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Abstract

Object-oriented heat-exchanger models were developed to simulate the dynamic thermal effects of dynamic changes in fluid composition and thus of fluid properties in a type of liquid typical for food products.
The models were written in the object-oriented language Modelica as objects in a library structure being developed to simulate complex liquid food process lines and their control systems. The models were based on moderate discretization of the heat exchanger into control volumes, and the fluid dispersion was modelled either as ideal mixing or as transport delay in each control volume. The transport delay model exhibited the best computational performance as well as affording flexibility in fluid dispersion modelling.

Keywords: Heat exchanger, Fluid property transitions, Dynamic model, Object-oriented, Liquid food, Dispersion

Nomenclature

See also Figure 1.

A Thermal contact area between the channels, m^2

A_c Cross-sectional area of a fluid channel, m^2

c_p Fluid specific heat capacity, J/kg K

C Concentration, i.e. mass fraction of components in fluid, -

$\hat{C}$ Concentration vector (in the present case a 5-element vector with mass fractions for water, carbohydrates, protein, fat and ash), -

$\vec{C}$ C at channel exit delayed by transport through the channel,

        i.e. $\vec{C}(t) = C(t - \tau)$, -

$\vec{\hat{C}}$ $\hat{C}$ at channel exit delayed by transport through the channel, i.e.

        $\vec{\hat{C}}(t) = \hat{C}(t - \tau)$, -

D_h Hydraulic diameter of channel, m

d Dispersion coefficient, m^2/s

F_w Wall friction force on fluid, N

H Enthalpy, J

f Coefficient of friction $f = 2\Phi$ (Fanning friction factor),

        defined by $\Delta p = 2fL\rho v^2 / D_h$, -

g Acceleration due to gravity, 9.80665 m/s^2

h Thickness of wall between channels, m

j Heat flux, W/m^2

K Consistency of fluid defined by $\sigma = K\dot{\gamma}^n$, Pa s^n

k Heat transfer coefficient between the channels, W/m^2 K

L Length of flow channel, m

m Mass, kg

N Discretization, i.e. the number of calculation cells (control volumes) for the heat exchanger

n Flow behaviour index of fluid defined by $\sigma = K\dot{\gamma}^n$, -

NTU_i Number of heat transfer units for channel i: $kA/W = kA/\rho c_p Q$, -

Nu Nusselt number defined as $\alpha\lambda/D_h$, -

P Heat flow or enthalpy flow, W

P_w Heat flow through wall, W

P_{w1} Heat flow from wall between channels to channel 1, W

P_{2w} Heat flow from channel 2 to wall between channels, W

Pr Prandtl number defined by $c_p\mu/\lambda$, -

Pe Péclet number $Q/Q_d = vL/d$, i.e. the ratio of flow rate to dispersive flow rate, -

Pe_h Péclet number W/W_d, i.e. the ratio of heat capacity flow to dispersive heat capacity flow, -

        Pe_h is identical to Pe since W originates from Q and W_d originates from Q_d

p Pressure, Pa

Q Volumetric flow rate vA_c, m^3/s

Q_d Dispersive volumetric flow rate dA_c/L, m^3/s

Re Reynolds number defined by $\rho D_h v/\mu$, -

T Temperature, K

T_{da} Average temperature difference in heat exchanger calculated as the arithmetic mean value of the terminal temperature differences, K

T_{dm}	Mean temperature difference in heat exchanger calculated as logarithmic mean temperature difference: $T_{dm} = \dfrac{(T_{21} - T_{11}) - (T_{22} - T_{12})}{\ln\left(\dfrac{T_{21} - T_{11}}{T_{22} - T_{12}}\right)}$, K
$\vec{T}$	$\vec{T}(t) = T(t - \tau)$, i.e. temperature at channel exit delayed by transport through the channel, K
T_{w1}	Temperature in wall half between channels closest to channel 1, K
T_{w2}	Temperature in wall half between channels closest to channel 2, K
t	Time, s
V	Volume, m^3
v	Mean velocity over a channel cross-sectional area, m/s
W	Heat capacity flow $Q\rho c_p$, W/K
W_d	Dispersive heat capacity flow: $Q_p \rho c_p = \lambda_d A_c/L$, W/K
x	Axial spatial coordinate (along the fluid channel), m or exponent in Equation (2)
y	Spatial coordinate perpendicular to x and z, m or exponent in Equation (2)
z	Vertical spatial coordinate, m or exponent in Equation (2)

Greek letters

α	Heat transfer coefficient, W/m^{2}K
$\dot{\gamma}$	Shear rate, s^{-1}
ΔX	Difference of X
ε	$(NTU_1 + NTU_2)/2$
λ	Thermal conductivity, W/m K
λ_d	Dispersive thermal conductivity due to flow dispersion defined by $Q_p \rho c_p = \lambda_d A_c/L \Rightarrow \lambda_d = Q_p \rho c_p L/A_c = d\rho c_p$, W/m K
μ	Dynamic viscosity defined by $\mu = \sigma / \dot{\gamma}$, Pa s
μ_w	Dynamic viscosity at wall, Pa s
ρ	Density, kg/m^3
σ	Shear stress, Pa
τ	Transport time (dwell time) for a fluid through a channel, $L/v = V/Q$, s More generally, to handle dynamic delay, i.e. varying velocities: $\tau(v(t)): L = \displaystyle\int_0^\tau v(t)dt$
Φ	Coefficient of friction $\Phi = f/2$, -

Other symbols

∇	Gradient vector operator $\left(\dfrac{\partial}{\partial x}, \dfrac{\partial}{\partial y}, \dfrac{\partial}{\partial z}\right)$
∇^2	Scalar operator $\dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2} + \dfrac{\partial^2}{\partial z^2}$

General subscripts

1	Channel 1
11	Channel 1 inlet
12	Channel 1 outlet

2	Channel 2
21	Channel 2 inlet
22	Channel 2 outlet
w	Wall between channels
w1	Wall surface to channel 1
w2	Wall surface to channel 2
2w	Channel 2 to wall surface

Other general symbols

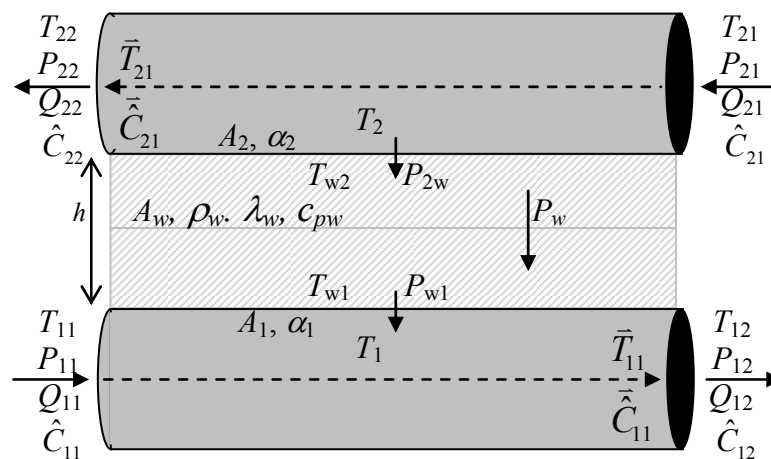|	
$\overline{X}$	Arithmetic mean value of X at inlet and outlet of channel
$\hat{X}$	Vector X
$\vec{X}$	X delayed by transport through the channel, i.e. $\vec{X}(t) = X(t - \tau)$
$\boldsymbol{X}$	Laplace transform of X

Figure 1. Principle of a heat exchanger with two channels and a separating heat transfer wall. This illustrates the principle of a finite volume element used in the dynamic model.

