INTEGRATED SOFTWARE ENVIRONMENT FOR BIOPROCESS SIMULATION

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Abstract

In development of the software applications object oriented transformation method was used. The objects of complex bioprocess are modeled by heterogeneous program packages. This development dynamics of the engineering program packages directly incorporated in software applications. Program components were generated with MathCAD program package. The new generating program components were integrated in MathConnex environment. MathConnex is a stable explorer for visual integration of heterogeneous program packages at creation the continual simulation. MathConnex totally integrates components generated by program packages MathCAD, Matlab, Excel and Axum and use program languages ConnexScript, VBScript and Jscript. The integration level may be enhanced with decreasing of a number used program packages. As a case study ethanol fermentation with free and immobilized cells *S.Cervisae* were simulated. In this paper, the bioprocess of ethanol production was simulated simultaneously with designing software applications. The complex bioprocess was decomposed to the object level by combination of the operational, transformational, and objection access. The complete plant model was then used to perform supply optimization, in which alternatives were evaluated. Several strategies were examined to find the best feed for the plant considering issues such as feed cost, product quality, and current product value in the market, and to analyze the operation of the plant to identify the optimum conditions under which to operate the plant. A simple economic objective function was defined. The obtained examples demonstrated there is a growth in the application of simulation as part of plant management. To perform on-line simulation the simulator needs to be interfaced to the plant to receive and transmit data.

Keywords: Object-oriented approach, Software development, Simulation model, Integrated environment.

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1 Introduction

Program packages usually do not satisfy high pretensions tools for process modeling and simulation, while special software packages are not commercial [1,2].

The integrated simulation systems development typically consist of phases such as requirements analysis,design, and implementation[3]. Requirements analysis investigates user needs and translates them into simulation model specifications, including performance requirements such as the response time of various outputs. In order to ensure a successful implementation of the system, these requirements are evaluated. Such an evaluation needs to be done during the requirements analysis phase because the cost of fixing the system at a later stage can be high due to design revision, code revision, retesting, and maintenance[4,5].

Simulation is widely used tool for checking the performance requirements [6,7]. It offers several benefits to the systems analyst and designer including the ability to identify the behavior and performance of the system prior to its design, and to check the efficiency of a system within a specific resource environment. I addition this system can be configured in several ways, with each configuration having varying performance and cost. The simulation of these configurations helps in understanding and evaluating the tradeoffs between performance and cost. Simulation can also aid in the design of information systems[8].

The current requirements or alternative energy sources have initialized the research of cellulose biomass conversion to the liquid fuel. In this paper integrated simulation system for the ethanol production were performed.

2 System network modelling

In order to simulate a system it is first necessary to construct an unit model of it.This model is then implemented in a high level purpose simulation language and the simulated features of the system observed. Formulation and building of the unit model of the system in perhaps the most unstructured, expensive, and less supported task in developing simulations. Through methods for building simulation models are available, there are no published studies on building simulation models for bioprocesses.

Specifically, in this article a network based approach to constructing a simulation model was described. The overall methodology consists of a two-step process, summarized in Fig.1.First knowledge pertaining to the target bioprocess system gathered by an analyst during requirements analysis is synthesized into a network model of the bioprocess. This model is then utilized for automatically building the simulation model. The approach has the benefits of shortening the system development cycle, economical and fast development of simulation model from the specifications obtained during requirements analysis, allowing analysts with little training in simulation to test the bioprocess.

