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Computational fluid dynamic (CFD) modeling of simultaneous extraction and fermentation process in a single sugar beet cossette

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Abstract

For simulations of flow and microbial conversion reactions, related to modeling of simultaneous extraction and fermentation process in a single sugar beet cossette a software package OpenFOAM was used. The mass transfer of the components (sucrose, glucose, fructose and ethanol) in the studied system was controlled by the convection and diffusion processes. Microbial conversion rates and yield coefficients were experimentally determined and/or estimated by mathematical simulation. Dimensions of the model sugar beet cossette (SBC) were: average length of cosettes 40.10 mm, average thickness 3.32 mm and average width 3.5 mm, and represented in the model as a square-shape cross-section cossette. The whole mesh domain was made of 32000 mesh cells and model sugar beet cossette was made up of 500 mesh cells. The finite volume method was used as a discretization scheme for calculations. The established CFD model was used to study the mass transfer and microbial conversion rates on the scale of single sugar beet cossette in the short time scales (up to 25 s). This model can be used for simulation of extractant flow around single sugar beet cossette as well as for description of simultaneous extraction and fermentation process in the studied system.

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Introduction

As prices of petroleum based fuels are changing on daily basis, and the whole "oil" based industry has an unpredictable future, the shortage of petroleum and other non-renewable material and energy resources, is a very certain scenario in the near future. One of the solutions for such problems is new economic models for alternative fuel production such as biofuels production from renewable materials. The technology for production of bioethanol from sugar and starch containing raw materials is well developed and established in industrial scale. The same is for biodiesel production from oilseeds and animal fats. Because of competition of bioethanol and food chain for starch and sugar containing raw materials, investigation of bioethanol production of second and third generation is intensively performed worldwide. The most important approach for design of more intensive and cost-effective bioprocess configuration is the integration of different technological operations included in the bioethanol production into one step (1). For example, integration of reaction and separation steps through the ethanol removing from the zone where the biotransformation takes place, offers several opportunities for increasing product yield and consequently reducing production costs. Other forms of integration may significantly decrease energetic costs of specific flow sheet configurations for ethanol production. Process integration is gaining more and more interest due to the advantages related to its application in the case of ethanol production: reduction of energy costs, decrease in the size and number of process units, intensification of the microbial and downstream processes (2-4). One of the integration approaches in development of new bioprocesses for ethanol production is combination of extraction process of sugars from renewable sugar containing raw materials (sugar beet) and simultaneous fermentation (5). This bioprocess can be carried out in a bioreactor system which combines tubular bioreactor with stirred tank bioreactor (6). Packed bed tubular bioreactors are a good alternative for semi-solid bioprocess as ethanol production from sugar beet cossettes (7).

For better understanding of new bioprocesses, and to gain an insight to microbial, physical and chemical parameters that significantly affect the bioprocess dynamics in bioreactor systems, mathematical models of the bioprocess combined with analysis of the mass transfer phenomena are studied. Mathematical models of microbial metabolism are useful tools in the optimization and control of ethanol production system (8-10). Combination of experiments with mathematical modelling has resulted in new aspects of microbial physiology, providing reasonable interpretations of experimental work with improvement of knowledge as well as the designing of new, more focused experiments (11). Very different model types can be applied for diverse bioprocess situations (cultivation techniques, mass transfer, microbial growth kinetics, metabolic network reaction kinetics; 12). Computational fluid dynamics (CFD) is based on the use of applied mathematics, physics and computational software to visualize the flow pattern of different medium components in the bioreactor system. CFD is mathematically based on the Navier-Stokes equations which describe correlations between different bioprocess parameters (e.g. velocity, pressure, temperature and density of moving fluids in the system). Mathematical modelling of biochemical reactions coupled with CFD can be simple to very complex, depending on the studied system. Complex metabolic models involve mimicking the metabolic pathways for product synthesis in a single cell, observing how simple changes to the environmental conditions have impact on the studied metabolic pathways (13). The key advantage of CFD as a modelling technique is visualization capability allowing detailed characterization of the local-scale phenomena in varying operating conditions. Hence, CFD can be used as a robust tool for the design of new efficient and energy optimised bioprocesses (14).

Materials and Methods

Microorganism and sugar beet cossettes

In this research, a fresh commercial culture of *Saccharomyces cerevisiae* (baker's yeast) was used as a working microorganism. Physical and chemical properties of sugar beet cossettes have to be determined in order to define the efficiency of sugar extraction process from sugar beet cossettes that are variable and irregular prism-like shapes. For this research, sugar beet cossettes were produced by cutting the beet in the barrel-shaped cutter ("Putsch" Hagen, Germany) in Sladorana d.o.o (Županja, Croatia). The average length of sugar beet cossettes (SBC) was 40.10 mm (range 5.7 to 145.5 mm), average thickness 3.32 mm and average width 3.57 mm, respectively. They had square-shape cross-section and Siline number (length of 100 g of sugar beet cossettes) was 10.2034 m. The content of soluble dry matter in the sugar beet cossettes was in the range of 14.5 - 18.5 % (w/w). Sugar content varies among different sugar beet batches. Sucrose content was 145-165 g/dm^3, glucose content 5.4-12.5 g/dm^3, fructose content 6.2-16.5 g/dm^3 and total sugars content 156.6-175.5 g/dm^3. Previously mentioned sugar beet cossettes characteristics are in agreement with required quality standards of sugar industry (15).