1. Introduction

In liquid food processing plants, e.g. dairies, the composition of the fluid varies and thus must be included in dynamic models used for simulation of the processes. We are engaged in developing such models [1,2] in the language Modelica[1] [3]. The Modelica language is non-causal, object-oriented, and suitable for physical modelling, where the tool itself (Dymola) handles the symbolic organisation of all the ordinary time-differential and algebraic equations, and solves them numerically using a method chosen by the user. (See the Appendix.)

In the liquid food industry, production lines have sequences for start-up and shut-down where, in the first case, water is run through the fluid channels in the plant followed by the food product, and in the second, shut-down, the procedure is reversed, i.e. the product is flushed out by water. Direct product change-over, 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 change-over of fluid

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

composition. These transients in composition cause changes in fluid properties that will influence plant parameters such as flow rates, temperatures and concentrations.

Heat exchangers are important components in process lines in the liquid food industry. In heat treatment processes such as pasteurisation and sterilisation temperature control loops are often used with heat exchangers to maintain an accurate and stable temperature. In the case of food heating e.g. cream pasteurisation, the temperature is a critical control parameter related to health and product quality since a possible presence of pathogenic microorganisms legally requires that the food is heated above a certain temperature, whereas too high a temperature will affect product quality (and increase the production costs).

The fluid composition in these systems affects both pressure drop and heat transfer. A sudden change of fluid composition could, for example, affect the temperature control, and since simulation is used to design equipment to avoid operational problems, it is important that simulation mimics the real dynamics correctly.

There is a great deal in the literature about dynamic modelling and simulation of heating and cooling processes within the food industry. Dynamic modelling has recently been reviewed by Wang and Sun [4], although their focus was on non-liquid food. The amount of work published on heating and cooling by heat exchangers is also very extensive. Furthermore, a considerable amount of scientific work has been performed on modelling tools. Examples of publications in various areas are given below.

- Analyses targeting various aspects such as static behaviour
  - Gut and Pinto [5]
  - Malinowski and Bielski [6]
- Configuration
  - Sahoo and Roetzel [27]
- Analytical (approximate) solutions
  - Abdelghani-Idrissi et al. [7]
  - Tan and Spinner [8]
  - Yin and Jensen [9]
- Linearized models
  - Luo et al. [10].
- Various transients such as response to step changes in flow or temperature
  - Tan and Spinner [8]
  - Yin and Jensen [9]
  - Luo et al. [10]
  - Romie [11-13]
  - Sharifi et al. [14]
  - Xuan and Roetzel [28, 29]
- Arbitrary temperature disturbances
  - Luo et al. [10]
  - Xuan and Roetzel [28, 29]
  - Lakshmanan and Potter [15]
  - Roetzel and Xuan [16]
- Simultaneous variation of flow and temperature
  - Abdelghani-Idrissi et al. [7]
- Frequency response of sinusoidal temperature inputs
  - Lakshmanan and Potter [15]
- Mal-distribution of flow
  - Sahoo and Roetzel [27]
  - Xuan and Roetzel [29]

- Axial heat dispersion
    - Sahoo and Roetzel [27]
    - Xuan and Roetzel [28, 29]
    - Roetzel and. Das [30]
    - Roetzel and Balzereit [31]
- Comparison of model results with experimental measurements
    - Abdelghani-Idrissi et al. [7]
    - Sharifi et al. [14]
    - Xuan and Roetzel [28]
    - Roetzel and Balzereit [31]
    - Kauhanen [17]
- Fluid dispersion, invetsigating axial dispersion and mal-distribution of flow
    - Sahoo and Roetzel [27]
    - Xuan and Roetzel [28, 29]
    - Roetzel and. Das [30]
    - Roetzel and Balzereit [31]
- Object-oriented dynamic modelling tools
    - Mattsson et al. [18]
    - Åström et al. [19]
    - Elmqvist et al. [20]
    - Tummescheit [21]
    - Wozny et al. [22]
- The modelling tool Modelica [3]
    - Åström et al. [19]
    - Wozny et al. [22]
    - Tiller [23]
    - Mattsson et al. [24]
    - Eborn [25]
    - Casella and Schiavo [26]
    - Skoglund [1] and [2]

A good coverage of the field of heat-exchanger dynamics is also given by Roetzel and Xuan [36].

To the best of our knowledge, no studies have been concluded on dynamic changes in fluid properties, although the related subject of fluid dispersion has been studied, e.g. Sahoo and Roetzel [27], Xuan and Roetzel [28, 29], Roetzel and Das [30] and Roetzel and Balzereit [31] to investigate both axial dispersion and mal-distribution of flow.

This paper describes how dynamic models can be constructed in a modern modelling language to simulate fluid composition transitions in a heat exchanger, events that are common in the liquid food industry and therefore important to understand. Based on these models, simulations of the fluid change-over *water to cream* and *cream to water* were performed.

2. Heat-exchanger models

In the present study the heat-exchanger models are built on the conservation of heat, mass and momentum related to flow acceleration and pressure. The correlation equations for heat transfer coefficients and pressure drop for a real industrial heat exchanger were employed.

The fluid properties of importance are: density, specific heat, thermal conductivity and viscosity. These have to be known, as well as their dependencies on temperature and fluid composition (the mass ratio of various components).

2.1 Fundamental equations

To perform simulations efficiently, it is often preferable to introduce approximations into the above mentioned balance and constitutive equations. In the present study the following approximations were made.

- The finite volume method (FVM) was used. Calculations were performed in a series of N control volumes, where N can be increased to decrease the size of the control volumes and thus achieve better accuracy.
- Within each control volume, the arithmetic mean value of the incoming temperature and outgoing temperature was used as the temperature for each side. This results in the "driving force" (T_{da}) for heat exchange with the adjacent channel. At steady state the generally valid logarithmic temperature difference is preferable, however in the present study it is not being used due to the following facts.
    - The logarithmic temperature difference (T_{dm}) is relevant during stationary conditions, whereas this study was focused on transient behaviour.
    - The logarithmic temperature difference differs by only approximately 1% from the above defined temperature difference (T_{da}) in the present study. The reason for this is explained by the ratio of T_{da}/T_{dm}, which can be expressed in terms of NTU values.