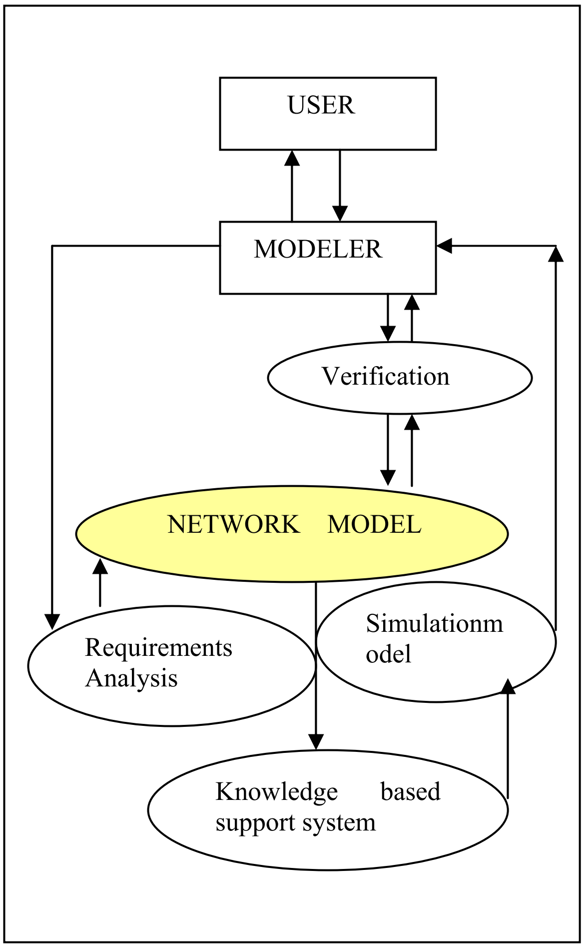


Fig.1 Simulation model construction

The next section discusses the properties desired of a modeling formalism in order to facilitates the derivation of a simulation model for the bioprocess systems.

3 Bioprocess systems network

Transaction that take place the environment affect the system as its inputs, while the outputs that leave the system affect its environment. A transaction entering a simulation model may pass through several processes before its transformation to an output. In addition to the input-process-output relationship, several complex relationships among these processes often exist (Fig.2). In general, any two processes may be mutually exclusive, order dependent, order independent, or concurrent. Two processes are mutually exclusive when only one of them can be performed. Two processes are order dependent when one must be performed before the other. Two processes are order independent when both can be performed in any order or simultaneously, i.e. performing one of these does not affect the other, and two processes are concurrent when both can be performed in any order but not simultaneously. Such processes complete for and utilize various resources.