Simultaneous extraction and fermentation in the vertical column bioreactor

Simultaneous extraction and fermentation (by yeast S. cerevisiae) of sugars (fructose, glucose and sucrose) from sugar beet cossettes was performed in the vertical packed-bed column bioreactor. This column bioreactor was 0.5 m in height and it has a cylindrical (upper) and conical (lower) part that is separated by perforated plate. The diameter of the column was of 5 cm and the height of sugar beet cossettes in the column was 0.45 m. The conical part of the column bioreactor was previously filled with glass beads (5 mm in diameters) to equalize the flow of extractant (60 g/dm^3 of yeast suspension) through cross section of the column. Perforated plastic circular plate was used to separate the top layer of cossettes from the layer of glass beads. Simultaneous extraction and fermentation process in the bioreactor were performed at 36°C that was maintained by water recirculation through the outer bioreactor coil.

Determination of bioprocess model parameters

Kinetic constants of microbial reactions and mass transfer coefficients are required so that the CFD model of simultaneous extraction and fermentation process in the vertical column bioreactor can be established. Therefore, diffusion coefficients for sucrose, glucose, fructose and ethanol were obtained from literature (15-18). Maximal yeast specific growth rate and Monod's substrate saturation constants were determined by Lineweaver-Burk- plots (ethanol production by different starting substrate concentrations). Maximal specific consumption rate for each sugar was determined from series of experiments where media with different substrate concentrations were inoculated with the same initial quantity of yeast cells taken from the middle exponential growth phase (5). Kinetic parameters originated from formal kinetic models of yeast growth and ethanol production described earlier by Levenspiel O. (19); Aiba and Shoda (20); Andrews (21) were determined by using a simulation software "Berkeley Madonna" (version 8.3.18.; 22) with variable integration step of Runge-Kutta fourth algorithm. The software function "Multiple curve fit" with "Monte Carlo" method for finding the absolute minimum and maximum was applied for the optimisation of model parameters (23). Stoichiometry yields were calculated from theoretical mass balances of microbial reactions. The CFD model parameters are presented in Table 1.

The CFD model for fluid flow and bioprocess description

Program package OpenFOAM (24) was used for computational fluid dynamic simulations of fluid flow and microbial reactions around single (one) sugar beet cossette. For post processing and visualisation of simulated data, program package ParaFOAM was used. For calculations integrated solver IcoFOAM, was adapted for simulation purposes. IcoFOAM solves the incompressible laminar Navier-Stokes equations using the PISO algorithm. The icoFOAM code can take mesh non-orthogonality into account with successive non-orthogonality iterations. The number of PISO corrections and non-orthogonality corrections are controlled through user input (25). PISO (Pressure implicit with splitting of operator; 26-27) algorithm is an extension of the SIMPLE algorithm used in the CFD to solve the Navier-Stokes equations. PISO is a pressure-velocity calcu-

Table 1. The CFD model parameters

Parameter	Symbol	Referent value	Unit
Diffusion coefficient of:			
- sucrose in SBC	D_{sb}	$1.43*10^{-08}$	m^2/s
- sucrose in fluid	D_{Suc}	$1.46*10^{-08}$	m^2/s
- fructose in fluid	D_{Fru}	$2.35*10^{-08}$	m^2/s
- glucose in fluid	D_{Glu}	$2.32*10^{-08}$	m^2/s
- ethanol in fluid	D_{ET}	$1.3*10^{-07}$	m^2/s
Yeast kinetic parameters:			
Maximal specific conversion rate	$q_{max.Suc}$	0.59	min^{-1}
Maximal specific conversion rate	$q_{max,Glu}$	0.01292	min^{-1}
Maximal specific conversion rate	$q_{max,Fru}$	0.0121	min^{-1}
Saturation constant	Ks	7	g/dm^3
Saturation constant	Km_{Glu}	21.192	g/dm^3
Saturation constant	Km_{Fru}	16.6318	g/dm^3
Inhibition constant	Ki_{Glug}	210	g/dm^3
Inhibition constants	Ki_{Fruf}	200	g/dm^3
inhibition constants	Ki	31.8551	g/dm^3
Maximal (critical) ethanol concentration	Et_{max}	128.35	g/dm^3
Biomass concentration	X	60	g/dm^3
Stoichiometric sucrose to glucose/fructose yield	Y	0.52632	-
Stoichiometric glucose to ethanol yield	$Y_{Et/Glu}$	0.51111	-
Stoichiometric fructose to ethanol yield	$Y_{Et/Fru}$	0.51111	-

lation procedure for the Navier-Stokes equations developed originally for non-iterative computation of unsteady compressible flow, but it has been adapted successfully to steady-state problems. The algorithm can be summed up as follows:

1. Set the boundary conditions.
2. Solve the discretized momentum equation to compute an intermediate velocity field.
3. Compute the mass fluxes at the cells faces.
4. Solve the pressure equation.
5. Correct the mass fluxes at the cell faces.
6. Correct the velocities on the basis of the new pressure field.
7. Update the boundary conditions.
8. Repeat from 3 for the prescribed number of times.
9. Increase the time step and repeat from 1.