      With $\varepsilon = \dfrac{NTU_1 + NTU_2}{2}$ it can easily be shown that:

      $$\frac{T_{da}}{T_{dm}} = \varepsilon \coth(\varepsilon) \tag{1}$$

      A graph of Eq. (1) is displayed in Figure 2. Note that the sign of the NTU values determines the direction of flow. This means that, in the case of counter-current flow with approximately equal magnitude of the NTU values, the value of the argument ε will be close to zero. This is the case in the present study, as well as normally in the food industry. Also, ε assumes small values if the size of the control volumes decreases, independent of the flow direction (co-current or counter-current). See also next point.
    - Increased discretization gradually reduces the error.
    - The model requires a temperature on each side, not the temperature difference.
    - The logarithmic temperature difference requires more computation.
- Axial heat flow (along the flow channels) in the fluid (dispersive and conductive) is neglected. As concluded by Xuan and Roetzel [29], this assumption is justified if the Péclet number $Pe_h > 55$, meaning that the dispersive heat capacity flow (W_d) is negligible compared with the heat capacity flow (W), see Eq. (20) and calculations thereafter. The main reason that this condition is fulfilled in this study is that both fluids (water and cream) flow under clearly turbulent conditions (Re > 4000) and that the heat exchanger geometry employed does not give rise to mal-distribution.
- Axial heat flow in the tube wall is neglected.
- The wall is simplified as two parts each with half the thickness (see Figure 1 and Eqs. 8 and 9) both with a homogeneous temperature, i.e. discretization degree 2 of the heat transfer through the wall. This is done as it provides a simple way of

handling the thermal dynamics of the wall, and to approximate the surface temperatures used for calculation of the heat transfer coefficients on each side. See Eq. (2). The reason for this is twofold:

  o   Firstly, the different surface temperatures are needed for correction factors for surface heat transfer coefficients.
  o   Secondly, the thermal dynamics of the wall is not negligible. In the present study the thermal capacity ratio for the tube wall compared with the tube volume filled with water is approximately 30%.

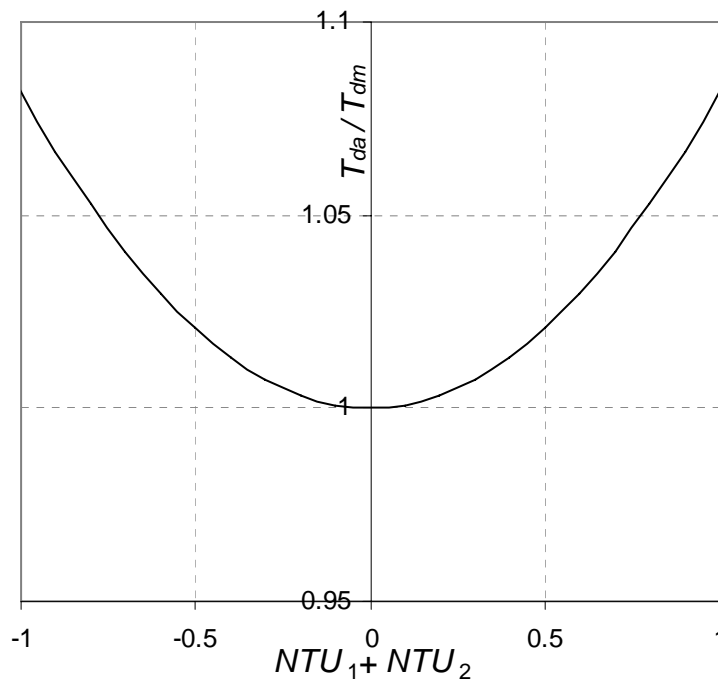• No heat is transferred to the environment.

Figure 2. Ratio of T_{da}/T_{dm} as a function of NTU_1+NTU_2 reflecting the error in the static temperatures in the heat exchanger when using T_{da} instead of T_{dm}.

2.1.1 Heat balance and heat transfer coefficient
The heat balance in one control volume of the heat exchanger involves three parts: i) the heat balance in the wall, ii) the heat balance in channel 1 and iii) the heat balance in channel 2 .

Heat balance in the wall
Heat conduction follows the fundamental heat diffusion equations (Fourier heat conduction). By above mentioned approximations, the fundamental heat diffusion equations through the heat exchanger wall become one-dimensional, perpendicular to the direction of fluid flow and involve three steps of heat transfer: i) From the fluid in channel 1 to wall surface 1, ii) from wall surface 1 to wall surface 2, and iii) from wall surface 2 to the fluid in channel 2.

Constitutive equations for the heat transfer from the fluid to the wall
Apart from heat conduction through the wall, there is the convective heat transfer between the fluids and the channel wall surfaces: $P = A\alpha\Delta T$

Here the value of the heat transfer coefficient α depends on the fluid properties, flow velocity and heat-exchanger geometry. The standard method is to use the dimensionless Reynolds, Nusselt and Prandtl numbers (*Re, Nu, Pr*). The relationship between the fluid properties together with the flow rate and the heat transfer coefficient can be expressed as a correlation between these numbers. The most-well known expression is the Dittus-Boelter correlation for turbulent flow.

$$Nu = C_{Nu}Re^x Pr^y \; (\mu/\mu_w)^z \qquad\qquad (2)$$

The constant (C_{Nu}) and exponents (x, y, z) may vary due to heat-exchanger geometry and whether the fluid is being heated or cooled. They also vary depending on the flow type, i.e. laminar, transition or turbulent. Correction factors are also sometimes used, e.g. if the channel length is short compared with the hydraulic diameter.

In this study the parameter values were taken from a company-owned database used for a commercial heat exchanger[2]. It has also been used to validate the dynamic models with respect to temperature and flow perturbations [17].

Fluid properties
As already mentioned, the heat transfer and temperature change depend on the fluid properties. Since the fluid properties depend on both the fluid temperature and the fluid type, this dependency has to be known. In the present work the fluid is described as a mixture of five typical food components: water, carbohydrates, protein, fat and ash. The concentration of each component is stored in a concentration vector, $\hat{C}$, with five elements of mass fraction. From this the fluid properties λ, c_p and ρ can be expressed as a function of $\hat{C}$ and *T*, see Heldman and Lund [32][3]. No general relation to concentration exists for the viscosity. Therefore a curve fitting model was derived from laboratory data from typical kinds of liquid foodstuffs, such as milk, cream and fruit juice. This means that for each type of fluid a relation between viscosity parameters and concentration (dilution with water) was fitted. See Figure 3 where the viscosity of water and 15% cream is shown as a function of temperature.

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[2] Tubular heat exchanger, model MT25/16S-6 manufactured by Tetra Pak Processing Components AB, Bryggareg. 23, SE-22736 Lund, Sweden.

