OPTIMAL OPERATION AND CONTROL OF A REACTIVE SIMULATED MOVING BED PROCESS

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Abstract: In this paper, we investigate the continuous production of High Fructose Corn Syrup (HFCS) in a Reactive Simulated Moving Bed process (RSMB). The RSMB process combines a quasi-continuous chromatographic separation with an enzymatic biochemical conversion of glucose to fructose. For the equilibrium limited glucose isomerization such an integration is suitable. The optimal operation of the RSMB process is determined using a sequential approach based on a rigorous mathematical model of the plant. In addition, we propose a new strategy to determine the distribution of the columns over the zones in the RSMB plant circumventing the solution of a Mixed Integer Nonlinear Problem (MINLP). During the operation of the RSMB process, disturbances occur (e. g. continuous decrease of the enzyme activity) which lead to an off-spec product. The control objective is to maintain the product purity while injecting a minimal additional amount of eluent. We propose a nonlinear model predictive controller which can deal with the complex hybrid dynamic of the RSMB plant as well as with hard constraints. The parameters of the non-linear process model are periodically estimated by least-squares fitting to online measurements. The efficiency of the whole control concept is shown in simulation studies for a 6-column RSMB plant.

Keywords: Simulated-Moving-Bed (SMB), Glucose Isomerization, High Fructose Corn Syrup (HFCS), Reactive Chromatography, Asynchronous Chromatography (VARI*COL*), Nonlinear model predictive control (NMPC).

1. INTRODUCTION

Glucose has only about 70% of the sweetness of sucrose and is less soluble in water. At the commercial concentration, glucose syrup must be kept above room temperature to prevent crystallization. Fructose is 30% sweeter than sucrose and twice as soluble as glucose at low temperatures. Using enzyme technology, by at least 50% conversion of glucose to fructose both problems can be overcome giving a stable high fructose corn syrup that is as sweet as a sucrose solution. The present world market for high fructose corn syrup is over 5 million tons and it is still expanding. This is due to the fact that the commercially available 'glucose isomerase' is remarkably resistant to changing temperatures and can be handled at high substrate concentrations. Most of the currently produced fructose syrups is obtained by the hydrolysis of starch into glucose followed by isomerization of glucose to fructose (Asif and Abaseed, 1998). This process produces syrups containing only about 42% fructose which has to be enhanced by selective removal of glucose or by applying multistage chromatographic separation methods.

A 3-zones-SMB process is proposed in this paper for the continuous isomerization of glucose, where reaction and separation are integrated in one apparatus leading to significant improvements in process performance. The optimization and the control of this complex hybrid system represent challenging tasks, and advanced strategies are required.

This work is structured as follows: in section I, the process is described and a detailed mathematical process model is presented. In section II, a mathematical model-based sequential optimization approach (Klatt *et al.*, 2001) is aplied to this process. In addition, we show how to use a new

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multicolumn continuous process called VARI*COL* which was recently introduced by (Ludemann-Hombourger and Nicoud, 2000), in order to determine the distribution of the columns over the zones of the RSMB plant. In section III, the control problem will be discussed. The objective is to maintain the desired product purity using a minimal amount of eluent. A nonlinear model predictive controller is developed, where at every sampling moment the optimal trajectory over a future control horizon is calculated online. The parameters of the rigorous process model are estimated periodically by least-squares fitting to online measurements. The efficiency of the control concept is shown in simulation studies for a 6-column RSMB plant.

2. THE RSMB PROCESS FOR GLUCOSE ISOMERIZATION

2.1 Process description

The process consists of a number of fixed beds, which are interconnected to form a closed-loop arrangement. All columns are homogeneously packed with an ion exchange resin (Amberlite CR-13Na) and the imobilized enzyme Sweetzyme T (supplied by Novo Nordisk Bioindustriale). A counter-current movement between the solid and the liquid phase is achieved by simultaneously advancing the inlet and outlet ports in direction of the liquid flow. In this special Simulated Moving Bed process, no attempt is made to achieve a complete separation of glucose and fructose, since the most common type of fructose syrup, usually called high-fructose syrup, is made in two categories: HFCS42 (42% fructose) and HFCS55 (55% fructose). For some purposes, a syrup with more than 55% fructose , called a higher-fructose syrup is desirable. Thus, the objective is to transform a syrup containing only pure glucose to one, where the glucose is **partially** converted to fructose.

