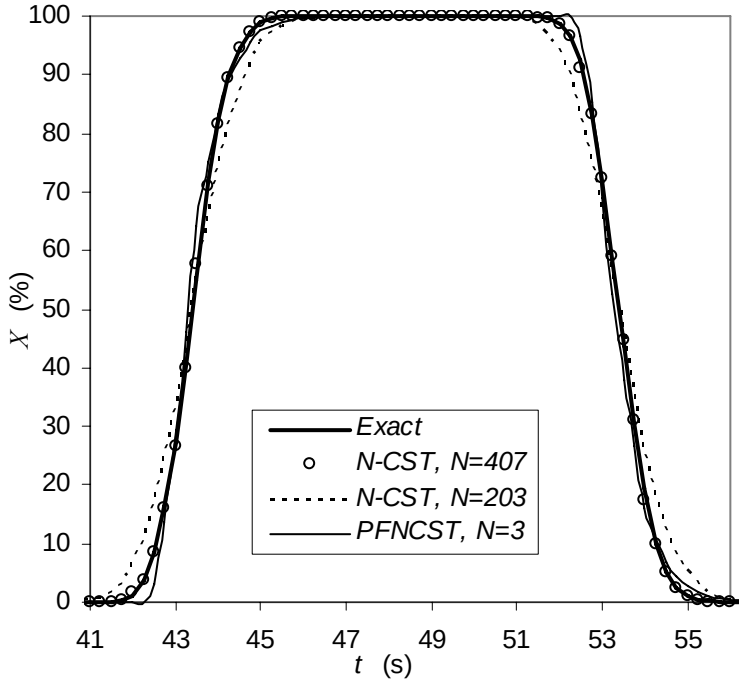

Fig. 9. Results of simulations of a 10 s wide pulse of cream-cream product change (D=0.037 m^2/s, Pe=814) showing the concentration at the pipe outlet using the new model (PFNCST, N=3) compared with the N-CST model (N=407 and N=203) and the exact solution of the ADPF model.

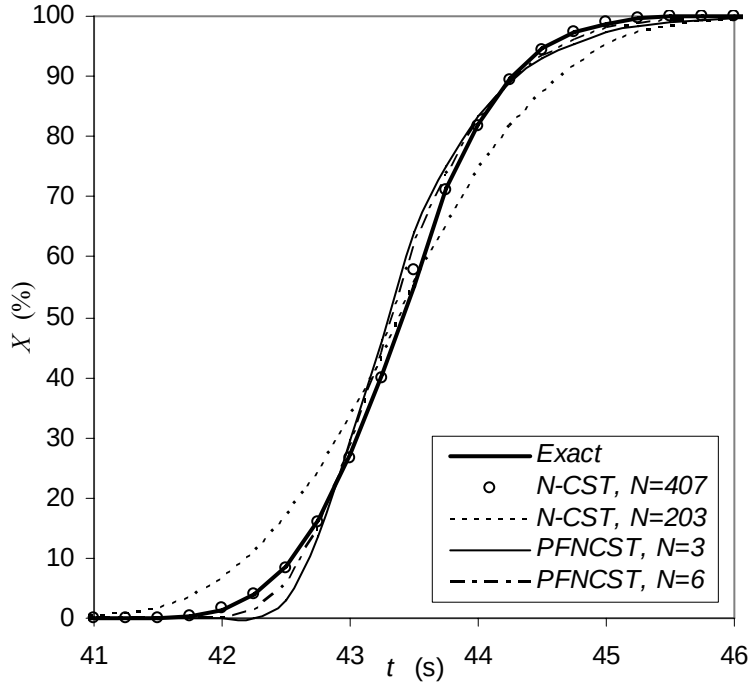

Fig. 10. The same results as in Fig. 9, showing the early phase and one more simulation (PFNCST, N=6).

