Mathematical modeling of mixing in a horizontal rotating tubular bioreactor: "Spiral flow" model

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Abstract A horizontal rotating tubular bioreactor (HRTB) was designed as a combination of a "thin-layer bioreactor" and a "biodisc" reactor whose interior was divided by O-ring shaped partition walls. For the investigation of mixing in HRTB the temperature step method was applied. Temperature changes in the bioreactor were monitored by six Pt-100 sensors (t₀ response time 0.08 s and resolution 0.002 °C) which were connected with an interface unit and a personal computer. In this work a modified "tank in series" concept was used to establish a mathematical model. The heat balance of the model compartments was established according to the physical model and the "spiral flow" pattern. Numerical integration was done by the Runge–Kutta–Fehlberg method. The mathematical mixing model called "spiral flow" model contained four adjustable parameters (N₁, Nᵢ, Fᵣ, and Fᵢ) and five parameters which characterized the plant and experimental conditions. The "spiral flow" model was capable to describe the mixing in HRTB properly, and its applicability was much better than with the "simple flow" model, presented earlier.

List of symbols

- \( A_{ui} \): m², ith part of inner surface of bioreactor's wall
- \( A_{vi} \): m², ith part of outlet surface of bioreactor's wall
- \( c_p \): kJ kg⁻¹ K⁻¹, heat capacity of liquid
- \( c_{pr} \): kJ kg⁻¹ K⁻¹, heat capacity of bioreactor's wall
- \( D \): h⁻¹, dilution rate
- \( E \): °C°C⁻¹ h⁻¹, error of mathematical model
- \( E_r \): dm³ s⁻¹, circulation flow in the model
- \( E_f \): dm³ s⁻¹, back flow in the model
- \( F_t \): dm³ s⁻¹, inlet flow in bioreactor
- \( I \): °C, intensity of temperature step, the difference in temperature between the temperature of the inlet liquid and the temperature of liquid in bioreactor before temperature step
- \( K_1 \): W m⁻² K⁻¹, heat transfer coefficient between the liquid and bioreactor's wall
- \( K_2 \): W m⁻² K⁻¹, heat transfer coefficient between the bioreactor's wall and air
- \( L \): m, length of bioreactor
- \( m \): kg, mass of bioreactor's wall
- \( n \): min⁻¹, rotational speed of bioreactor
- \( n_i \): number of temperature sensors
- \( N_1 \): number of compartments inside cascade
- \( N_i \): number of cascades
- \( r_{wi} \): m, inner diameter of bioreactor
- \( r_{o} \): m, outside diameter of bioreactor
- \( s(t) \): step function
- \( t \): s, time
- \( T \): °C, temperature
- \( T_c \): °C, calculated temperature
- \( T_m \): °C, measured temperature
- \( T_{N1,Ni} \): °C, temperature of liquid in defined compartments inside the cascade
- \( T_{N1,S} \): °C, temperature of surrounding air
- \( V_1 \): dm³, volume of liquid in the bioreactor
- \( V_i \): dm³, volume of liquid in bioreactor

Matrix coefficients

- \( B = \frac{F_t N_1 N_i}{V_1} \)
- \( C = \frac{F_r N_1 N_i}{V_1} \)
- \( D = \frac{F_r N_1 N_i}{V_1} \)
- \( E = B + C + D \)

- \( G_1 = K_1 \frac{2 r_i I L N_i}{V_1} \)
- \( G_2 = K_1 \frac{2 r_i I L N_i}{V_1} + K_2 \frac{2 r_i I L N_i}{V_1} \)
- \( G_3 = K_2 \frac{2 r_i I L N_i}{V_1} \)
- \( A_{wi} = \frac{2 r_i I L N_i}{V_1} \)
- \( A_{vi} = \frac{2 r_i I L N_i}{V_1} \)

1 Introduction

In a previous work [1], we presented the construction and technical details of a horizontal rotating tubular bioreactor (HRTB). Furthermore, in the same work, we presented...
a mathematical mixing model which we named a "simple flow" model. Results of mixing simulation achieved by the "simple flow" model were not fully satisfactory in the whole range of explored variables and parameters. In the real system, the forward flow ($F_t$) caused by the inlet flow is influenced further by the rotational speed and the friction of liquid on the surfaces of rotating O-rings and bioreactor wall. The friction forces turn the forward flow into the circulation flow. As a consequence, the resulting flow should be a sum of both effects and it was named the "spiral" flow. This fact was not taken into account in the "simple flow" model [1]. In order to be able to implement the combined "spiral" flow in forward direction, we developed the "spiral flow" model (Fig. 1) with the intention to obtain better agreement between measured and simulated data as well as better correlation between experimental (operation) and model parameters.