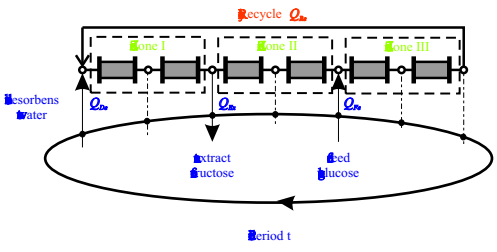

Figure 1. Schematic diagram of the 3-zones RSMB process for glucose isomerization

After start-up, a reactive True Moving Bed unit would achieve a steady-state, in which every process variable remains constant in time at any spatial location. In contrast, due to the discrete switching of the columns, SMB units do not reach a steady-state but rather a *cyclic* steady or periodic one (see figure 2).

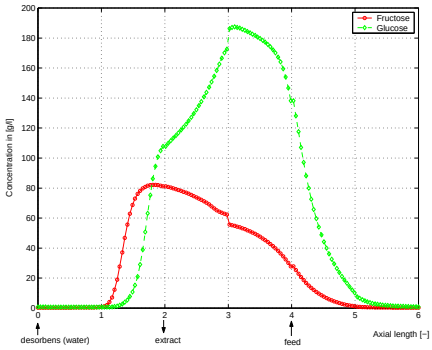

Figure 2. Axial concentration profile at the begin of the period for $Pur_{Ex} = 70\%$

2.2 Mathematical Modeling

A lot of work has been published on modeling of chromatographic processes (Gu, 1995). Accurate dynamic models of multi-column continuous chromatographic processes consist of coupled dynamic models of each column under consideration of the periodic port switching. A single chromatographic column is described by the *General Rate Model* which accounts for all important non-idealities of the column, axial dispersion, pore diffusion and the mass transfer between liquid and solid phase:

$$\begin{aligned} \epsilon_b \frac{\partial c_{b,i}}{\partial t} + \frac{(1-\epsilon_b)3k_{l,i}}{R_p}(c_{b,i} - c_{p,i}|_{r=R_p}) \\ + \epsilon_b r^{\text{liq}}_{\text{kin},i} = \epsilon_b D_{ax} \frac{\partial^2 c_{b,i}}{\partial x^2} + \epsilon_b u \frac{\partial c_{b,i}}{\partial x} \\ (1-\epsilon_p)\frac{\partial q_i}{\partial t} + \epsilon_p \frac{\partial c_{p,i}}{\partial t} = \epsilon_p D_{p,i} \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c_{p,i}}{\partial r}\right). \end{aligned} \quad (1)$$

The model is completed by the mass balances at the nodes, and boundary and initial conditions which represent the switching process. The adsorption equilibrium and the reaction kinetic have to be determined experimentally. For the adsorption isotherm we assume a parabolic behavior:

$$q_i = H_i c_{b,i} + k_i c_{b,i}^2 + k_{ij} c_{b,i} c_{b,j},\ i,j = A,B. \quad (2)$$

The reaction kinetic can be accurately described by a first order pseudo-kinetic model (Fricke and Schmidt-Traub, 2002):

$$r^{\text{liq}}_{\text{kin},i} = \nu_i \frac{k_m (c_{b,i} - c_{b,j})}{k_{eq}},\ i,j = A,B. \quad (3)$$

The parameters are taken from (Fricke and Schmidt-Traub, 2002) and are listed in Appendix A. The resulting system of coupled partial differential equations can be solved efficiently using the approach introduced by (Gu, 1995), where a finite element discretization of the bulk phase is combined with an orthogonal collocation of the solid phase.

