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Research Article

Novel Study of Reaction Kinetics and Mass Transfer in Bioreactor Modelling: Prediction of Bioethanol Fermentation Performance by Saccharomyces cerevisiae on Continuous Fixed Bed Biofilm Plug Flow Reactor

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S1. Pressure Drop Analysis and Optimization of Reactor Configuration

Based on the calculations that have been carried out, the required reactor length is very high, which can reach hundreds of meters. Longer reactors result in higher pressure drop throughout the reactor. At default conditions (temperature 31°C, substrate concentration 100 g/L, cell concentration 10 g/L, superficial flow rate 3.2 cm/s, reactor diameter 20 cm, and solid particle diameter 2 cm), the pressure loss value as a function of reactor length shown in Figure S1. Based on Figure S1, the pressure loss value is very high, reaching 5 bar for a 600 m long reactor. Moreover, the fermentation is done at atmospheric pressure (nearly 1 atm), so increasing the feed pressure to more than 5 bar can potentially change the fermentation performance. Apart from that, a 600 m long reactor makes the maintenance and preparation very difficult. Moreover, a fixed bed pipe reactor needs to be designed vertically to facilitate bed entry and exit, so a 600 m high pipe reactor is not feasible. This shows the need to optimize operating conditions and optimum reactor configuration.

Based on the analysis that has been carried out, in terms of operating conditions, it is recommended to reduce the substrate concentration in the feed solution to reduce the required reactor length. However, the water usage of this system will be higher, so it must be considered for the next step process, namely purification step. Besides, biocatalyst levels also need to be increased. The feed volumetric flow rate (resulting in the feed superficial flow rate) can also be reduced to reduce the reactor length at the same residence time. Furthermore, it is possible to reduce the solid particle diameter and increase the reactor diameter.

Several other options that can be used to overcome the pressure loss problem are increasing the feed pressure and changing one large reactor into several small reactors arranged in series with a pump between the reactors. However, the feed pressure should not be increased too much, because it can reduce fermentation performance [SI-1]. Based on Galanakis *et al*., the pressure loss value significantly influences fermentation in the range of 3-7 atm, but is still not significantly different in the range of 1-3 atm [SI-1]. Therefore, the feed pressure can still be increased to 3 atm to overcome the pressure loss problem. Furthermore, it is important to divide the reactors into several reactors in series configuration, then place several pumps throughout the systems in an optimum placement.

To make the reactor easier to design and operate, the reactor length should not be too large. Industrial-scale tubular reactors can have a length-to-diameter ratio of 50 [SI-2]. For a diameter of 30 cm (large diameter variation), the reactor length is 1500 cm (15 m). However, for vertical reactors, this reactor is too long, so it can make the maintenance process difficult, especially when removing and filling the bed. In addition, the typical height of industrial buildings is approximately 10 m [SI-3], which means that the reactor length must be designed to be lower than this value. Therefore, the length of 1 reactor is reduced from 15 m to 5 m. This value is half the length of industrial scale tubular reactors [SI-4].

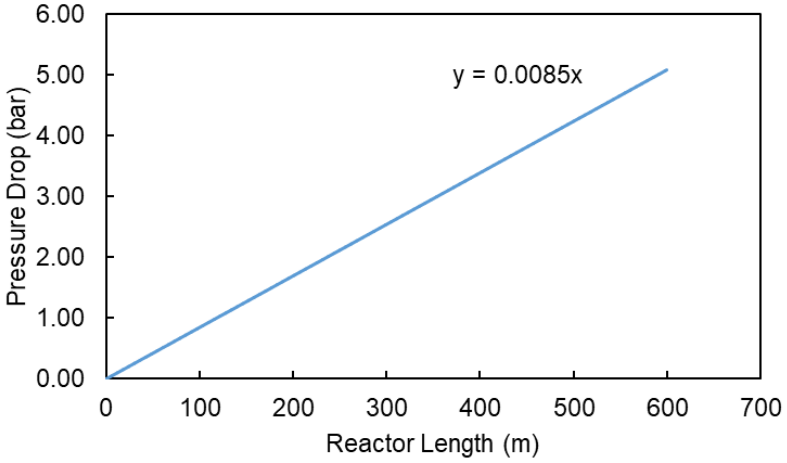

Figure S1. Pressure loss value throughout the reactor at default conditions

Cited Literatures in Supporting Information (SI)

[SI-1] Galanakis, C.M., Kordulis, C., Kanellaki, M., Koutinas, A.A., Bekatorou, A., Lycourghiotis, A. (2012). Effect of pressure and temperature on alcoholic fermentation by *Saccharomyces cerevisiae* immobilized on γ-alumina pellets. *Bioresource Technology*, 114, 492–498. DOI: 10.1016/j.biortech.2012.03.010.

