MODELLING EFFECTS OF MICROMIXING ON PERFORMANCE OF CONTINUOUS BIOREACTORS

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Abstract: *Effects of micromixing on performance of continuous bioreactors is investigated by determination of upper and lower boundary of substrate conversion. The bounds are evaluated on basis of limiting micromixing dynamics, i.e. as completely segregated flow and as maximum mixidness flow. Applied is probability density function of residence time (RTD) corresponding to "tank in series" model. Numerical evaluation of the bounds is obtained by solving a set of nonlinear differential equations with asymptotic split boundary conditions. Dependence of the bounds in substrate conversion as functions of Damkohler number are graphically presented.*

Keywords: residence time distribution, chemostat, micromixing

1. Introduction

Modelling complex hydrodynamic behaviour is one of the most difficult numerical problems, but at the same time it is of fundamental importance to many aspects of engineering. It requires solution of Navier-Stokes equation with rheological and/or turbulence models. CFD - computational fluid dynamic methods are based on extensive space and time meshing and use of finite element approximation of solution of Navier-Stokes equation. From reactor engineering aspect, hydrodynamic effects in a reactor are due to flow, pumping and impeller rotation in vessels, and is usually described on macroscopic scale by probability residence time density function (Danckwerts,1958; Zwietering, 1959; Westerterp *et. al.* 1963). However, hydrodynamic effects chemical and biochemical reaction on microscopic scale and knowledge of RTD function does not suffice for evaluation of reactor performance. In this work is applied a numerical method based on mass and energy balances for the boundary cases of the earliest and the latest micromixing. The boundary cases of micromixing correspond to maximum mixidness and segregated flow respectively. On macroscopic scale, the model of "tanks in series" is applied for numerical evaluation of RTD function.

2. Mathematical model

RTD function $E(\theta)$ of the series of equal volume perfectly mixed tanks is obtained by the inverse of Laplace transform of the product of N individual transfer functions:

$$E(\theta) = \mathrm{L}^{-1}\left[\prod_{i=1}^{i=N}\left(\frac{1}{\frac{1}{N}\cdot s+1}\right)\right] \qquad (1)$$

In Eq. 1. RTD is expressed as function of dimensionless time θ defined as the ratio of real time and the average residence time, which equals to the ratio of a vessel volume and volumetric flow rate through the vessel. The function is model for a very broad spectrum of RTD functions ranging from ideally continuous stirred tank reactors (CSTR), various packed bed reactors, and in the limiting case for $N \to \infty$ it corresponds to a response of a plug flow in a hollow tube. In Fig. 1. are depicted typical RTD profiles obtained by Eq. 1.

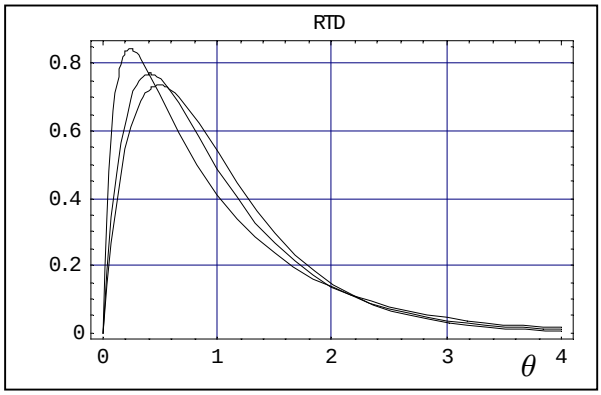

Fig. 1.Residence time distributions RTD for the

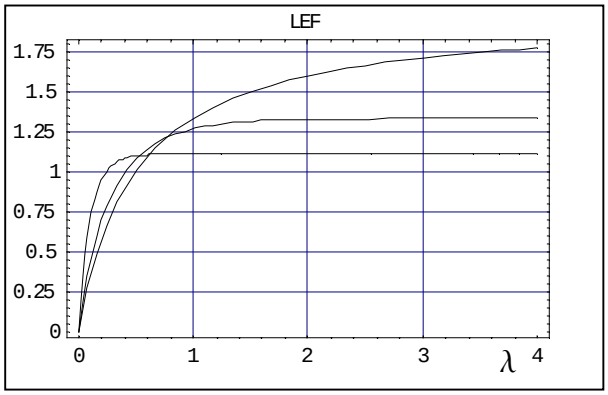

Fig. 2. Life expectancy functions LEF for the variances: 0.1, 0.25, 0.5.