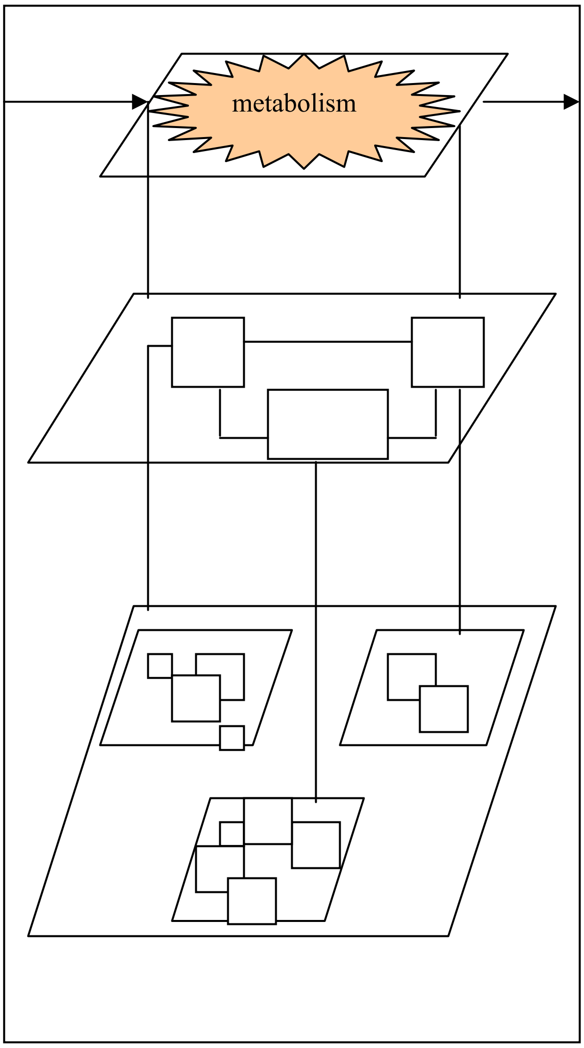


Fig.2 A bioprocess system synthesizing

There are many approach to model integrated networks. Two of them are frequently used: hierarchical and Petri net approach. Petri nets have been utilized extensively in a number of application areas, including design of distributed computing systems, general purpose information systems, production planning, and flexible manufacturing systems. In this paper the hierarchical approach for bioprocess system was employed (Fig.2).

In ethanol fermentation the biotransformational way have two alternatives *aerobic* and *anaerobic*. In operation can be employed batch and continuous bioprocesses and bioprocesses with free and immobilized cells.

4 A simulation model

In general, modeling begins with an observation of the system and then translating these observations into a model. Some systems such as manufacturing systems may be modeled by beginning with the print of the facilities, followed by defining the materials flow, and then defining the interfaces between system components.

Mutually exclusive processes are represented by making a place that has a single token become an input to multiple transitions corresponding to these mutually exclusive processes. Places that are outputs of a transition but not inputs to any transition indicate the transactions that leave the system. These places define boundary of the system and help identify system interfaces with the environment. A model that is too abstract may be refined to show greater detail.

Developing simulation models hierarchically offers several advantages such as hierarchically simplification and ease of simulation.

In the development of software application object oriented transformation method was used. The objects of complex bioprocess are modeled by heterogeneous program packages. Development of the engineering program packages directly incorporated in software applications.

In this paper the program components were generated in MathCAD program package. The generated program components were integrated in MathConnex environment [6]. MathConnex is a stable explorer for visual integration of heterogeneous program packages at creation the continual simulation. MathConnex totally integrates components generated by program packages MathCAD, Matlab, Excel and Axum as well as program languages ConnexScript, VBScript and Jscript[7]. The integration level may be enhaced with decreasing of a number the used program packages.