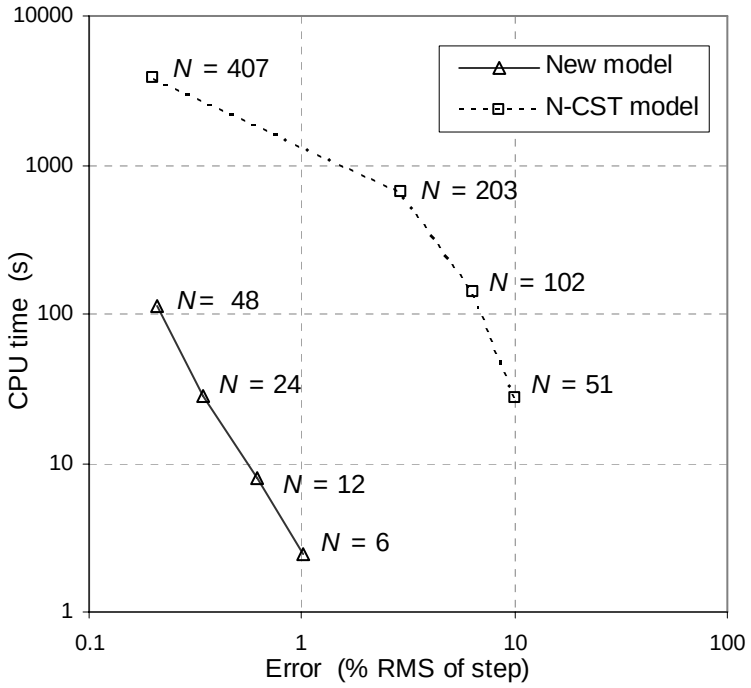

Fig. 11. CPU time vs. error for a number of simulations carried out with the proposed model (PFNCST) and the N-CST model. The error and CPU time were calculated over the simulation period of 30-60 s in the simulations shown in Fig. 9. The diagram shows that for a certain demand on the error, the new model requires considerably less computational power (a factor of 30-500).

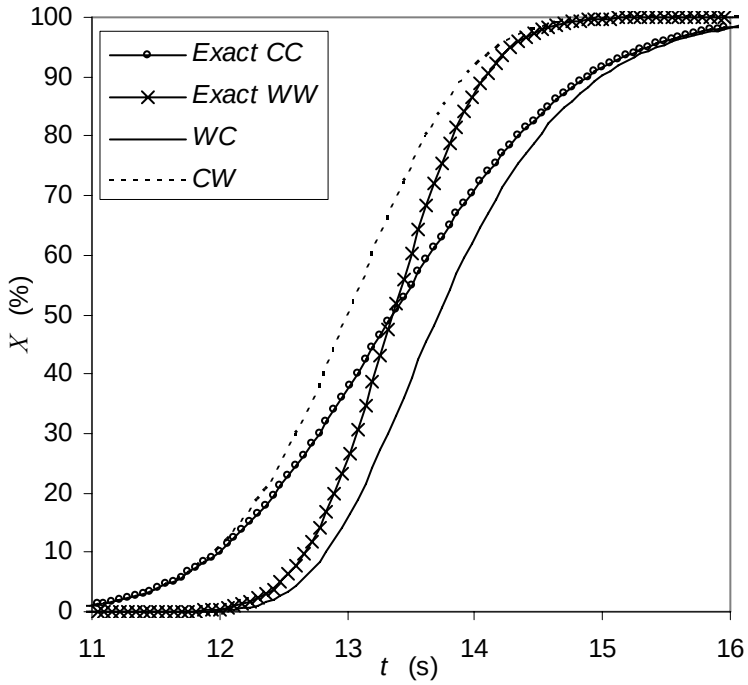

Fig. 12. Exact step response of cream-cream (CC) changeover with 30% fat and water-water (WW) changeover compared with the simulated step response of water-cream (WC) and cream-water (CW) changeovers using the proposed model (PFNCST) with N=48. The model uses dynamic adaptation of the dispersion coefficient D by using Eq. (35). The diagram clearly shows the ability of the new model to handle dynamic variations of the dispersion coefficient.

5. Conclusions and discussion

A new fluid dispersion model for turbulent flow has been presented as an approximation of the axial-dispersed plug-flow model. The new model consists in principle of an ideal plug-flow pipe followed by N ideally mixed volumes (continuously stirred tanks). To dynamically handle pressure drop and momentum balance as fluid properties change, the model was rearranged to represent N sets of one plug-flow pipe combined with one ideally-mixed volume.