2 Materials and methods

The horizontal rotating tubular bioreactor (HRTB) was made of a plastic tube. The technical characteristics were described earlier [1]. For mixing investigations in HRTB the temperature step method was used. The temperature change in the bioreactor was detected by six Pt-sensors ($t_{res}$ response time 0.08 s and resolution 0.002 °C) connected with an interface unit and a personal computer. Operation conditions for the investigation of combined influence of dilution rate and rotational speed were the same as for the previously described "simple flow" model [1]. According to the physical model shown in Fig. 1, dividing the bioreactor into ideally mixed compartments, the heat balance was established for each compartment inside the model. The obtained system of differential equations is analogous to the "simple flow" model and can be expressed as follows:

$$\frac{d}{dt} \begin{bmatrix} T_{1,1} \\ \vdots \\ T_{N1,1} \\ T_{1,Ni} \\ \vdots \\ T_{N1,Ni} \\ T_{1,s} \\ \vdots \\ T_{N1,s} \end{bmatrix} = A_2 \begin{bmatrix} T_{1,1} \\ \vdots \\ T_{N1,1} \\ T_{1,Ni} \\ \vdots \\ T_{N1,Ni} \\ T_{1,s} \\ \vdots \\ T_{N1,s} \end{bmatrix} + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$[T(t)]$$

A2 is a corresponding model matrix and has the form as presented below. Coefficients inside the matrix are listed in the above list of matrix coefficients. Heat transfer coefficients were defined in the same manner as earlier [1]. The Runge–Kutta–Fehlberg numerical integration method was applied for the solution of the system of differential equations [2]. A sensitivity analysis of the model [3–5] was undertaken for all model parameters. The "spiral flow" model contains four adjustable parameters ($N_1$, $Ni$, $F_t$, and $F_p$) and five fixed parameters ($I$, $F_c$, $V_t$, $K_1$ and $K_2$), respectively. For the evaluation of successfulness of simulation two criteria were applied [1]:

\begin{align*}
T_{1,1} &
T_{1,2} \\
& \vdots \\
T_{N1,1} \\
T_{1,Ni} \\
& \vdots \\
T_{N1,Ni} \\
T_{1,s} &
T_{1,s} \\
& \vdots \\
T_{N1,s} \\
& 
\end{align*}

\begin{align*}
T_{1,1} &
T_{1,2} \\
& \vdots \\
T_{N1,1} \\
T_{1,Ni} \\
& \vdots \\
T_{N1,Ni} \\
T_{1,s} &
T_{1,s} \\
& \vdots \\
T_{N1,s} \\
& 
\end{align*}

\begin{align*}
T_{1,1} &
T_{1,2} \\
& \vdots \\
T_{N1,1} \\
T_{1,Ni} \\
& \vdots \\
T_{N1,Ni} \\
T_{1,s} &
T_{1,s} \\
& \vdots \\
T_{N1,s} \\
& 
\end{align*}

\begin{align*}
T_{1,1} &
T_{1,2} \\
& \vdots \\
T_{N1,1} \\
T_{1,Ni} \\
& \vdots \\
T_{N1,Ni} \\
T_{1,s} &
T_{1,s} \\
& \vdots \\
T_{N1,s} \\
& 
\end{align*}

\begin{align*}
T_{1,1} &
T_{1,2} \\
& \vdots \\
T_{N1,1} \\
T_{1,Ni} \\
& \vdots \\
T_{N1,Ni} \\
T_{1,s} &
T_{1,s} \\
& \vdots \\
T_{N1,s} \\
& 
\end{align*}

\begin{align*}
T_{1,1} &
T_{1,2} \\
& \vdots \\
T_{N1,1} \\
T_{1,Ni} \\
& \vdots \\
T_{N1,Ni} \\
T_{1,s} &
T_{1,s} \\
& \vdots \\
T_{N1,s} \\
& 
\end{align*}