For given RTD function uniquely is defined the life expectancy f unction LEF as function of the expectancy variable (also named "intensity function"), Λ (λ), given by:

$$\Lambda(\lambda) = \frac{E(\lambda)}{1 - \int_0^{\lambda} E(\theta) \cdot d\theta} \qquad (2)$$

Distributions of the life expectancy functions, which correspond to the RTD functions, are depicted in Fig. 2. Mass balances for reacting species in a bioreactor under batch conditions are expressed in the matrix form:

$$\frac{d}{d\theta}\vec{c} = Da \cdot \boldsymbol{\alpha}^T \cdot \vec{r}(\vec{c}) \qquad (3)$$

Stoichiometric matrix for a set of reactions is given by $\boldsymbol{\alpha}$, and volumetric reactions are given as components of the vector $\vec{r}$. Applied is the relative time scale leading to introduction of Damkohler dimensionless number defined as the ratio of maximum rate of reaction and maximum rate of convection through reactor. The balances (3) apply for homogeneous and structured models of microorganism metabolism. However, it is a custom to replace volumetric rates r by specific rates μ expressed per unit dry mass of cells:

$$\vec{r} = \vec{\mu}(\vec{c}) \cdot c_X \qquad (4)$$

The balances (3) are integrated for given initial conditions c(0) = c_0 and a specified *Da*, yielding the solutions c(θ, *Da*). The initial concentrations for batch balances (3) are identical to concentrations in a feeding stream in case of continuously flow through reactor.

For the limiting case of completely segregated flow, which for given RTD distribution can be interpreted as the case of the latest mixing, mass balance in steady state is given by the convolution of RTD and concentration profile:

$$\vec{c} = \int_0^{\infty} E(\theta) \cdot \vec{c}(\theta, Da) \cdot d\theta \qquad (5)$$

The opposite boundary case is defined by assumption of the earliest mixing, when the maximum mixidness is achieved. In this case the mass balances involve the life expectancy function and are evaluated by a set of nonlinear differential equations:

$$\frac{d}{d\lambda}\vec{c}(\lambda) = -Da \cdot \boldsymbol{\alpha}^T \cdot \vec{r}(\vec{c}) + \Lambda(\lambda) \cdot (\vec{c}(\lambda) - \vec{c}_0) \qquad (6)$$

with the asymptotic right hand boundary condition:

$$\frac{d}{d\lambda}\vec{c}\ (\lambda)\Big|_{\lambda=\infty} = 0 \qquad (7)$$

The solution of the steady state problem is given by the initial condition:

$$\vec{c}_S = \vec{c}(\lambda = 0, Da) \qquad (8)$$

Integration of (6) has to be evaluated in the reverse direction (from right to left) with the initial condition determined from the nonlinear algebraic equation:

$$0 = -Da \cdot \boldsymbol{\alpha}^T \cdot \vec{r}(\vec{c}, \lambda = \infty) + \Lambda(\infty) \cdot (\vec{c}(\lambda = \infty) - \vec{c}_0) \qquad (9)$$

In view of the relative time scale, when mean residence time is equal to 1, the limiting vale for $\lambda \to \infty$ is replaced by a number for which RTD is practically negligible, for example for $\lambda = 4 (or\, 8)$. The nonlinear problem (9) requires an iterative procedure such as Newton algorithm, and since system of differential equation is "stiff" and requires backward integration, it has to be executed with a robust ODE integrator, such as LSODE.

3. Results

The model for effects of degree of mixing on performance of continuously operated bioreactors is analysed. The problem is motivated by the importance of evaluation of boundaries of conversion (or productivity) based only on RTD information without prior knowledge of actual degree of mixidness, or the need for solution of Navier-Stokes equation by CFD software. The marginal error is determined for a range of Damkohler numbers in a practical region, from the wash-out state when conversion is approaching zero, to the upper values of Damkohler number for which conversion is approaching 100 %. In view of applicability of simulation results it essentially to have the evaluation in the full space of parameters, which is accomplished by rending the problem in dimensionless form. The dimensionless form of the model equations also improves numerical stability of integration algorithm.

Investigation of RTD on performance of bioreactors has been of a continuous interest to biochemical engineers working with non-Newtonian liquids in reactors of large volumes (Kelly and Humphrey, 1998), in cases of complicated flow patterns occurring in open containers for biodegradation of polluted waters (Newell *et al*., 1988), or in multiphase aerated bioreactors (Pollard *et al*. 1997; Gavrilescu *et. al*., 19086; Ruffer *et al*. 1994). In this work is investigated performance of chemostat, i.e. continuously and isothermally operated liquid phase bioreactor with suspended microorganisms. The balances are accounted by the rate limiting substrate (y) and biomass (z). Dimensionless balances in the batch mode of operation, corresponding to Eq. (3), are:

$$\frac{d}{d\theta} y = -\beta \cdot Da \cdot \mu(y) \cdot z \qquad (10)$$

$$\frac{d}{d\theta} z = Da \cdot \mu(y) \cdot z \qquad (11)$$

$$\mu(y) = \frac{y}{\gamma_S + y + \frac{y^2}{\gamma_I}} \qquad (12)$$

The initial conditions are provided by the dimensionless values of the feeding concentrations $y(0)=1 \;\; z(0)=1$.