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[SI-3] Mavridou, T., Doulos, L. (2019). Evaluation of different roof types concerning daylight in industrial buildings during the initial design phase: Methodology and case study. *Buildings*, 9(7), 170. DOI: 10.3390/buildings9070170.

[SI-4] Marvast, M.A., Sohrabi, M., Zarrinpashne, S., Baghmisheh, G. (2005). Fischer-Tropsch synthesis: modeling and performance study for Fe-HZSM5 bifunctional catalyst. *Chemical Engineering & Technology*, 28(1), 78–86. DOI: 10.1002/ceat.200407013.

Table S1. Influence of fermentation temperature on reactor design and performance

Fermentation Temperature (^oC)	Residence Time (minute)	Reactor Length (m)	Reactor Volume (m^3)	Product Concentration (g/L)	Product Productivity (g/(L.h))	Pressure Drop (bar)
5	4580.9	21666	680.3	44.3	0.6	194.9
10	1950.4	9224	289.6	43.9	1.3	81.7
15	907.3	4291	134.7	43.5	2.9	37.5
20	421.3	1992	62.6	43.3	6.2	17.2
22.5	292.3	1383	43.4	43.2	8.9	11.9
25	208.0	984	30.9	43.1	12.4	8.4
27	164.0	776	24.4	43.1	15.8	6.6
29	137.3	649	20.4	43.0	18.8	5.5
31	126.8	600	18.8	43.2	20.4	5.1
33	131.2	620	19.5	43.3	19.8	5.2
35	152.6	722	22.7	43.6	17.2	6.1
37.5	202.0	956	30.0	44.5	13.2	8.0
40	263.5	1246	39.1	45.6	10.4	10.4

Table S2. Influence of initial substrate concentration on reactor design and performance

Initial Substrate Concentration (g/L)	Residence Time (minute)	Reactor Length (m)	Reactor Volume (m^3)	Product Concentration (g/L)	Product Productivity (g/(L.h))	Pressure Drop (bar)
50	60.0	284	8.9	21.6	21.6	
75	92.0	435	13.7	32.4	21.1	
100	126.8	600	18.8	43.2	20.4	
125	164.8	779	24.5	54.0	19.7	
150	206.6	977	30.7	64.8	18.8	

Table S3. Influence of cell concentration on reactor design and performance

Cell Concentration (g/L)	Residence Time (minute)	Reactor Length (m)	Reactor Volume (m^3)	Product Concentration (g/L)	Product Productivity (g/(L.h))
3.75	253.1	1197	37.6	43.2	10.2
5.63	168.7	798	25.1	43.2	15.3
7.50	126.8	600	18.8	43.2	20.4
9.38	101.5	480	15.1	43.2	25.5
11.25	84.7	401	12.6	43.2	30.6

Table S4. Influence of superficial flow rate on reactor design and performance

Superficial Flow Rate (cm/s)	Residence Time (minute)	Reactor Length (m)	Reactor Volume (m^3)	Product Concentration (g/L)	Product Productivity (g/(L.h))
1.6	127.1	301	9.4	43.2	20.4
2.4	126.9	450	14.1	43.2	20.4
3.2	126.8	600	18.8	43.2	20.4
4.0	126.7	749	23.5	43.2	20.4
4.8	126.5	898	28.2	43.2	20.5

Table S5. Influence of reactor diameter on reactor design and performance

Reactor Diameter (cm)	Void Fraction	Residence Time (minute)	Reactor Length (m)	Reactor Volume (m^3)	Product Concentration (g/L)	Product Productivity (g/(L.h))
10	43.6%	136.9	600	4.7	43.2	18.9
15	41.3%	129.6	600	10.6	43.2	20.0
20	40.4%	126.8	600	18.8	43.2	20.4
25	39.9%	125.4	600	29.4	43.2	20.7
30	39.7%	124.5	600	42.4	43.2	20.8