3. OPTIMAL OPERATION

3.1 Optimizing the operating parameters

The goal is to minimize specific separation costs for a given plant meeting the required product purities after the process has reached the cyclic steady state (CSS). For the description of the CSS, the operator Φ is introduced which represents the process dynamics $\mathbf{f}(\mathbf{x}, \mathbf{u})$ and the switching operations between two switching intervals:

$$\mathbf{x}_{k+1} = \Phi(x_k) \Leftrightarrow \begin{cases} \mathbf{x}^*_{k+1} &= \int_{t=0}^{\tau} \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t))dt, \\ \mathbf{x}_0 &= \mathbf{x}_k, \\ \mathbf{x}_{k+1} &= \mathbf{P}\mathbf{x}^*_{k+1}. \end{cases} \tag{4}$$

The switching operation causes a re-initialization of the initial value of the dynamic simulation and is represented by the permutation matrix $\mathbf{P}$. In the CSS, the axial concentration profile $\mathbf{x}_k$ at the end of period k does not change from period to period, which can be checked numerically as:

$$\|\Phi(\mathbf{x}_k) - \mathbf{x}_k\| \leq eps_{steady}. \tag{5}$$

Then, given a SMB process with a *fixed* column partition, the optimization problem can be stated as follows:

$$\begin{aligned} \min_{Q_{De}, Q_{Ex}, Q_{Fe}, Q_{III}, \tau} \quad & \text{Cost}_{spec}(k) \\ \text{s.t.} \quad \|\Phi(\mathbf{x}_k) - \mathbf{x}_k\| &\leq eps_{steady}, \\ Pur_{Ex,k} &\geq Pur_{Ex,min}, \\ Q_I &\leq Q_{max}. \end{aligned} \tag{6}$$

An inequality constraint is imposed on the product purity. Since the flow rate in zone I is the highest one in the plant, it is constrained in order to avoid violation of the maximal pressure drop delivered by the pumps. The objective function must be specified based on the available data on the operating cost.

The natural degrees of freedom are the flow rates of desorbent Q_{De}, feed Q_{Fe}, recycle Q_{III} and the switching period τ. In the framework of optimization, they are transformed to the β-factors (Hashimoto *et al.*, 1983), where the apparent solid flow rate Q_S is introduced:

$$\begin{aligned} Q_S = \frac{(1-\epsilon_b)A\ L}{\tau}, \beta_1 = (\frac{Q_1}{Q_S} - \frac{1}{F})/H_A \\ \beta_2 = (\frac{Q_2}{Q_S} - \frac{1}{F})/H_B, \frac{1}{\beta_3} = (\frac{Q_3}{Q_S} - \frac{1}{F})/H_A, \end{aligned} \tag{7}$$

and which reflects the fact that in SMB processes absolute flow rates are less important as their relative values. H_A and H_B denote the slope of the isotherm for the different species at the feed concentrations.

We use a direct sequential algorithm for the solution of the problem (6). The process is simulated until the cyclic steady state is reached. The constraints and the objective value are then evaluated and given back to a non-linear optimizer FFSQP (Zhou *et al.*, 1997).

3.2 Optimizing the distribution of the columns

For this purpose, we first introduce the VARI*COL* process developed by (Ludemann-Hombourger and Nicoud, 2000), where in contrast to the SMB process the ports are shifted asynchronously (see figure 3).

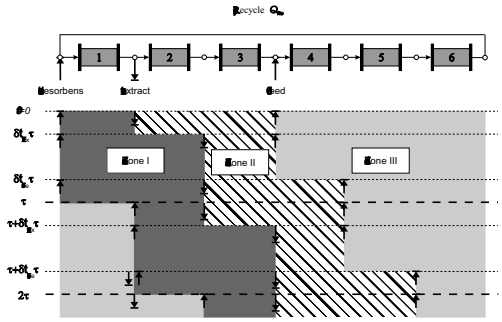

Figure 3. 3-zone VARI*COL* process for glucose isomerization

The numbers of columns per zone change during the period. E. g. the number of columns in zone I is one during a quarter of the period and two for the rest of the period. This corresponds to an average length of

$$\overline{N}_1 = 1 \cdot \frac{1}{4} + 2 \cdot \frac{3}{4} = \frac{7}{4} \tag{8}$$

for zone I. Analogously, $\overline{N}_2 = \frac{6}{4}, \overline{N}_3 = \frac{11}{4}$ result. While the SMB process is described by an integer column distribution, the asynchronous VARI*COL* process corresponds to a *real* number of columns in each zone.

Thus, the VARI*COL* process is more flexible than the SMB process. From the optimization point of view, the zone lengths $\overline{N}_i$ can be simply integrated as further degrees of freedom in the NLP formulated in equation 6 (Toumi *et al.*, 2002*a*; Toumi *et al.*, 2002*b*).