The model expresses the relationship between the model parameters (τ_0, τ_N and N) and the system parameters (τ and Pe), (Eqs. 9, 10 and 20). For any value of N, the relationships give an optimal value of the model parameters, i.e. the volumes of the plug-flow pipe (V_0) and the N tanks (V_N). The value of N can be chosen to obtain desired accuracy.

Mathematical frequency analysis (Section 2.2) and mathematical step-response analysis (Section 2.3) were applied to demonstrate the validity of the approximation. In simulations the model showed good agreement with the exact solution of the ADPF model at typical values of Pe, even for moderate values of N. This demonstrates that the new model is computationally efficient and suitable for simulations of large systems that are typical for many liquid food processing systems. Implementation of the model showed its ability to handle dynamic variations in the dispersion coefficient. Furthermore, the model gave good predictions of breakthrough time for typical cases in liquid food applications (Section 2.4). Simulations also showed that the new model is well suited for implementation in Modelica.

It is proposed that in future work the model be implemented in more complex fluid channels. In our group the model is currently being implemented in heat exchanger models.

Notation

$C(x,t)$ Volumetric concentration, kg/m^3
C_b Definition of the volumetric concentration at which breakthrough takes place (see Section 2.4), kg/m^3
$C_{in}(t)$ Volumetric concentration at the channel inlet, $C(0,t)$, kg/m^3
$C_{out}(t)$ Volumetric concentration at the channel outlet, $C(L,t)$, kg/m^3
$\boldsymbol{C}$ Laplace transform of C
D Dispersion coefficient in axial direction, m^2/s
$\boldsymbol{G}$ Transfer function, i.e. ratio of Laplace transforms for output and input signals,

$$\boldsymbol{G} = \frac{\boldsymbol{C}_{out}(s)}{\boldsymbol{C}_{in}(s)}$$

i Imaginary part of complex numbers, -
L Length of flow channel, m
L_0 Length of channel with ideal plug flow, m
N Number of continuously-stirred tanks in the dispersion model, -
Pe Péclet number defined by vL/D (the ratio of convective flow rate to dispersive flow rate), -
Q Volumetric flow rate, m^3/s
R Radius or hydraulic radius, m
Re Reynolds number defined by $2\rho Rv/\mu$, -
s Complex argument of the Laplace transform, s^{-1}

s^* Dimensionless argument of the Laplace transform, $Ls/v = \tau s$, -

t Time, s

t_b Breakthrough time, s

t_p Duration of pulse, s

t^* Dimensionless time, $t^* = \frac{t}{\tau}$, -

t_b^* Dimensionless breakthrough time, $t_b^* = \frac{t_b}{\tau}$, -

t_p^* Dimensionless duration of pulse, $t_p^* = \frac{t_p}{\tau}$, -

V Volume, m^3

V_0 Volume of channel with ideal plug flow in the new model (see Fig. 1), m^3

V_N Volume of one of the N continuously stirred tanks, m^3

v Mean velocity over a channel cross-sectional area, m/s

X Relative mass concentration, i.e. mass fraction, C/ρ, -

X_b Definition of the mass fraction at which breakthrough takes place, (see Section 2.4), C_b/ρ, -

x Axial spatial coordinate (along the fluid channel), m

Greek letters

ξ Dimensionless variable defined by $\xi = \frac{L - vt}{\sqrt{4Dt}} = \frac{\sqrt{Pe}}{2}\frac{\left(1 - t^*\right)}{\sqrt{t^*}}$, -

ρ Density, kg/m^3

τ Average transport time (dwell time) for a fluid through a channel (see Fig. 1), V/Q or L/v, s
More generally, to handle dynamic delay, i.e. varying velocities:

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

τ_0 Transport time (dwell time) for a fluid through the channel with ideal plug flow in the new model (see Fig. 1), $L_0/v = V_0/Q$, s
More generally, to handle 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 (dwell time) for a fluid through one of the N continuously stirred tanks in the new model (see Fig. 1), V_N/Q, s
More generally, to handle dynamic delay, i.e. varying flow rates:

$$\tau_N = \tau_N(Q(t)): V_N = \int_0^{\tau_N} Q(t)dt$$

ω Angular frequency, radians/s

ω^* Dimensionless angular frequency, $L\omega/v = \tau\omega$, -

General superscripts

A^* Dimensionless form of variable A (further explained above for each variable)