The IcoFAOM solver solves incompressible Navier-Stokes equation:

$$\nabla \bullet u = 0 \qquad [1]$$

$$\frac{\partial u_x}{\partial t} + \nabla \bullet (u\ _x) = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \nu \nabla^2 u_x \qquad [2]$$

$$\frac{\partial u_y}{\partial t} + \nabla \bullet (u\ _y) = -\frac{1}{\rho}\frac{\partial p}{\partial y} + \nu \nabla^2 u_y \qquad [3]$$

$$\frac{\partial u_z}{\partial t} + \nabla \bullet (u\ _z) = -\frac{1}{\rho}\frac{\partial p}{\partial z} + \nu \nabla^2 u_z \qquad [4]$$

where non-linear convection terms (∇*(uu)) is handled using a iterative solution technique and pressure equation is derived by using continuity and momentum equation (25).

Mathematical equations for microbial reactions of medium components (sucrose, glucose, fructose and ethanol) were incorporated in the IcoFOAM solver. Mathematical formulations are as follows:

Sucrose:

$$\frac{\partial \rho Suc}{\partial t} + \nabla \bullet \phi * Suc - \nabla \bullet D_{sb} * \nabla Suc = \frac{-X * q_{max,Suc}}{Ks + Suc * (1 + \frac{Suc}{Ki})} * \frac{1}{Y} \qquad [5]$$

Fructose:

$$\frac{\partial \rho Fru}{\partial t} + \nabla \bullet \phi * Fru - \nabla \bullet D_{Fru} * \nabla Fru =$$

$$= \frac{X * q_{max,Suc}}{Ks + Suc * (1 + \frac{Suc}{Ki})} - q_{Fru,max} * \frac{X * Fru}{Km_{Fru} + Fru * \left(1 + \frac{Fru}{Ki_{Fruf}}\right)} * \left(1 + \frac{Et}{Et_{max}}\right) * \frac{1}{Y_{Et/Fru}} \qquad [6]$$

Glucose:

$$\frac{\partial \rho Glu}{\partial t} + \nabla \bullet \phi * Glu - \nabla \bullet D_{Glu} * \nabla Glu =$$

$$= \frac{X * q_{max,Suc}}{Ks + Suc * (1 + \frac{Suc}{Ki})} - q_{Glu,max} * \frac{X * Glu}{Km_{Glu} + Glu * \left(1 + \frac{Glu}{Ki_{Glug}}\right)} * \left(1 + \frac{Et}{Et_{max}}\right) \frac{1}{Y_{Et/Glu}} \qquad [7]$$

Ethanol:

$$\frac{\partial \rho\, Et}{\partial t} + \nabla \bullet \phi * Et - \nabla \bullet D_{Et} * \nabla Et = \quad [8]$$

$$= q_{Glu,\max} * \frac{X * Glu}{Km_{Glu} + Glu * \left(1 + \frac{Glu}{Ki_{Glug}}\right)} * \left(1 + \frac{Et}{Et_{\max}}\right) * \frac{1}{Y_{Et/Glu}} +$$

$$+ q_{Fru,\max} * \frac{X * Fru}{Km_{Fru} + Fru * \left(1 + \frac{Fru}{Ki_{Fruf}}\right)} * \left(1 + \frac{Et}{Et_{\max}}\right) * \frac{1}{Y_{Et/Fru}}$$

where ∂ - partial derivative, ∇ - nabla operator, $\bullet$ - dot (inner vector) operator, ϕ - viscosity (kg/s m), ρ - density (g/dm^3), Suc - sucrose (g/dm^3), Glu - glucose (g/dm^3), Fru - fructose (g/dm^3), Et - ethanol (g/dm^3) and X - yeast concentration (g/dm^3)

Microbial reaction equations of the CFD model were solved in two steps. In the first step, equations of continuity and flow were solved

$$\frac{\partial \rho C}{\partial t} + \nabla \bullet \phi * C \quad [9]$$

in order to obtain complete flow pattern in terms of distribution of fluid pattern. The established flow pattern was used for calculation of diffusion ($-\nabla \bullet D_C * \nabla C$) and related microbial reaction terms (equations 5-8).

Mesh was created with Mesh generation with the blockMesh utility supplied with OpenFOAM. The blockMesh utility creates parametric meshes with grading and curved edges. The mesh is generated from a dictionary file named blockMeshDict located in the constant/polyMesh directory of a case. blockMesh reads this dictionary, generates the mesh and writes out the mesh data to points and faces, cells and boundary files in the same directory. The principle behind blockMesh is to decompose the domain geometry into a set of 1 or more three dimensional, hexahedral blocks. Each block of the geometry is defined by 8 vertices, one at each corner of a hexahedron. The vertices are labeled via automatic algorithm for labeling in the program itself, and then written in a list of vertices (in the blockMesh dictionary) so that each vertex can be accessed and drawn using its label. Each block has a local coordinate system (x1,x2,x3) that must be right-handed. A right-handed set of axes is defined such that to an observer looking down the Oz axis, with O nearest them, the arc from a point on the Ox axis to a point on the Oy axis is in a clockwise sense. Fluid flow around single sugar beet cossette tested was vertical (upwards) and horizontal (from side; **Fig. 1**).