[3] It should be noted that Table 2, p. 251 in reference [32] includes an error. The second term in the formula for calculation of the thermal conductivity of fat, $2.7604*10^{-3}T$, should read $2.7604*10^{-4}T$.
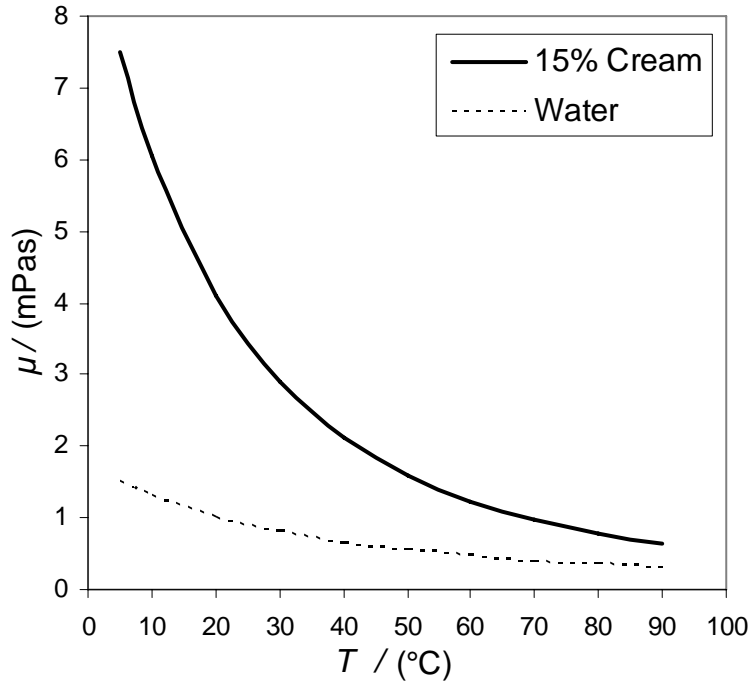
Figure 3. Viscosity of water and cream as a function of temperature.

Heat balance in the control volume
By considering one small volumetric part of the heat exchanger, and using the above equations and approximations, the heat balance equations become (see Figure 1):

$$\bar{\rho}_1 \bar{c}_{p1} V_1 \frac{dT_{12}}{dt} = P_{11} - P_{12} + P_{w1} = \rho_{11} \bar{c}_{p1} Q_{11} T_{11} - \rho_{12} \bar{c}_{p1} Q_{12} T_{12} + P_{w1} \tag{3}$$

$$\bar{\rho}_2 \bar{c}_{p2} V_2 \frac{dT_{22}}{dt} = P_{21} - P_{22} - P_{2w} = \rho_{21} \bar{c}_{p2} Q_{21} T_{21} - \rho_{22} \bar{c}_{p2} Q_{22} T_{22} - P_{2w} \tag{4}$$

with heat flow into and out of the wall surfaces:

$$P_{w1} = (T_{w1} - \bar{T}_1)\alpha_1 A_1 \tag{5}$$

$$P_{2w} = (\bar{T}_2 - T_{w2})\alpha_2 A_2 \tag{6}$$

and with heat transfer through the wall:

$$P_w = (T_{w2} - T_{w1})\frac{\lambda_w}{h} A_w \tag{7}$$

(Note that the heat transfer equation must cover the whole thickness (using h, not h/2).

The heat balance for the wall:

$$A_1 \frac{h}{2} \rho_w c_{pw} \frac{dT_{w1}}{dt} = P_w - P_{w1} \tag{8}$$

$$A_2 \frac{h}{2} \rho_w c_{pw} \frac{dT_{w2}}{dt} = P_{2w} - P_w \tag{9}$$

If the geometry is planar then $A_1=A_2=A_w$, but if we have a tubular geometry, as in this study, we get the logarithmic wall area.

$$A_w = \frac{(A_2 - A_1)}{\ln\left(\dfrac{A_2}{A_1}\right)}$$ (10)

It should be noted that the models developed allow all the above physical properties, except geometrical parameters, to be varied during simulation. Hence not only $\hat{C}_{11}$ and $\hat{C}_{21}$ may be varied as in the present study, but also T_{11}, T_{21}, Q_1 and Q_2 may be varied arbitrarily. Thus, since the heat transfer coefficient and the fluid properties depend on $\hat{C}$, T and Q, they will vary accordingly.

2.1.2 Mass and momentum balance

In addition to the heat transfer dynamics, the dynamics of the flow rate also has to be modelled appropriately in a full-scale simulation. This is done in the models used here. However, since this is not in the focus of interest in the present study, the details are not given here. It should, however, be mentioned that the basic conservation laws used are mass balance and momentum balance.

- Mass balance

$$\frac{\partial(\rho A_c)}{\partial t} + \frac{\partial(\rho A_c v)}{\partial x} = 0$$ (11)

This is also valid for each fluid component individually (water, protein, fat, carbohydrates and ash) and has to be accounted for, particularly in one of the models. (See below where Eq. (14) describes the mass balance in an ideally mixed volume.)

With a constant cross-sectional area and a density depending on the temperature and concentration, and assuming the fluid to be incompressible Eq. (11) becomes:

$$\frac{\partial\rho}{\partial T}\left(\frac{\partial T}{\partial t} + v\frac{\partial T}{\partial x}\right) + \sum_{i=1}^{5}\frac{\partial\rho}{\partial\hat{C}[i]}\left(\frac{\partial\hat{C}[i]}{\partial t} + v\frac{\partial\hat{C}[i]}{\partial x}\right) + \rho\frac{\partial v}{\partial x} = 0$$ (12)

Thus a temperature change will give rise to a velocity change as the temperature change causes expansion or contraction of the fluid. Further simplifications are possible but they are not presented here.

- Momentum balance, Thomas [33]

$$\frac{\partial(\rho v A_c)}{\partial t} + \frac{\partial(\rho v^2 A_c)}{\partial x} + A_c\frac{\partial p}{\partial x} + F_w + A_c\frac{\partial(z\rho g)}{\partial x} = 0$$ (13)

This equation is used with some approximations such as:

$$\frac{\partial(\rho v^2 A_c)}{\partial x} \approx 0$$

Constitutive equations for components, such as pressure drop equations, are also used in the models [1, 2].

2.2 Alternative models for fluid property propagation

In a liquid food plant, a common procedure is to start up equipment (e.g. a pasteuriser) on water and proceed with the product when the equipment is ready (e.g. pre-sterilised). When production is completed, the reverse procedure takes place, i.e. water is flushed through the plant to remove the product, while maintaining production conditions. To be able to simulate this, the fluid properties must be varied accordingly. The change in fluid data during the simulation can be implemented in different ways.

Model I – "Instantaneous property change"
The simplest method is to instantaneously change the fluid properties in the whole heat exchanger as soon as the new fluid is introduced.

Model II – "Ideally mixed volumes"
This is a "classical" finite volume model where we regard the control volumes as ideally mixed volumes, gradually replacing the old fluid data with new, following the ideal mixing equation for the concentration vector, $\hat{C}$, of the fluid components (water, protein, fat, carbohydrates and ash):

$$\rho_{out} V \frac{d\hat{C}_{out}}{dt} = \rho_{in} Q_{in} \hat{C}_{in} - \rho_{out} Q_{out} \hat{C}_{out} \qquad (14)$$

where the subscripts "in" and "out" denote flow into and out of the volume. The heat balance is treated in the same way as above. In this case the fluid properties will change gradually in each control volume as the concentrations of fluid components change. See above under "Fluid properties".