Table S6. Influence of solid particle diameter on reactor design and performance

Solid Particle Diameter (cm)	Void Fraction	Residence Time (minute)	Reactor Length (m)	Reactor Volume (m^3)	Product Concentration (g/L)	Product Productivity (g/(L.h))
1.0	39.4%	123.4	598	18.8	43.2	21.0
1.5	39.8%	124.7	599	18.8	43.2	20.8
2.0	40.4%	126.8	600	18.8	43.2	20.4
2.5	41.1%	129.2	601	18.9	43.2	20.0
3.0	41.9%	132.1	603	18.9	43.2	19.6

Supporting Information (FlexPDE6 Script)

```
{ Fill in the following sections (removing comment marks ! if necessary),
  and delete those that are unused.}
TITLE 'Continuous Fixed Bed Biofilm Plug Flow Reactor'        { the problem
identification }

COORDINATES cartesian1 { coordinate system, 1D,2D,3D, etc }
VARIABLES        { system variables }
Cs (0.001)
Csb (0.001)
Tr (0.001)

SELECT         { method controls }
ngrid=1
errlim=1e-2
penwidth=3

DEFINITIONS    { parameter definitions }
!Reactor dimension
dre=0.3 !m
are= 3.14*dre*dre/4 !m2

!Temperature
TempC = 31 !degC
TempK = TempC+273.15 !K

!External diffusion
psiwtr = 2.6
Mrwtr = 18 !g/mol
viscwtr = 0.7843e-3 !Pa.s
vaglu = (14.8*6+3.7*12+7.4*5+7.4)*10^(-3) !m3/kmol
Daq = 1.173e-16*(psiwtr*Mrwtr)^0.5*TempK/viscwtr/(vaglu^0.6) !m2/s

!Feed flow
Fin =1e-3 !m3/s
uz = Fin/are !m/s

!Fluid hydrodynamics
viscf = viscwtr !Pa.s
rhof = 995.34 !kg/m3
dp = 1e-2 !m
ratiod=dre/dp
e=0.39+1.74/(ratiod+1.140)^2
ap= 6*(1-e)/(dp) !m2/m3

!Reynold number
Re = rhof*uz*dp/viscf

!Schmidt
Sc = viscf/rhof/Daq

!Colburn factor
Jd=1/e*(0.765/(Re^0.82)+0.365/(Re^0.386))

!Sherwood
Sh = Jd*Re*Sc^(1/3)

!kc
kc = Sh*Daq/dp !m/s
kcmnt = kc*60 !m/minute

!Internal diffusion
koefDe = 0.3
```

```
De=koefDe*Daq !m2/s
Demnt = De*60 !m2/minute

!Operating condition
tau = 100 !minute
Cs0=50 !g/L

!Biofilm and cell
Cx = 11.25 !g/L
rhocell = 1.0952*1000 !kg/m3
Lbf = Cx/ap/rhocell

!Reaction rate and yield
miumax=0.339/60 !/minute
Yps= 0.436

Ypx= 3.787

Ksb=150/1000 !g/L
rm = miumax*Ypx/Yps*Cx !/g/L.minute

!Product concentration
Cp = Yps*(Cs0-Cs)

!Product inhibition
Cpmax=170 !g/L
fp = 1-(Cp/Cpmax)

!Substrate concentration in the biofilm
a = kcmnt*ap
b = kcmnt*ap*Ksb+rm*fp-kcmnt*ap*Cs
c = -kcmnt*ap*Cs*Ksb
Csbi = (-b+(b^2-4*a*c)^0.5)/(2*a) !g/L

!Conversion
conv = (Cs0-Cs)/Cs0*100
conv_value = globalmax(conv)

!Reactor length
z = tau*60/e*uz !m

!Reactor volume
vre = are*z !m3

!Productivity
Cpout=globalmax(Cp) !g/L
productivity = Cpout/(tau/60) !g/L.h

INITIAL VALUES
Cs = Cs0
Tr=304.15

EQUATIONS        { PDE's, one for each variable }
Cs:  Csbi = Cs + e/(kcmnt*ap)*dt(Cs)
Csb: Demnt*dxx(Csb) = rm*Csb/(Ksb+Csb)*fp

!CONSTRAINTS    { Integral constraints }
BOUNDARIES       { The domain definition }
  REGION 1       { For each material region }
    START(0)
      point value (Csb) = Csbi
      LINE TO (Lbf)
      point natural (Csb) = 0
```

```
TIME 0 TO tau     { if time dependent }

MONITORS          { show progress }

PLOTS             { save result displays }
for cycle = 1

SUMMARY

HISTORIES
history (Cs) at (0)
!export file = 'Cs.dat' format '#t#r     #i'
END
```