In table 1 (second column), the optimal operating point for the VARI*COL* process is listed. In this study, the objective was to minimize the desorbens consumption for an extract purity of 70%. The optimal distribution obtained in the VARI*COL* case is $[0.99, 1.6, 3.4]$, i. e. the zone III should be chosen much larger than the zones I and II. In comparison to the optimal operating point of the SMB-process with the configuration [2,2,2] (first column), **40%** less desorbens consumption is reached. If the optimal VARI*COL* distribution is rounded to the *next* integer distribution, an SMB process with section lengths $[1, 2, 3]$ results. By this distribution, the desorbens consumption can

Table 1. Optimization of the distribution of the columns among the zones for Pur_{Ex}=70%

	SMB I	VARICOL	SMB II
rel. Q_{De} [%]	100.00	60.00	74.00
Pur_{Ex} [%]	70.00	70.00	70.00
Q_{Fe} [ml/min]	1.30	1.30	1.30
Q_{De} [ml/min]	3.70	2.26	2.31
Q_{Re} [ml/min]	17.60	15.51	15.25
τ [min]	10.40	12.12	12.26
Q_{Ex}	5.00	3.56	3.61
β_i	**[1.04,0.79,1.63]**	**[0.97,0.84,1.50]**	**[0.97,0.82,1.53]**
N_i	**[2,2,2]**	**[0.99,1.61,3.4]**	**[1,2,3]**

be reduced by **26%** in comparison to the original [2,2,2]-configuration.

This approach led us to a considerably better SMB distribution after only two optimization runs. Even if mathematically this approach can lead to a sub-optimal distribution, the search space can be reduced when the optimal distribution of the VARI*COL* process is known. It can be assumed, that the optimal SMB distribution is one of the edges in the neighborhood of the optimal VARI*COL* distribution. In addition, since the VARI*COL* process includes all possible SMB-configurations, we know now a-priori the maximal attainable performance in term of desorbens consumption for a given plant (i. e. a given number of columns).

4. CONTROL STRATEGY

Automatic control of the SMB process was applied to the separation of aromatic hydrocarbons where on-line Raman spectroscopy can be utilized to measure the concentration of the compound at the outlet of the chromatographic columns (Marteau *et al.*, 1994). However this as well as the geometric nonlinear control concept described in (Kloppenburg and Gilles, 1999) are mainly based on a model for the corresponding true moving bed (TMB) process, where the cyclic port switching is neglected. In the case of SMB processes with a few number of columns (e. g. less than 8), the TMB process does not approximate the SMB process accurately, so that the applicability of this control scheme to plants with few columns seems problematic.

(Natarajan and Lee, 2000) investigated the application of the repetitive model predictive control (RMPC) technique on SMB processes. RMPC is a model-based control technique developed by incorporating the basic concept from repetitive control into model predictive control technique. In order to apply this technique, the switching period of the process is assumed to be constant. This is limiting, since the switching time can be used as another manipulated variable to control the process. The rigorous model was then linearised along the optimal trajectory. Afterwards it was reduced to a low dimensional linear model, based on which a linear MPC controller scheme was developed.

(Schramm *et al.*, 2001) presented a model-based control approach for direct control of the product purities of SMB processes. Based on wave theory, they derived relationships between the front movements and the flow rates for the equivalent TMB process. Based on these relationships, they developed a simple concept with two standard PI controllers. This concept is very easy to implement. However, similar relationships are difficult to determine analytically in the case of nonlinear reactive chromatography.

(Klatt *et al.*, 2001) proposed a two-layer control architecture where the optimal operating trajectory is calculated off-line by dynamic optimization based on a rigorous process model. The parameters are adapted based on online measurements. The low-level control task is to keep the process on the optimal trajectory despite disturbances and plant/model mismatch. The controller are based upon identified models gained from simulation data of the rigorous process model along the optimal trajectory. For the linear (linear adsorption isotherm) case, linear ARX models are sufficient (Klatt *et al.*, 2001), whereas in the nonlinear case neural networks (NN) were applied successfully (Wang *et al.*, 2002). A disadvantage of this two-layer concept is that the stabilized front positions may not guarantee the product purities if plant/model mismatch occurs.