Results and Discussion

In this research, the CFD model of simultaneous extraction and fermentation process around single sugar beet cossette was established in order to define transport and microbial conversion phenomena of this bioprocess in the vertical packed bed column bioreactor. This CFD model is based on the experiments performed in the column bioreactor by extractant

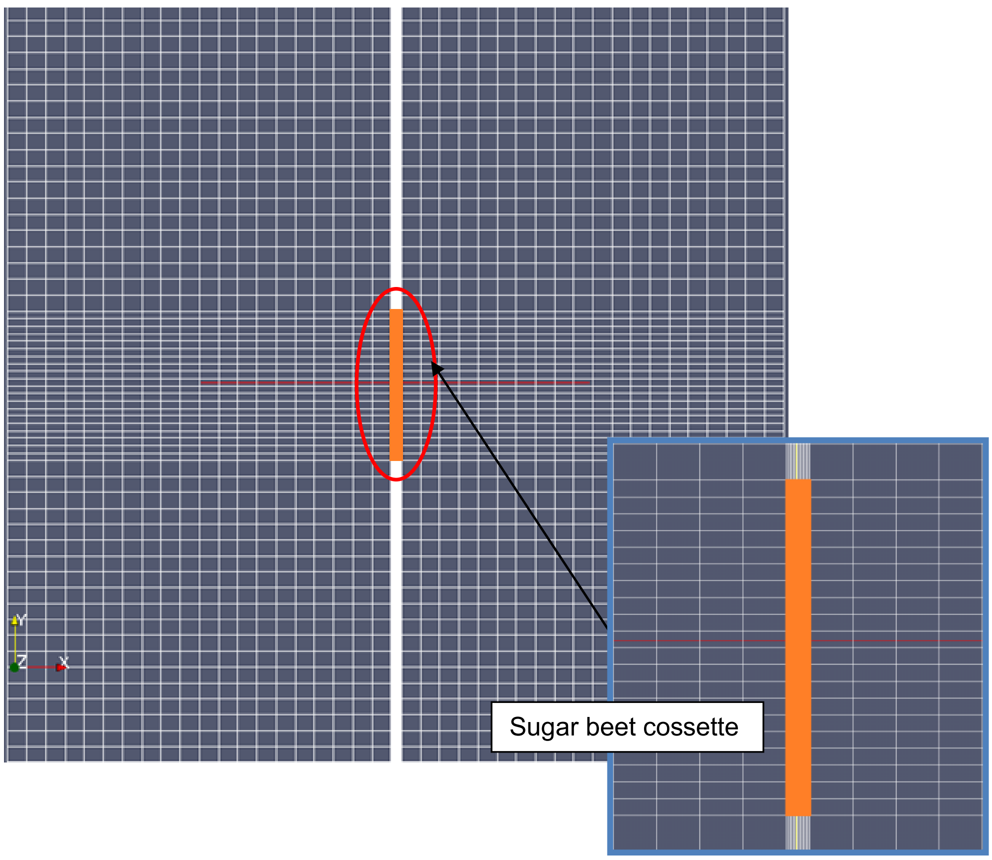

Figure 1. Wireframe of mesh used for the CFD simulations.

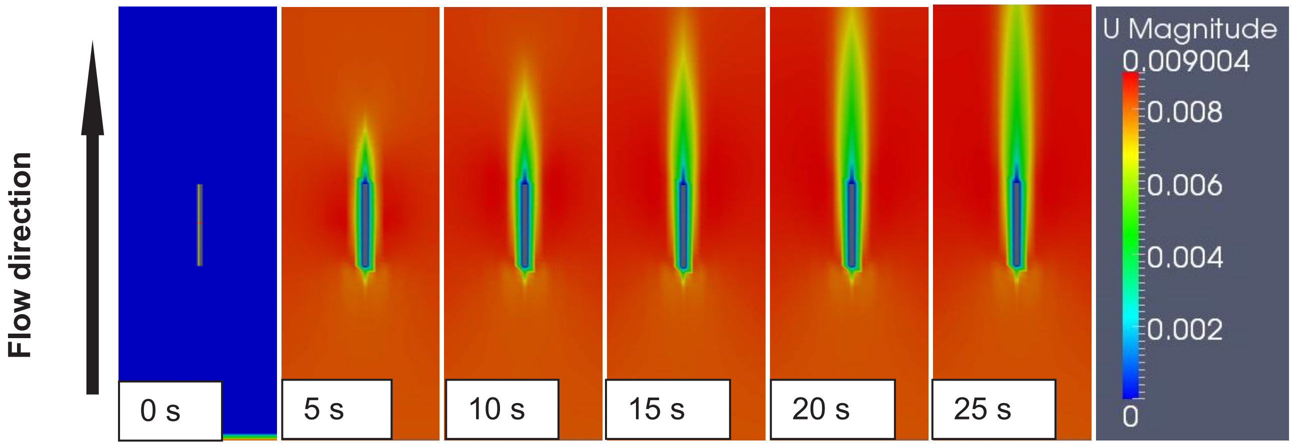

Figure 2. Model velocity profile (U magnitude in m/min) of extractant flow around single sugar beet cossette.