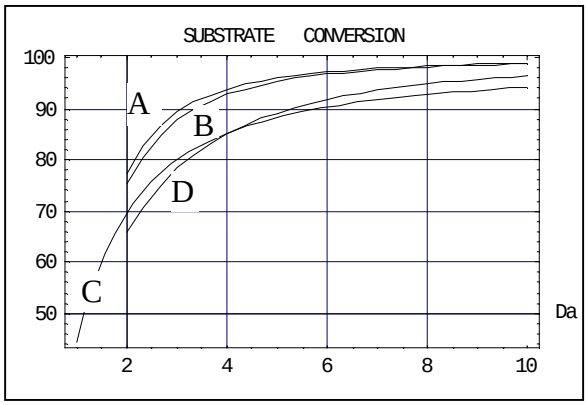

Figure 3. Substrate conversion as function of Damkholer number at mixing conditions: B) maximum mixidness; B) true (test case); C) ideally mixed; D) segregated flow.

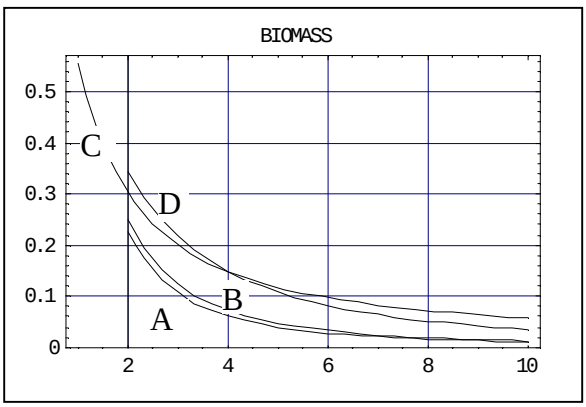

Figure 4. Biomass produced as function of Damkholer number at mixing conditions: A) maximum mixidness; B) true (test case); C) ideally mixed; D) segregated flow.

The process kinetics is given by the dimensionless growth function (12) for which the kinetics order changes in the range from + 1 to -1 with increase of substrate concentration y. This information is sufficient for proving that maximum mixidness will provide the upper bound for substrate conversion, while the segregated flow correspond to the lower bound.

In Fig. 3-4 are presented results obtained for the following set of parameters: γ_S =1, γ_I =10, β = 0,8, and variance of RTD σ^2 (θ) = 0,5. The software *Mathematica* v. 4.0.(Wolfram, 1996) has been used for numerical evaluation of the substrate and biomass balances (5-6). The batch mode balance (3) is evaluated numerically by use of *NDSolve* with *Da* as a variable parameter. For the segregated balance (5) numerical integration by adaptive Gauss quadrature is applied as provided by the *NIntegrate* program. The nonlinear equation for determination of the missing right hand boundary value is calculated by Newton algorithm as given in *NSolve*. The critical step is the backward integration of the nonlinear set of stiff equations (6). Applied is the powerful adaptive integrator *NDSolve* which encompasses LSODE algorithm. In order to provide analysis of degree of mixidness at a range of *Da* number, the integrals are defined as a function *Da*. On Fig. 3-4 are also shown results obtained from the test problem (exact solution), and the case for assumed ideally mixing (ideal chemostat). The errors for the upper and lower bound with respect to the exact solution are also given in Table 1.

	Percentage error in substrate conversion	
Da	upper bound error maximum mixidness	lower bound error segregated flow
2	2,077	-9,477
4	1,049	-7,701
6	0,444	-4,926
8	0,223	-3,303
10	0,128	-2.345

Table 1. Comparison of errors in substrate conversion for upper and lower bound of mixidness.

The results prove that for mixing in bioreactors defined by the test model of "tanks in series" the maximum mixidness model will provide very accurate upper bound on substrate conversion for the whole practical range of Damkohler number. Maximum err of the upper bound is +2% at the point close to "washout" , and with further increase of Da the error decreases to 0,1 % when conversion is practically 100%. Error of the lower bound are for a degree off order larger.

4. Conclusions

Solutions of the numerically intensive problems of mixing in bioreactors based on Navier-Stokes equation and the computational fluid dynamics (CFD) can be effectively approximated by evaluation of upper and lower bounds of conversions based on the assumptions of maximum mixidness and segregation.

The approximation requires numerical integration of stiff equations for substrate and biomass with backward integration and an asymptotic right hand boundary conditions.

Numerical methods provided by *Mathematica* v 4.0 proved to be robust and effective.
The simulation results are compared with the exact test case.

Errors of the upper bound are at most of order 2 % and are for order of magnitude smaller than for segregated flow.

The results have a very practical value since a simple method can provide sufficient accuracy for prediction of performance of industrial bioreactors based just on RTD function.

Acknowledgement

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5. References

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