Model III – "Transport delay"
A third and novel alternative is to allow the concentration vector to propagate along the flow channel with the fluid velocity, and use the concentration data at the inlet of each control volume. This method requires that the model can simulate the transport delay dynamically as the flow velocity changes. (See definition of τ.) This is important even though the flow rate in the present study was kept constant. With this method, the fluid properties depend on the dynamically delayed concentration in each control volume for each channel.

$$\hat{C}_{12}(t) = \vec{\hat{C}}_{11}(t) = \hat{C}_{11}(t - \tau) \qquad (15)$$

$$\hat{C}_{22}(t) = \vec{\hat{C}}_{21}(t) = \hat{C}_{21}(t - \tau) \qquad (16)$$

This affects the fluid properties ρ, λ, c_p and μ (or K and n) as mentioned above, e.g.

$$\lambda_{12} = \lambda(\hat{C}_{12}, T_{12}) = \lambda(\vec{\hat{C}}_{11}, T_{12}) \qquad (17)$$

Since the tool employed, Dymola, provides an efficient function for simulating dynamic transport delays, this is easily implemented in the model. The reason for doing this is that we want to *separate the fluid propagation model, including possible dispersion, from the heat transfer model*. It can also be justified to assume plug flow in the present study. To do so, the Péclet numbers, *Pe* and *Pe*$_h$, have been calculated according to Taylor dispersion (Taylor [34] Eqs. 5.1 and 5.3):

$$d = 10.1 \frac{D_h}{2} v \sqrt{\frac{f}{2}} = 3.57 D_h v \sqrt{f} \qquad (18)$$

The value of *f* can be derived from [34] Eq. 5.4, but simplified according to Blasius (e.g. Coulson & Richardson [35] Eq. 3.11) for turbulent flow with $Re<10^5$ (Note $\Phi=f/2$)

$$f = 2\Phi = 0.0792 Re^{-0.25} \tag{19}$$

This gives:

$$Pe = vL / d = \frac{L}{3.57 D_h \sqrt{0.0792 Re^{-0.25}}} \approx \frac{L Re^{0.125}}{D_h} \tag{20}$$

The actual values of *Re* and *Pe* are calculated at the inlet of the tube for cream which is the case where the viscosity is highest, thus giving the lowest value of both the Reynolds number and the Péclet number that occur in the heat exchanger.
The tube side (channel 1):
Re = 4110 with cream at 10 °C
D_h = 0.014 m
L = 12 m
Pe = 2420
Hence *Pe*>55 is satisfied, as concluded by Xuan and Roetzel [29] as a condition for negligible axial dispersion. It can thus be concluded that the axial dispersion due to fluid dispersion is negligible in this study.

Comparison between Models II and III
In the present study, as in many food applications, the heat exchanger is assumed to be working in a turbulent region with a high Péclet number, as shown above. Hence the liquid propagates with negligible axial dispersion, i.e. the turbulent flow profile can, to a good approximation, be replaced by plug flow as in Model III. Accordingly, a relevant case to study when separating heat transfer and fluid propagation, is the case of ideal plug flow. Model II has the drawback that it causes a "numerical fluid dispersion", i.e. property propagation due to limited discretization. Only when the discretization approaches infinity does the property propagation approach plug flow behaviour. This fact is well known and can be seen by a Laplace transform of Eq. (14).

$$\hat{C}_{out} = \frac{1}{1 + s\tau} \hat{C}_{in} \tag{21}$$

Here we have simplified the situation by assuming the density, ρ, to be constant and by replacing *V/Q* with τ. When the control volume is discretized into *N* control volumes, each with the volume *V/N*, it corresponds to the Laplace transform:

$$\hat{C}_{out}(N) = \left(\frac{1}{1 + s\frac{\tau}{N}} \right)^N \hat{C}_{in} = \left[\left(1 + s\frac{\tau}{N} \right)^{\frac{-N}{s\tau}} \right]^{s\tau} \hat{C}_{in} \tag{22}$$

and we see that

$$\underset{N \to \infty}{\text{Lim}}\, \hat{C}_{out}(N) = e^{-s\tau} \hat{C}_{in} \xrightarrow{Laplace^{-1}} \hat{C}_{in}(t - \tau) = \vec{\hat{C}}_{in} \tag{23}$$

Hence an infinite discretization of Model II corresponds to ideal plug flow with only a transport delay in the concentration. The "numerical fluid dispersion" due to the finite value of *N* is clearly visible in Figure 6.

This means that, while Model III only requires sufficient discretization for the thermal balance equations, Model II also requires discretization to mimic plug flow well. Therefore Model III is advantageous with regard to the amount of computation required.

2.3 Discretization in Modelica

The dynamic models in the present work is built in a tool (Dymola) based on the Modelica language. Modelica is described briefly in the Appendix, where an example of code from a heat exchanger model is also given.

To solve the system of partial differential equations (PDE) and algebraic equations (AE), discretization of space (the axial coordinate only) is required to convert the system into a system of ordinary differential equations (ODE) and AEs, which can be handled by a Modelica-based tool. The finite volume method was used since it has good properties in respect of maintaining the conserved quantities. The heat balance equations above are approximations that become better as the control volumes become smaller. Therefore, to solve the heat transfer problem, the heat exchanger has to be discretized into smaller volumes. This is done by splitting up the whole heat exchanger model into N volumes. Figure 4 shows a system where $N=2$. Furthermore, the Modelica language supports vectors of models, a possibility that was used in the present work as a convenient way to discretize the heat exchanger models.
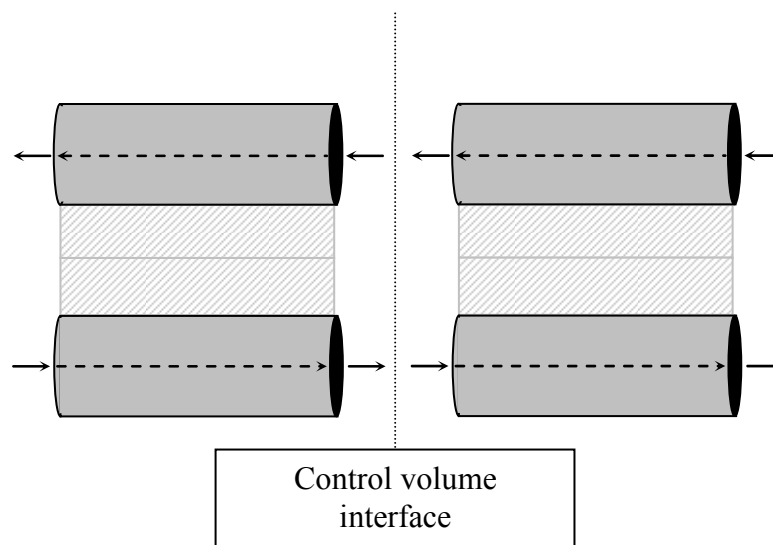

Figure 4. Principle of two heat-exchanger control volumes with a counter-current flow interface where variables are set equal.

3. Calculation set-up – system model

In the present study a complete system of component models was set up to simulate the heat exchanger during fill-up and purging. See Figure 5. The dynamic heat exchanger model has been validated previously with transients in temperature and flow [17].

The data used in the system were as follows.