General subscripts

$_{ADPF}$	Axial-dispersed plug-flow (ADPF) model
$_{N\text{-}CST}$	N-continuously-stirred-tanks (N-CST) model
$_{PFNCST}$	New proposed model combining plug flow with the N-continuously-stirred-tanks (PFNCST) model
$_{i}$	Continuously stirred tank number i
$_{in}$	Into the system
$_{out}$	Out of the system
$_{b}$	Breakthrough

Other general symbols

$\boldsymbol{A}$	Laplace transform of A

Model acronyms

ADPF	Axial-dispersed plug flow
N-CST	N continuously stirred tanks
PFCST	Plug flow combined with 1 continuously stirred tank
PFNCST	Plug flow combined with N continuously stirred tanks (= new model)

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References

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.

Bischoff, K. B., Levenspiel, O., 1962a. Fluid Dispersion-Generalization and Comparison Of Mathematical Models - I. Generalization of Models. Chemical Engineering Science, 17, 245-255.

Bischoff, K. B., Levenspiel, O., 1962b. Fluid Dispersion-Generalization and Comparison Of Mathematical Models - II. Comparison of Models. Chemical Engineering Science, 17, 257-264.

Bäckman, J., Edvall, M., 2005. Using Modelica and Control Systems for Real-time Simulations in the Pulp. Proceedings of the 4th International Modelica Conference, 579-583, Hamburg, March 7-8, 2005, Organized by Modelica Association and Hamburg University of Technology, Germany (http://www.modelica.org)

Casella, F., Otter, M., Proels, 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 2006, 631-640, Vienna, Austria, September 4-5, 2006, Organized by Modelica Association and Arsenal Research, Vienna, 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, 1542-1552.

Elmqvist, H., Tummescheit, H., Otter, M., 2003. Object-Oriented Modeling of Thermo-Fluid Systems. Proceedings of the 3rd International Modelica Conference, 269-286, Linköping, Sweden, November 3-4, 2003, Organized by Modelica Association and Linköping University, Sweden (http://www.modelica.org).

Hopkins, M. J., Sheppard, A. J., Eisenklam P., 1969. The use of transfer functions in evaluating residence time distribution curves. Chemical Engineering Science, 24, 1131-1137.

Levenspiel, O., Smith W., 1957. Notes on the diffusion-type model for the longitudinal mixing of fluids in flow. Chemical Engineering Science 6, 227-233.

Levenspiel, O., Bischoff, K. B., 1963. Patterns of flow in chemical process vessels. Advances in Chemical Engineering, 4, 95-198.

Marquardt, W., 1996. Trends in Computer-Aided Process Modeling. Computers and Chemical. Engineering, 20, 591-609.

Modelica Association, -. Modelica and the Modelica Association. Available from <http://www.modelica.org>.

Råde, L., Westergren B., 2001. Mathematics Handbook for Science and Engineering, Studentliteratur, ISBN 91-44-00839-2

Serpemen, Y., Deckwer, W-D., 1974. Instationary Dispersed Plug Flow Model with Linear Rate Processes. Ind. Eng. Chem. Fundam., 13, 399–400.

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. Organized by Modelica Association and Linköping University, Sweden. Available from <http://www.modelica.org>.

Skoglund, T., 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, Organized by EUROSIS.

Skoglund, T., Årzén, K-E., Dejmek P., 2006. Dynamic object-oriented heat-exchanger models for simulation of fluid property transitions. International Journal of Heat and Mass Transfer 49, 2291-2303.
Taylor, G., 1953. Dispersion of soluble matter in solvent flowing slowly through a tube. Proceedings of the Royal Society of London Series A, 219, 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, 446-468.
Taylor, G., 1954b. Diffusion and Mass Transport in Tubes, Proceedings of the Physical Society of London, 67, 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.
Wen, C. Y., Fan, L. T., 1975. Models for Flow Systems ad Chemical Reactors. Marcel Dekker, New York. ISBN 0-8247-6346-7.