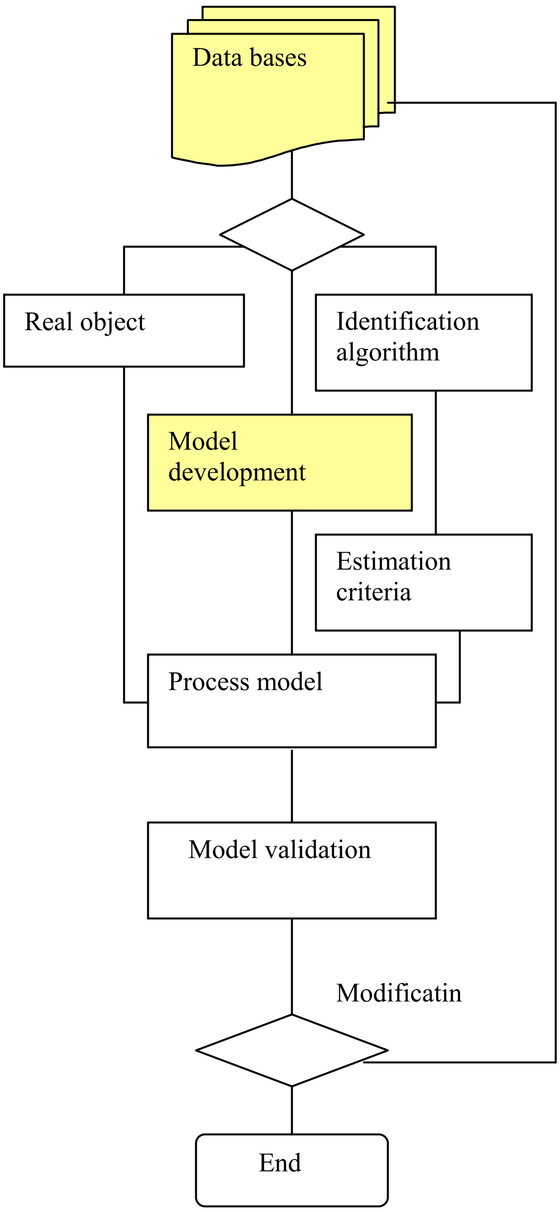


Fig.3 Flowchart of modeling methodology

For all study phases the owns program components may be generated by heterogeneous program packages. The program components include the structure of mathematical model, the algorithm for model identification and parameters estimation as well as validity testing model. Integrated structure of program components is shown in Fig.3. The base program components were generated in MathCAD program package.

All program components are integrated in MathConnex environment. The logic flow diagram of the program structure integration is shown in Fig.4. Several software segment may be independently executed, to the objective of studying of the bioprocess phases, the software development and a fresh integration.

5 The bioprocess simulation

The generic models were illustrated by actually implementation of continuous anaerobic fermentation.

By analysis the ethanol production system, following phases were identify: biocatalyst synthesis, hydrodynamic operation and diffusion phenomena, biochemical kinetic and operational stability and productivity in the packed bed column.

The program components include the structure of mathematical model, the algorithm for model identification and parameters estimation, as well as validity model testing.

Mathematical model of the flow bioreactor with free or immobilized cells(Fig.5) was derived from mass balance of cells, substrate and product, respectively, including of reaction rates[1].

$$F_0 X_0 - F_0 X + (r_x)V_L = V_L \frac{dX}{dt} \qquad (1)$$

$$F_0 S_0 - F_0 S + (r_S)V_L = V_L \frac{dS}{dt} \qquad (2)$$

$$F_0 P_0 - F_0 P + (r_p)V_L = V_L \frac{dP}{dt} \qquad (3)$$

Mathematical model of packed bed column reactor with constant immobilized cells concentration was obtained by balance equations including effectiveness factor η for bead

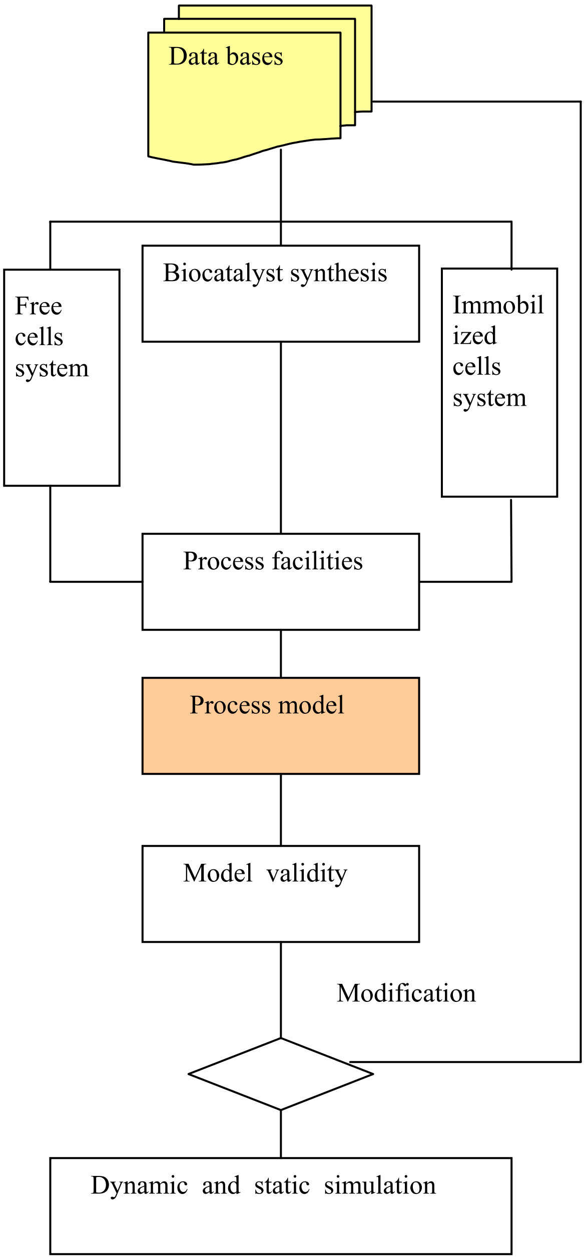


Fig.4 Program structure integration in the MathConnex environment for the ethanol process production

geometry, fluid fraction ε for column design and dilution rate D for v_0/V_L ratio.