- Tube & shell heat exchanger model Tetra Pak MT 25/16S-6 with 2 sections. This is a concentric type of heat exchanger with one smooth (non-corrugated) tube. The tube has an outer diameter of 16 mm and is made of 1 mm thick stainless

steel. The shell has an outer diameter of 25 mm and is made of 1.2 mm thick stainless steel. Each section is 6 m long.

- Fluid channel 1 (tube) with two fluids in three phases:
    - Phase 1: Fluid 1 = water, 10 °C
    - Phase 2: Fluid 2 = cream, 15% fat, 10 °C
    - Phase 3: Fluid 1 again
- Fluid channel 2 (shell): Water, 95 °C all the time
- Flow rate channel 1: 1000 l/h (controlled by a PID controller, stable during fluid transition)
- Flow rate channel 2: 1300 l/h (controlled by a PID controller, stable during fluid transition)
- *NTU* value in channel 1: $NTU_1 = 1.45$ during the water phases (= phase 1 and 3) and 1.63 during the cream phase (= phase 2)
- *NTU* value in channel 2: $NTU_2 = -1.16$ where the minus sign indicates counter-current flow. Note that the maximum value of $NTU_1 + NTU_2 = 1.63 - 1.16 = 0.47$. Using Figure 2 this gives $T_{da}/T_{dm} \approx 1.01$
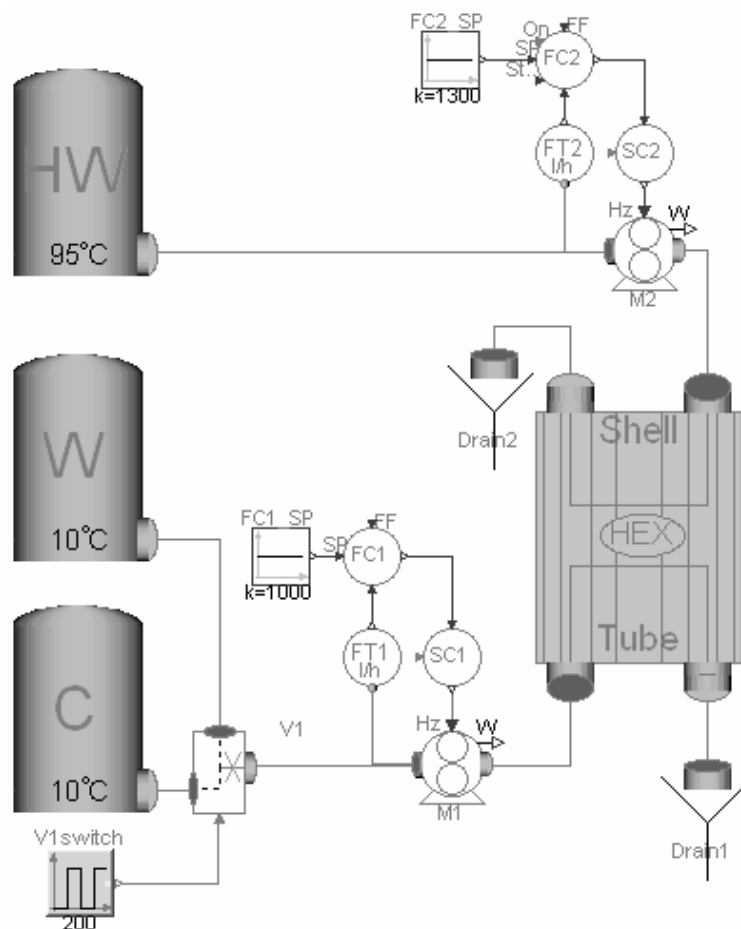

Figure 5. The design of a theoretical experiment as a system of dynamic models, whereof one, denoted "HEX", is the heat-exchanger model that can be defined as Model I, II or III. Depending on the change-over valve, V1, channel 1 (Tube) is connected to either a water source denoted "W" or a cream source denoted "C". Channel 2 (Shell) is connected to a hot-water source denoted "HW". The temperatures in the fluid sources are constant. The flow rate control loop for the tube side (channel 1) includes a sensor (FT1), a PID controller (FC1), a flow set point (FC1_SP), an inverter (SC1) and a pump (M1). The corresponding units on the shell side are FT2, FC2, FC2_SP and M2.

4. Results

Simulation was carried out by numerically solving the system of model equations using the solver Dassl in Dynasim's Modelica based program Dymola version 5.3a. The following simulations were run with all three models I, II and III described above.

Step 1 (0-100 s):   Start-up of the system with fluid 1 (water) in both channels to allow flow to stabilise.

Action 1 (at 100 s):   Changeover from fluid 1 (water) to fluid 2 (cream) at the tube side (channel 1) inlet. The action time for the changeover valve (V1 in Figure 5) is 0.1 s.

Step 2 (100-200 s):   Continue to allow the transient to stabilise.

Action 2 (at 200 s):   Change over from fluid 2 (cream) to fluid 1 (water) at the tube side (channel 1) inlet. The action time for the changeover valve (V1 in Figure 5) is 0.1 s.

Step 3 (200-300 s):   Continue to allow the transient to stabilise.

The simulations gave the following results:

Exit concentration in channel 1

The fluid transition, expressed as concentration of fat (15% fat = 100 % cream) is plotted in Figure 6. The exit curves differ for the three models. For Models I and III the degree of discretization makes no difference. While Model I has an exit concentration identical to the entrance concentration, Model III shows a dwell time difference of 6.3 s between the two curves. Model II is plotted with discretization of $N=5$ and 15, showing the dependency of exit concentration on the discretization.

Exit temperatures

The temperature transients occurring as a result of the fluid changeover are plotted in Figures 7 and 8. Figure 7 shows an overview of the results of all three models with discretization $N=15$. Both outlet temperatures (T_{12}, T_{22}) covering fill-up and purging are displayed. Model I is obviously far too simple a model to simulate the behaviour correctly. Figure 8 shows an expanded view of the fill-up transient of T_{12} and with more discretization cases simulated ($N=2$, 5 and 80) for Models II and III. Figure 8 shows that Model III converges faster, as N increases, than Model II.

To further analyse the transient behaviour, the temperature profiles in the channels are plotted in Figure 9 at different moments in time. The fluid transition can be seen as a temperature wave propagating through channel 1 before the new steady state is established. Since the heat transfer is worse with cream, the front zone of cream will not be heated as much as the preceding water. The water in channel 2 will not be cooled down as much for the same reason. Furthermore, since the temperature difference at the beginning of the transient is less than at the end of the transient, the front zone of cream experiences a smaller driving force, and therefore leaves the heat exchanger at a lower temperature than later when a greater temperature difference will drive more heat to the cream than initially. In Figure 9 the curve for channel 1 at 108.8 s shows this decrease in exit temperature. In Figures 7 and 8 the same

temperature drop, below the new steady state, is clearly visible as undershoot in the first transient. In the second transient in Figure 7 there is a corresponding overshoot.