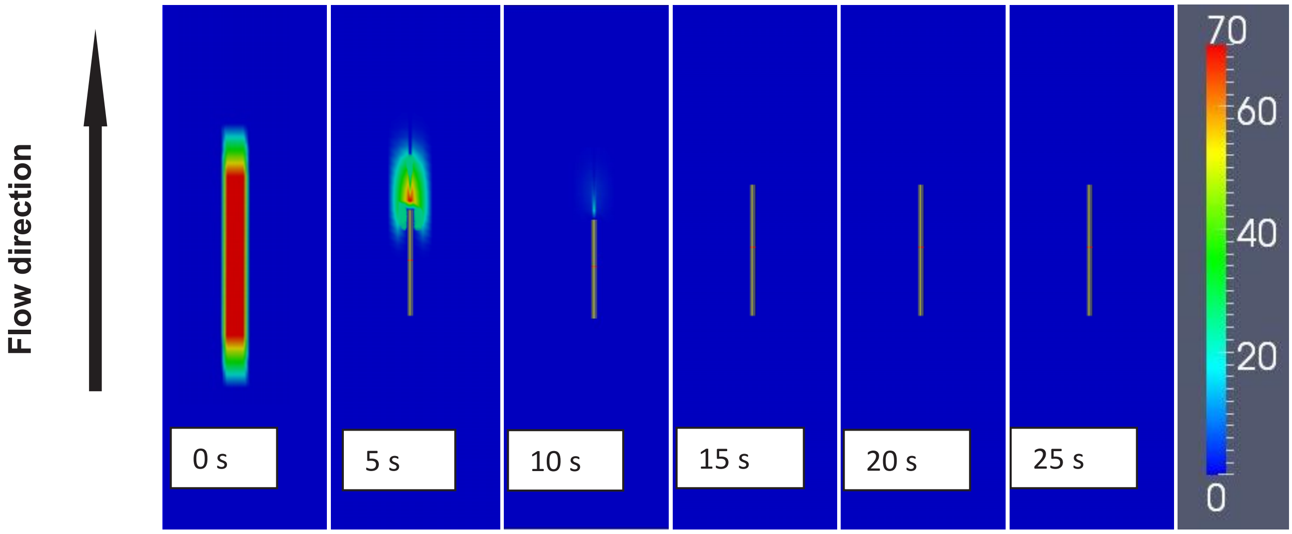

Figure 3. Concentration profile g/dm³ of sucrose around single sugar beet cossette.

(yeast suspension of 60 g/dm³) flow velocity of 0.008083 m/min. The CFD model parameters are presented in Table 1. The mass transfer of the medium components (sucrose, glucose, fructose and ethanol) in the studied system was controlled by the convection and diffusion processes. For solving the reactions in the CFD models that are used to describe the microbial conversion of substrate into product, experimental microbial conversion rates and yield coefficients are required to relate the physical phenomena of bioprocess to the computational flow field. In this CFD model microbial conversion rates and yield coefficients were taken from the structured mathematical model of mass transfer and microbial conversion of sugars into ethanol during simultaneous extraction and fermentation process of sugar beet cossettes (5). Dimensions of the model sugar beet cossette as average length of cosettes 40.10 mm, average thickness of 3.32 mm and width of 3.5 mm are represented in the model as a square-shape cross-section cossette. The domain for the CFD simulation was defined as a two dimensional plane mesh with height to width aspect ratio of 1:1. The whole mesh domain was made of 32000 mesh cells and model sugar beet cossette was made up of 500 mesh cells (**Fig. 1**). For perpendicular flow beside the surface of one single cossette (**Fig. 2**) velocity inlet conditions were applied to the mesh at the bottom of the mesh.

The top boundary was defined as empty space. The extractant (fluid) enters through the bottom surface and leaves the domain through the top surface as a flux. The remaining boundaries were treated as walls, where no fluxes were defined i.e. were specified as zero without gradients. The sugar beet cossette domain was treated as walls with zero gradients for velocity field, and with pre-set concentration field for substrates (a boundary layer for the concentration of substrate on the surface) and product (**Fig. 3**).

A steady-state simulation was performed, due to the fact that steady-state simulations greatly reduce the complexity and computing time (14). Kinetic model parameters are temperature dependent, but temperature variations in the system were negligible and consequently energy balance was not solved. For longitudinal stream of extractant to the surface of single cossette (**Fig. 4**) velocity inlet conditions were applied to the mesh at the lateral sides (left and right) and the remaining boundaries (bottom and top) were treated as walls.