$$DS_0 - DS + \frac{\eta}{\varepsilon}(v_S)S = \frac{dS}{dt} \qquad (4)$$

$$DP_0 - DP + \frac{\eta}{\varepsilon}(v_P)P = \frac{dP}{dt} \qquad (5)$$

6 The bioprocess scheme

An integrated system approach for a multiscale and multipurpose process simulation involving approaches at the different length scales from micro-scale to macro-scale was employed.

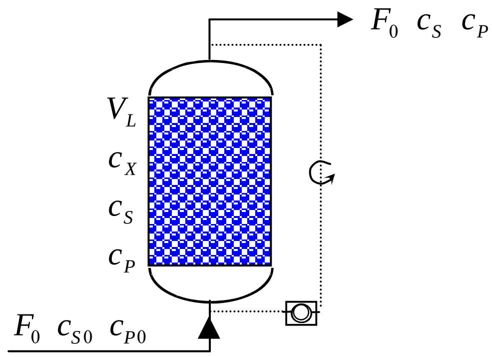
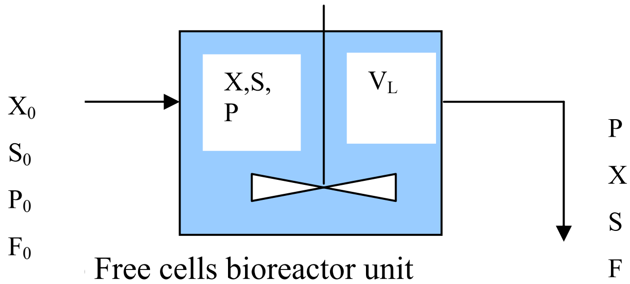