4.1 Formulation of the control problem

The essence of model predictive control (MPC) is to optimize, over the future values of the inputs, the future process behavior. The future process behavior is analyzed with a process model over a finite time interval which is called the *prediction horizon*. The first input of the optimal input sequence, which spans the *control horizon*, is applied to the plant and the problem is solved again at the next time interval using updated process measurements and a shifted horizon. In

the framework of MPC control, it is simple to include hard constraints on the state and input variables. Furthermore, the process behavior can be predicted using a linear model or a nonlinear model. However, in the latter case, getting the *exact global* solution of a non-convex optimization problem requires formidable efforts and can not be achieved within a fixed sampling time. Even with state-of-the-art optimization algorithms, this seems to be practically impossible. Therefore we modify the nonlinear model predictive algorithm: we are calculating a *suboptimal* but *feasible* solution which can be applied in real-time.

We propose to solve the following optimal control problem over the finite *control horizon* H_r:

$$\begin{aligned}
\min_{[\beta_k,\ldots,\beta_{k+H_r}]} \quad & J = \sum_{j=k}^{k+H_p} \left(Cost(i) + \mathbf{\Delta}\beta_j^T \mathbf{R}_j \mathbf{\Delta}\beta_j \right) \\
\text{s.t.} \quad & \begin{cases} \dot{\mathbf{x}}_j = \mathbf{f}(\mathbf{x}_j, \beta_j), \\ \mathbf{x_{j+1,0}} = \mathbf{P}\mathbf{x}_j(\tau(j)), \\ j = k, \cdots, k+H_p. \end{cases} \\
& Pur_{Ex,H_r} + \Delta Pur_{Ex} \geq Pur_{Ex,min}, \\
& Pur_{Ex,H_p} + \Delta Pur_{Ex} \geq Pur_{Ex,min}, \\
& Q_{I,j} \leq Q_{max}, \\
& \mathbf{g}(\beta_j) \geq \mathbf{0}, j = k, \cdots, k+H_p.
\end{aligned} \tag{9}$$

We discretize the *prediction horizon* in cycles, where a cycle is a switching time $\tau(k)$ multiplied by the total number of columns. Eq. 9 consists of a dynamic optimization problem including the transient behavior of the process. The objective function J is a sum of stages costs (e. g. desorbens consumption) and a regularizing term added in order to smooth the input sequence avoiding high fluctuations in the input sequence from cycle to cycle. The first equality constraint represents the plant model evaluated over the finite prediction horizon H_p. The switching dynamic is introduced vice the permutation matrix $\mathbf{P}$. Since the maximal attainable pressure drop has not to be exceeded, constraints are imposed on the flow rates in zone I. Further inequality constraints $\mathbf{g}(\beta_j)$ are added in order to avoid negative flow rates during optimization.

The control objective is introduced by the purity constraint over the control Horizon H_r which is additionally corrected with a bias term ΔPur_{Ex} resulting from the difference between the last simulated and the last measured process output. A second purity constraint over the whole prediction horizon acts as a terminal (stability) constraint forcing the process to converge towards the optimal cyclic steady state. It has to be pointed out that the control goal (i. e. to fulfill the extract purity) is introduced as a constraint. We are using a feasible path SQP algorithm for optimization (Zhou *et al.*, 1997), which generates a feasible point before it starts to minimize the objective function.

4.2 Parameter Estimation

We assume that the concentration profiles in the recycling line are measured during a cycle. Since this measurement point is fixed in the closed-loop arrangement, the sampled signal includes information of all three zones. At every cycle and during the start-up phase an on-line estimation of the actual model parameters is started. The quadratic cost functional $J(\mathbf{p})$

$$J(\mathbf{p}) = \sum_{i=1}^{nsp} \left(\int_0^{N_{col,ges}} (c_{i,meas}(t) - c_{i,Re}(t))^2 \, dt \right) \tag{10}$$

is minimized with respect to the parameters $\mathbf{p}$. For this purpose, the Least-Squares solver E04UNF from the NAG-library is used. A by-product of the parameter estimation is the actual value $\mathbf{x}_0(k)$ which is given back to the NMPC controller.