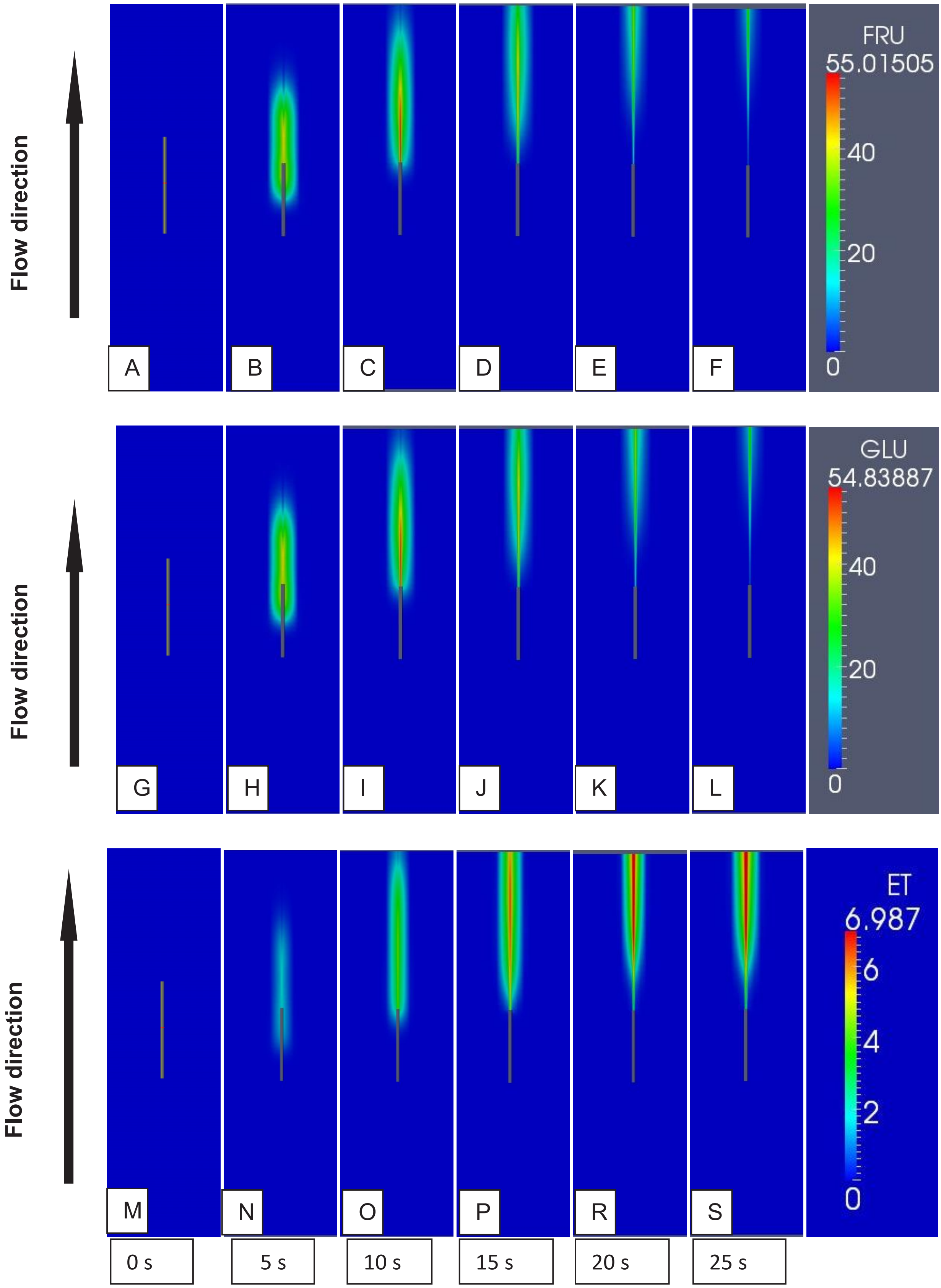

Figure 4. CFD simulation of the concentration of fructose (A, B, C, D, E, F), glucose (G, H, I, J, K, L) and ethanol (M, N, O, P, R, S) around single sugar beet cossette in simultaneous extraction and fermentation process.

Also the same statements for sugar beet cossette domain were used with the same assumptions (**Figs. 5-9**). The set of equations were solved numerically in 9 steps. It is important to (i) establish suitable grid system, (ii) to convert the equations into algebaric equations, (iii) to select the discretization sheme for formulation of equations at every single grid location, (iv) to establish pressure equation and (v) finally to develop suitable iteration scheme for obtaining a solution. The finite volume method was used as a discretization scheme. The finite-volume method (FVM) is a method for representing and evaluating partial differential equations in the form of algebaric equations. Similar to the finite difference method or finite element method, values are calculated at discrete places on the meshed geometry. "Finite volume" refers to the small volume surrounding each node point on the mesh. In the finite volume method, volume integrals in a partial differential equation that contain a divergence term are converted to surface integrals, using the divergence theorem (25). These equations are then evaluated as fluxes at the surfaces of each finite volume. Since the flux inlet of a given volume is identical to the outlet the adjacent volume, these methods are conservative. Another advantage of the finite volume method is that it can be easily formulated for unstructured meshes. The method is often used in different computational fluid dynamics packages as OpenFOAM (28).

In order to understand the mass transfer in the simultaneous extraction and fermentation process of ethanol production (i.e mass transfer and microbial conversion of sugars from sugar beet cossettes into ethanol), only macro scale simulations are not sufficient. Microbial conversion flow models of the micro scale (single sugar beet cossette acts as a microreactor) are indispensable to capture all scales of the process. As it was proven above, low reactants transport rate (diffusion) affects the microbial conversion rates. The use of compartment type structured mathematical model for description of bioprocesses in tubular reactors was not sufficient to examine the mass trasfer and microbial conversion rates on the scale of one sugar beet cossette in the short time scales (0-25 s; 5). The established CFD model with microbial conversion phenomena can be used for simulation of: perpendicular stream (**Figs. 2-4**) of extractant to the surface of one single cossette and longitudinal flow (Figs. 5-9) beside the surface of one single cossette. As it can be seen in **Fig. 2** the flow pattern was established after 5 seconds and velocity field is increasing around the sugar beet cossette as well as a wake is formed "behind" the cossette in the flow direction. Differences in velocities around the sugar beet cossette and outside are not so expressed (0.006 and 0.007 m/min) without cavity phenomenon, what means that recirculation zone was not established behind the cossette. At low Reynolds numbers of the flow arround single sugar beet cossette, hydrodynamics are controled mainly by viscous effects (creeping type flow; 29). For sucrose concentration field at t=0 s (**Fig. 3**) it can be seen that maximal sugar concentration is in the middle of the cossette and that the gradient of concentration is established along the cossette width (established boundary concentrations). After 5 s of reaction time, concentration diminishes, with its maximum at the "top" of the cossette in the flow direction. This information confirms that the sucrose hydrolysis by yeast invertase is rapidly carried out. Furthermore, it is obvious from the study of the established concentration field after 15 s of microbial conversion that sucrose is almost completely converted into fructose and glucose. The study of concentration fields for fructose (**Fig. 4 A-F**) and glucose (**Fig 4. G-L**) pointed out that the increase of fructose and glucose concentration was related to the sucrose diminishing effect. The increase of ethanol concentration was notable in the flow direction (**Fig. 4 M-S**).