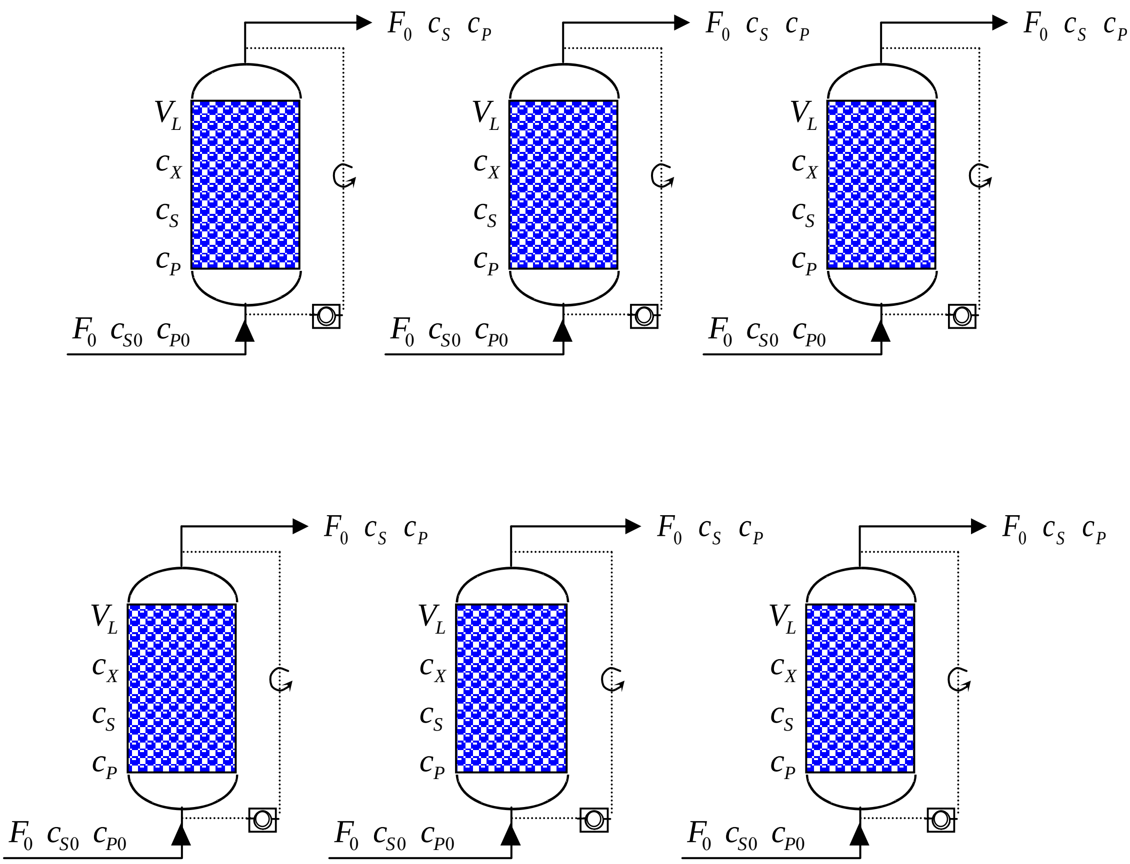
Fig.5 Immobilized cells bioreactor unit



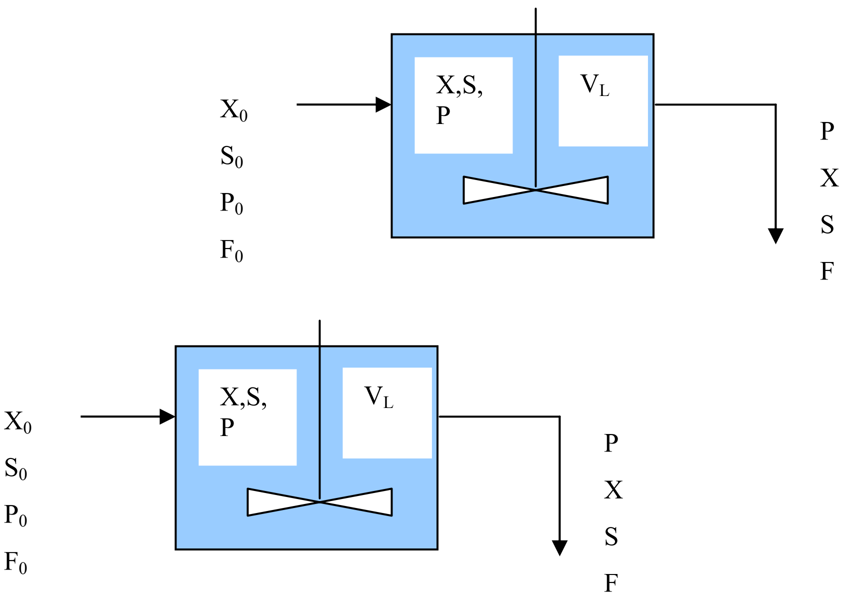
Free cells bioreactor unit

One of most interesting and encouraging trends in process simulation is its use in many more of the total range of activities concerned with process plant design and operation. Thus application of a flowsheeting system is no longer confined to use by engineers in the development of a new design or revamp. This still remains an important purpose of simulation but is now joined by range of other functions so that the overall value of process modeling is of benefit throughout the full life cycle of the plant.