The different convergence rates of Models II and III were analysed by plotting the temperatures at 110 seconds, where the temperature dip occurs, as a function of N. Figure 10 clearly shows the asymptotic behaviour, where Model III conspicuously converges faster than Model II, as N increases. The combined plot shows that, for a given level of accuracy, Model II requires approximately 10 times more CPU time than Model III.
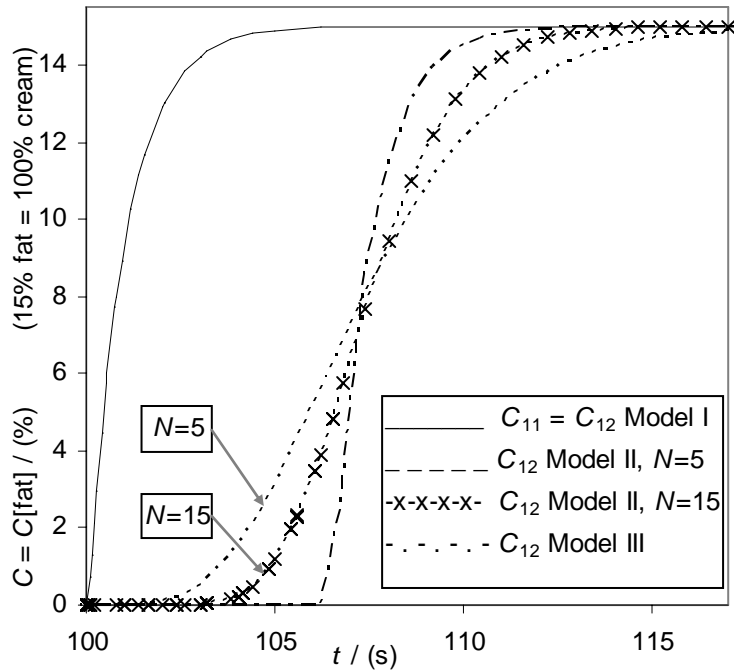

Figure 6. Detailed view of the concentration at the tube inlet (C_{11}) and the tube outlet (C_{12}) during cream filling (15% cream displacing water). The inlet transition represents a realistic changeover due to fluid dispersion in the upstream equipment. In this case it is the result of a valve with an ideal mixing volume of 0.278 litres and a change-over time of 0.1 sec. The curves for C_{11} and C_{12} are identical in Model I since in that case a fluid change is assumed to take place instantaneously in the whole heat exchanger. The curve shape for C_{12} is equal to C_{11} for Model III but delayed by a time corresponding to the dwell time in the heat exchanger, independently of the degree of discretization. The curve for C_{12} predicted by Model II depends on the degree of discretization.
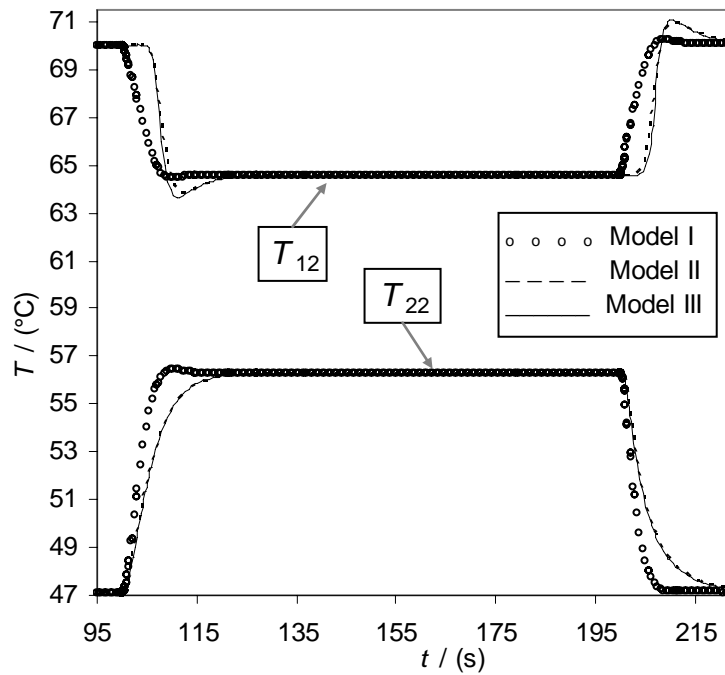
Figure 7. Overview of temperatures at the outlet of the tube side (T_{12}) and the shell side (T_{22}) throughout the whole course of cream filling and purging. The simulation shows the results from all three models and with N=15.
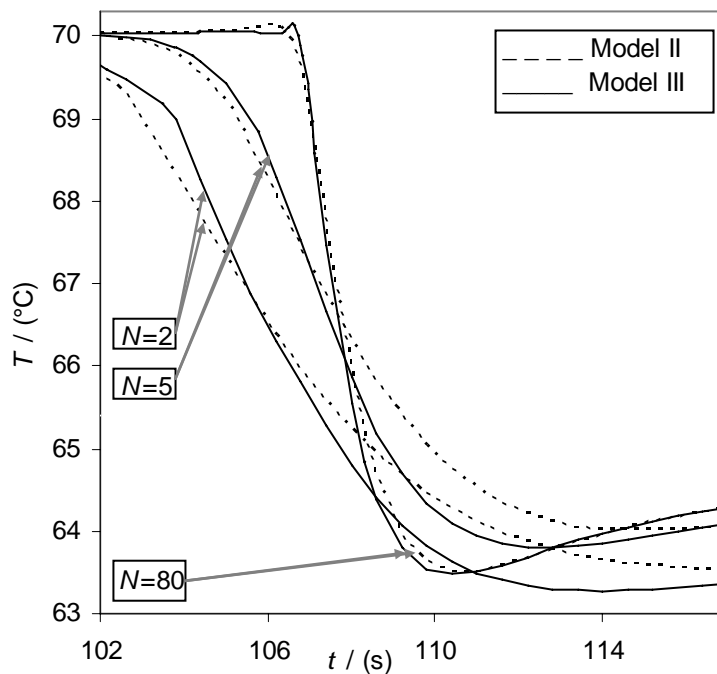