4.3 Simulation study

Figure 4 shows a simulation scenario where the desired extract purity was set to 70% at the beginning of the experiment. At cycle 60, the desired extract purity is then changed to 60%. At cycle 120, the extract purity is increased to 65%. A fast response of the controller in both directions can be seen. Compared to the uncontrolled case, the control concept can keep the desired product purity rejecting a disturbance in the enzyme activity. The evolution of the optimizer-iterations are plotted as dashed-lines and shows that a feasible solution can be found rapidly and that the concept can be realized in real time. In this example the *control horizon* was set to 2 cycles and the *prediction horizon* to 10 cycles. A diagonal matrix $R_j = 0.02 I_{(3,3)}$ was chosen for regularization.

We assumed an exponential drift in the enzyme activity which corresponds to a drift in the reaction rate. Figure 5 shows the result of the parameter estimation. A good fitting was achieved and the estimated parameter follows the drift of the real parameter adequately.

5. CONCLUSIONS AND FUTURE WORK

The optimal operating point, as well as the distribution of the columns over the zones, of a RSMB plant were determined using a model-based mathematical approach. A nonlinear model predictive controller is presented which maintains the product purity while using a minimal additional amount of desorbens.

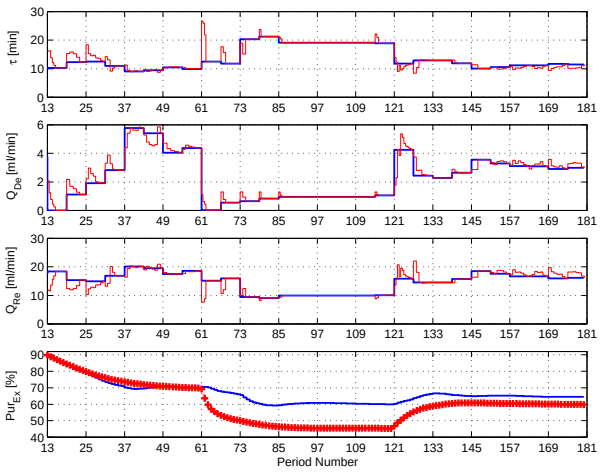

Figure 4. Control scenario: $H_r = 2, H_p = 10$

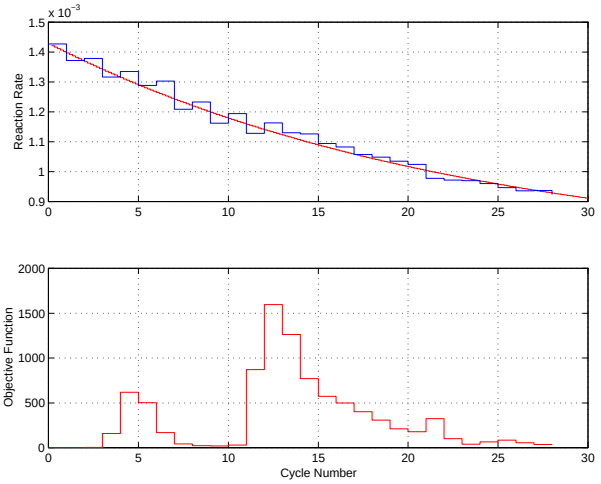

Figure 5. Estimation of the reaction rate

VARI*COL* is still **14%** better in term of desorbens consumption than the best SMB distribution [1,2,3] (see table 1). Therefore, it becomes more attractive to use the VARI*COL* concept, where in fact no additional investments are needed (despite programming the logical control system).

Appendix A. SYSTEM PARAMETERS

L=60.0 [cm]	k_i=[1.46E-07,1.33E-07]
D=2.6 [cm]	k_{ij}=[2.90E-07,9.30E-08]
ϵ_p=0.01 [–]	X=0.1 [-]
ϵ_b=0.4 [–]	k_0=24
D_p=16.25 [mm]	k_m=1.43E-03
k_{eff}=8.88E-05	k_{eq}=1.079 8 [–]
r=1.0 [g/cm^3]	Q_f=1.3 [ml/min]
h=5.8E-3 [g/(cm s)]	c_f=0 0.3 [g/cm^3]
D_p=1.0E-3 [cm^2/s]	Pur_{Ex}=60.0% or 70.0%
ν_i=[+1,-1] [–]	N_i=[2 2 2] or [1 2 3]
H_i=[0.47,0.27]	Δp_{max}=50 [bar]

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