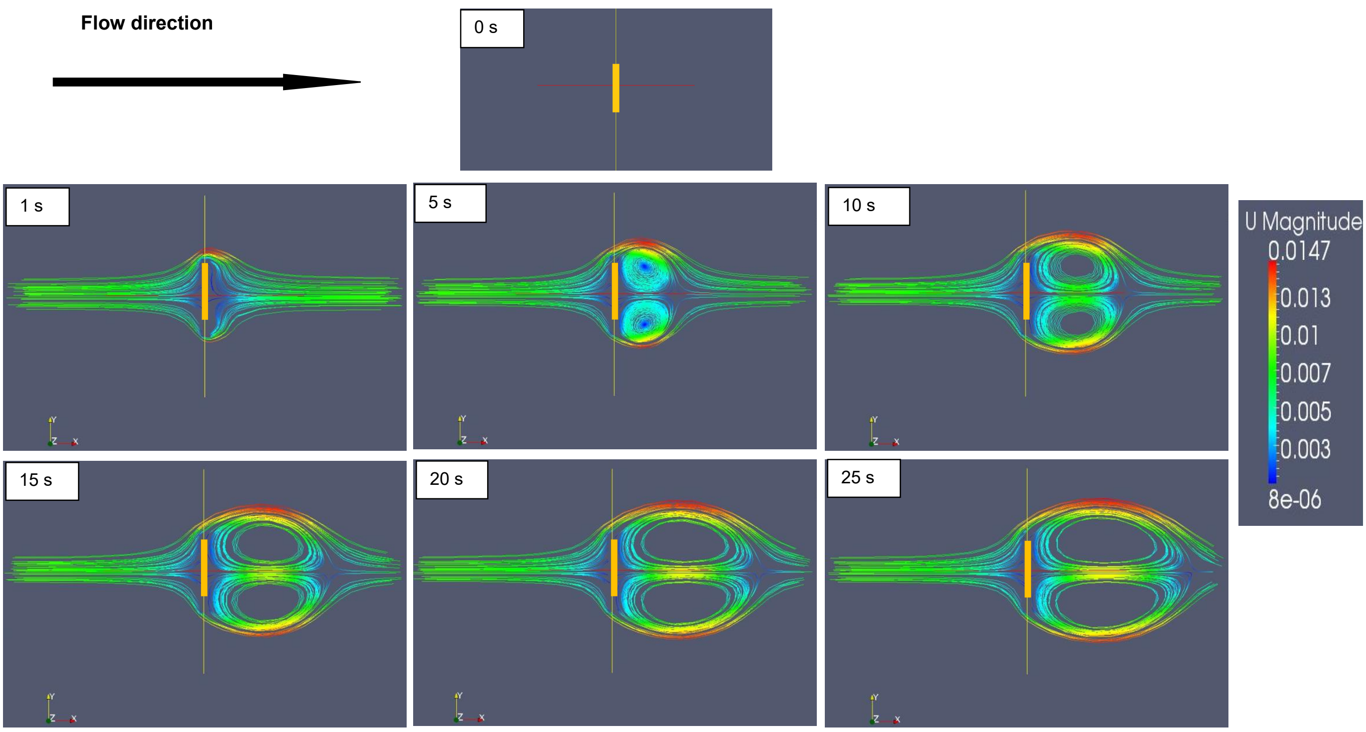

Figure 5. Model velocity profile (U magnitude) m/min of extractant flow around single sugar beet cossette.

For longitudinal flow (**Fig. 5**), it can be seen that after formation of fluid flow around the sugar beet cossette, the flow past the wake zone is enlarged with time. Due to the fact that difference between velocities are obvious, recirculation zone behind the sugar beet cossette was formed. The development of recirculation zones is in agreement with increase of Re number for fluid flow (29). The zone consists of two symmetric circulation cells. Although the cavities (the circulation zones) are increased in time, after 25 s flow pattern is fully established (non–stable flow pattern was not present), and consequently no vortex shedding was observed.

Changes of sucrose, glucose and fructose concentration fields follow the same pattern as velocity fields. Sucrose is (**Fig. 6**) diminished after 5 s due to the relatively high yeast invertase activity and consequently the enlargement of fructose (**Fig. 7**) and glucose (**Fig. 8**) concentration was observed. Ethanol concentration increases with decrease of glucose and fructose concentration (**Fig. 9**), and reaches its maximum after 25 s. The maximal ethanol concentration was detected in the recirculation zones behind the sugar beet cossette. This observation can be useful due to the fact that yeast cell could be inhibited if it is "caught" in these circulation zones because of relatively high local ethanol concentrations.