Design of various capacity plant using serial or parallel process systems schemes is shown in Fig.7



(a) immobilized cells process units network



(b)free cells process units network

Fig.7 Simulation flow diagrams

From a definition of the process a rigorous model is developed that permits use steady state design, for dynamic simulation and in optimization. The creation of that model may be motivated initially by use in the development of a new process design. However rather than generation of those results being the end of the exercise, they become just the starting point for fuller use of the process model.

The opportunity for this wider applicability is derived largely from technological advance in simulation technology itself, and especially from the emergence of equation-solving systems. The established technology employs the sequential modular approach and its use is widespread. In the sequential modular approach the calculations proceed successively from unit operation to unit operation to arrive at final answer. By contrast the equation-oriented technique represents a complete plant as a large global set of equations, all of which are then solved simultaneously.

7 Results and discussion

The advantage of the equation-oriented technique is its flexibility. No constraints are imposed on the type of problem to be tacked. A single problem definition may be used for study of steady state or dynamic behavior and it can also be used for optimization purposes. However the technique is much more demanding in terms of numerical technique and it is only in recent years that such systems have maturated sufficiently for use as a day-to-day production tool.

The simulation of outlet ethanol concentration, as a function of inlet substrate concentration and dilution rate were provided. Cells productivity simulation for different inlet substrate concentration and process parameters, in the continuous flow reactor with free cells was performed.

The optimal process parameters for volumetric ethanol productivity as a function o inlet substrate concentration and dilution rate are shown in Fig.8

The adequate contour map was used for estimating the optimal values by canonic analysis.

8 Conclusions

Deriving a simulation model from an understanding of the system to be simulated is perhaps the most complex and time consuming task of the simulation life cycle. This paper has been focused upon the development of simulation models for bioprocess of ethanol production in the integrated MathCAD and MathConnex environment. The models for free cells and immobilized cells in anaerobic conditions were developed.

Future research can investigate the derivation of simulation models in other simulation software.

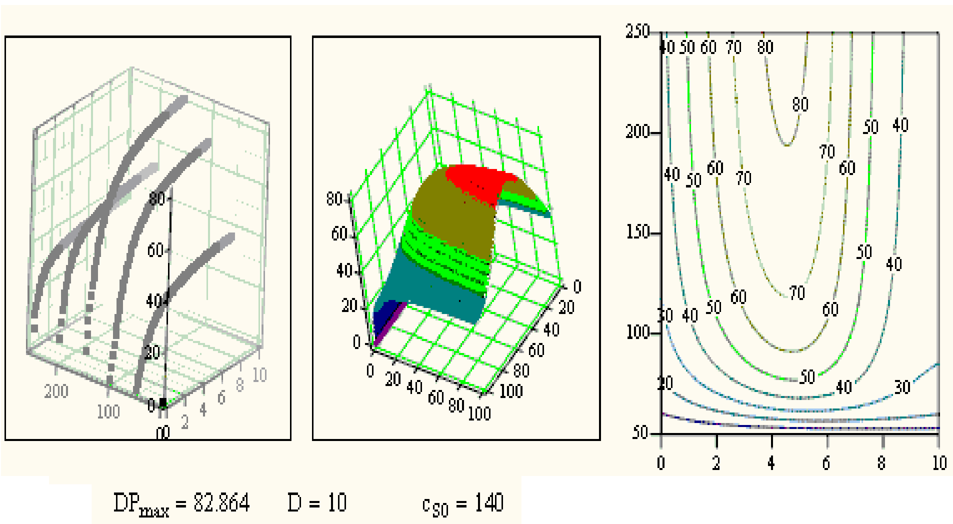


Fig.8 Product progress vs. dilution rate D

Thus, this multiscale integrated approach will also be of great help, in responding to the increasing environmental, societal and economic requirements.

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Notation

c-concentration kg/dm^3

D-dilution rate

F-flow rate,m^3/h

P-product

S-substrat

V-volume

X-biomass

η -effectiveness factor

ε- fluid fraction

Subscript

L-liquid

0-initial

P-product

S-substrate

X-biomass

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