Figure 8. Detailed view of the outlet temperature at the tube side (T_{12}) during cream filling (cream displacing water) for Models II and III with different degrees of discretization.
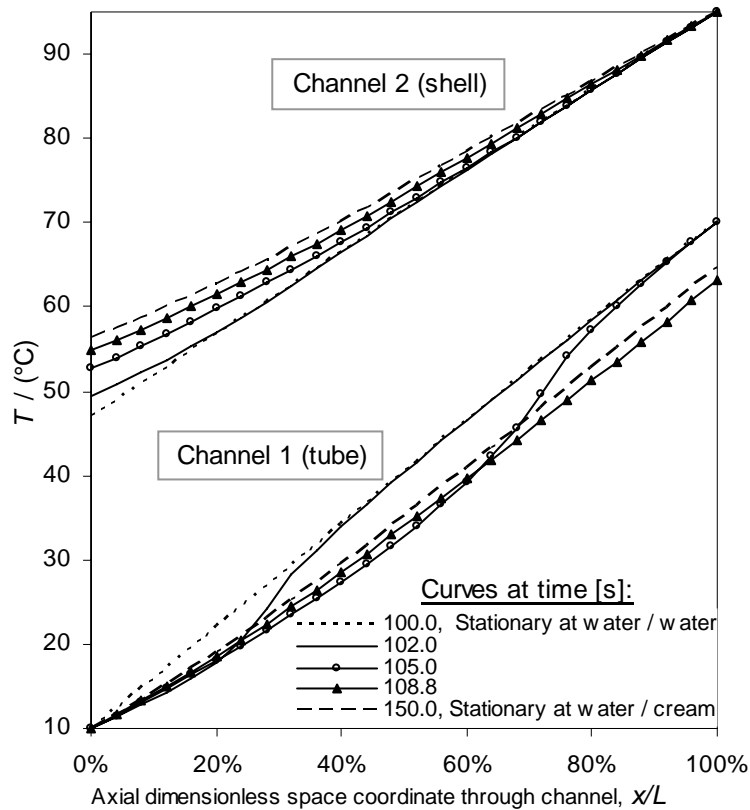
Figure 9. Temperature profiles in the channels, at different instances in time, during the transition where cream is being pumped into the heat exchanger. The degree of discretization is *N*=25. (In this particular case the fluid transition at the tube inlet was an ideal step instead of the change shown in Figure 6.)
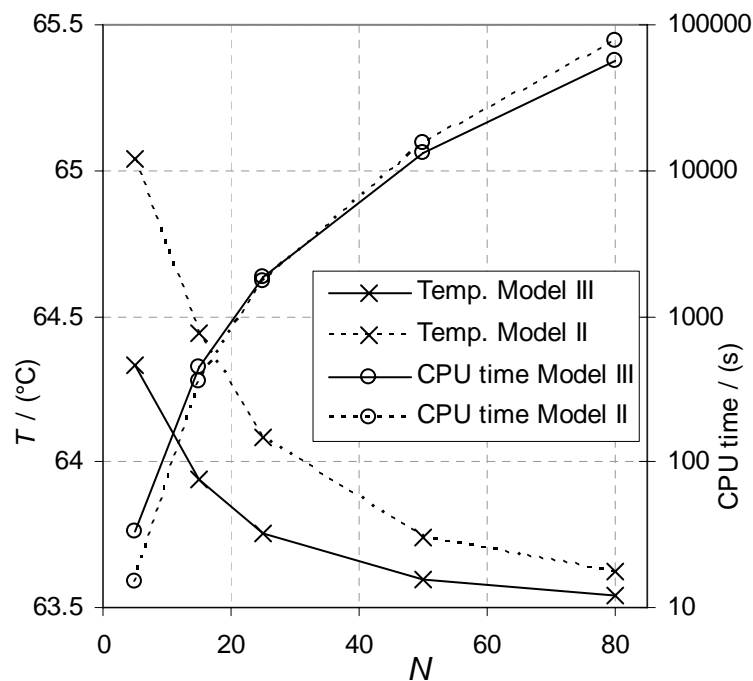

Figure 10. Convergence and required computational power. As an indication of convergence the temperature at 110 s is shown for Models II and III as a function of degree of discretization. The required CPU time (in a PC of model Dell Optiplex SX270) is also shown as a function of degree of discretization. It is clearly visible that Model II requires a higher degree of discretization than Model III for the same accuracy. Model II requires approximately 10 times more CPU time than Model III.

5. Conclusions

To be able to use simulation in liquid food process design it is important to model fluid transitions to capture dynamic characteristics such as temperature transients, for example the dip occurring in the present study (Figure 8). If simulation does not provide such details, the plant, including its control, is likely to fail or perform badly.

Three models were formulated to describe fluid transfer effects on the dynamics of the thermal behaviour in a heat exchanger. A simple model (I, "Instantaneous property change") was compared with a more traditional one (II, "Ideally mixed volumes") and a new model (III, "Transport delay"). Simulation showed that Model I is too simple, while Model III was the best.

A high Péclet number is common for tubular heat exchangers in liquid food processes, i.e. little axial dispersion takes place. Model II gives a "numerical fluid dispersion" due to limited discretization, whereas model III has a constant dispersion ($d = 0$ m^2/s) independent of the discretization. Hence, while Model III only has to be discretized for heat transfer calculations, Model II also must be discretized to reduce the "numerical fluid dispersion". Therefore Model III requires less discretization and therefore less computation time (a factor ≈ 10) than Model II. Model III is also easily implemented in a Modelica tool with true transport delay functionality.

Furthermore, separating the fluid transition model from the heat transfer model, as in Model III, provides the freedom to handle other fluid dispersion models than plug flow as an add-on to the plug flow model, without affecting the heat transfer model. This will be investigated in future work.

Appendix – The Modelica modelling language

The Modelica language [3, 23] is an object-oriented, dynamic modelling language designed to allow for component-oriented modelling of complex physical systems.

Models in Modelica are mathematically described by a mixture of ordinary *differential equations* (ODE) via the language element *der(<variable>)*, *algebraic equations* (AE) and *discrete equations*. A Modelica-based tool handles and sorts the equations symbolically and eventually solves them numerically. No particular variable needs to be solved manually, as a Modelica-based tool solves all variables.

The interfaces between model components are "connectors" in which the variables to be communicated between the components are defined. The instruction *connect* is used to create a connection. There are two types of variables in connectors:

- *across variables* whose values are set equal in a connection point (e.g. voltage) and
- *flow variables* whose values are summed and set equal to zero at a connection point (e.g. electrical current).

  The statement *connect(*a,b*)* means that the variables in the connectors "a" and "b" follow the above rules.

Models can be constructed in a hierarchy with inheritance (by instantiation or extensions).

The example below shows part of the code used in the present study. In the code, `HEX[]` is one complete heat exchanger control volume model, defined as a vector (see Figures 1 and 4). The variables, such as temperature, flow, pressure concentration, etc., are built into the "connectors" of that control volume model. The "connectors" are `HEX[i].PrIn1` for channel 1 inlet and `HEX[i].PrOut1` for channel 1 outlet in element *i* of `HEX[]`. The corresponding connectors are defined for channel 2. By "connecting" *N* elements of `HEX[]`, as in the code below, a counter current heat exchanger is generated.

```
for i in 1:N - 1 loop
  // Connectors channel 1
    connect(HEX[i].PrOut1, HEX[i + 1].PrIn1);
  // Connectors channel 2
    connect(HEX[i].PrIn2, HEX[i + 1].PrOut2);
end for;
```

Using this feature it is easy to declare *N* as a parameter that can be decided just before simulation. Hence, in this study, *N* is the length of a heat-exchanger array. As a consequence, some heat-exchanger parameters for the elements in the array have to depend on *N*, for example the channel volume of each element is $1/N$ of the total volume. The Modelica language also supports handling of this parameter dependency.

It should be noted that even though Figure 1 shows polarity (co-current or counter-current), this does not exist for a single control volume, i.e. both sides are equal. What creates the polarity is the order in which the inlets and outlets of adjacent control volumes are connected. Thus, by changing the statement for channel 2 above to the following, a co-current heat exchanger is created instead.

```
    connect(HEX[i].PrOut2, HEX[i + 1].PrIn2);
```

The corresponding change could also have been implemented in channel 1 instead.

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