The CFD approach to model complex microbial conversion and flow patterns in the packed bed bioreactor is not an easy task. Modeling flow patterns and microbial conversion arround a single sugar beet cossette is only a first step in development of more complex flow for the metabolic reaction systems of the whole bioprocess.

Conclusions

Formal kinetic model of microbial sugars conversion from sugar beet cossette into ethanol was combined with the PISO algorithm and it was used in the computational fluid dynamics calculations. After post processing of data two-dimensional concentration fields for sucrose, glucose, fructose, ethanol as well as the extractant velocity field were obtained. The longitudinal flow in the surrounding of sugar beet cossette is characterised by development of recirculation zones (concur with increase of Reynolds number) and two symmetric circulation

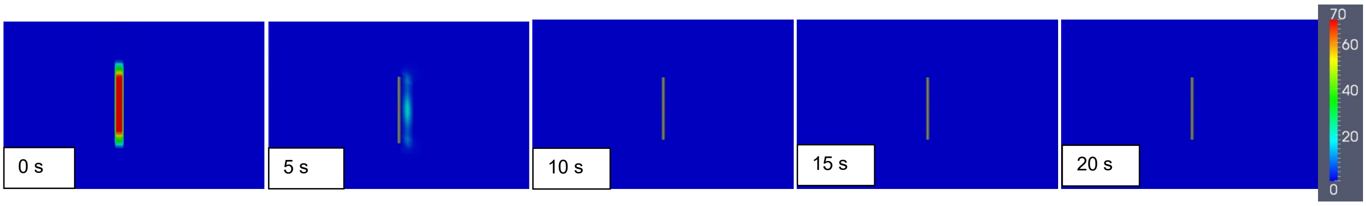

Figure 6. Model concentration profile g/dm³ of sucrose around single sugar beet cossette. Flow horizontal laterally from left.

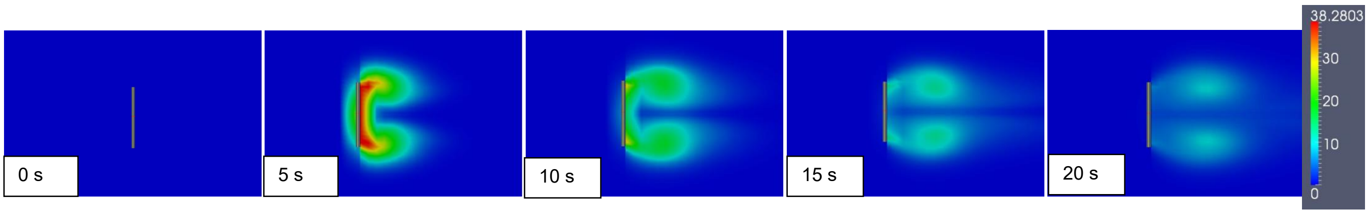

Figure 7. Model concentration profile g/dm³ of fructose around single model sugar beet cossette. Flow horizontal laterally from left.

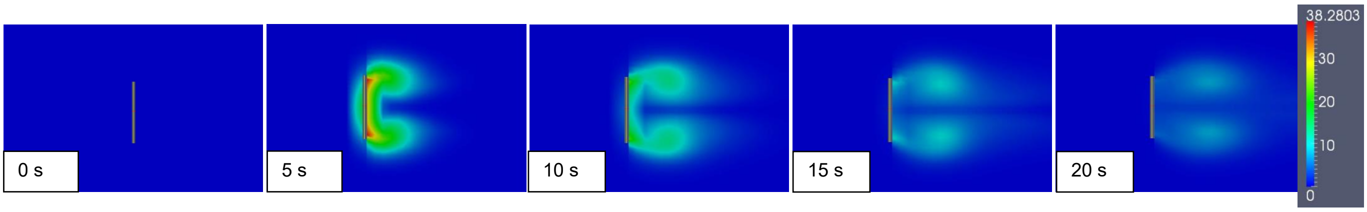

Figure 8. Model concentration profile g/dm³ of glucose around single sugar beet cossette. Flow horizontal laterally from left.

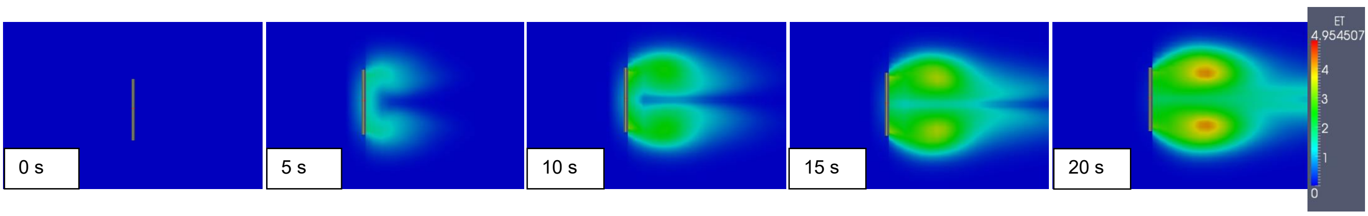

Figure 9. Model concentration profile g/dm³ of ethanol around single sugar beet cossette. Flow horizontal laterally from left.

cells (vortex). For perpendicular streams near the cossette the wake is formed "behind" the cossette in flow direction without cavity occurrence. The flow around the single sugar beet cossette was also characterised by relatively low Reynolds numbers as well as liquid phase physico-chemical properties.

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Conflict of interest statement

The authors declare no commercial or financial conflict of interest.

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