# Process and Control Design for a Novel Chemical Heat Exchange Reactor

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# PROCESS AND CONTROL DESIGN FOR A NOVEL CHEMICAL HEAT EXCHANGE REACTOR

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*Abstract:* A new chemical reactor, the Open Plate Reactor (OPR), is being developed by Alfa Laval AB. It has a very flexible configuration with distributed inlet ports, cooling zones and internal sensors. This gives the OPR improved control capabilities compared to standard chemical reactors in addition to better heat transfer capacity. In this paper, we address the relationship between the process design, the number of actuators used and how to use these actuators in feedback control to be able to use the full potential of the OPR. The performance of the OPR can be significantly improved by using additional inlet ports and cooling zones. However, this may also require multivariable control methods to actually achieve this improvement in presence of model uncertainty and disturbances.

*Keywords:* process control, process design, optimization, operating conditions, model predictive control, process intensification

## 1. INTRODUCTION

The syntheses of fine chemicals or pharmaceuticals, widely carried out in batch or semi-batch reactors, are often strongly limited by constraints related to the dissipation of the heat generated by the reactions. A common solution is to dilute the chemicals to have lower concentrations, thus ensuring that the reaction rate and the subsequent heat release is lower than the heat transfer capacity of the reactor. After the reaction stage, the solvent is removed in a separation stage to provide a high-concentrated product of good quality. This separation process is both time and energy consuming, thus very expensive.

A new concept of compact heat exchange reactors, the Open Plate Reactor (OPR) is being developed by Alfa Laval AB, a leading manufacturer in heat exchangers. The key feature is to combine good micro-mixing conditions with high heat transfer capacity into *one* operation.

It allows complex chemical reactions to be performed with a very accurate thermal control, by combing high heat transfer capacity with improved micro-mixing conditions. Therefore OPR appears particularly suited to process intensification, as it allows at the same time an increase of reactant concentration and a desired reduction of the solvent consumption. The reduced need of down-stream separation results in large savings in time and money.

The modelling of the OPR and some results on the control design have been presented in (Haugwitz *et al.*, 2006) and (Haugwitz, 2005). In this paper, we will focus on the early part of the design phase, more specifically, the initial process design, the choice of operating points and the selection of control variables and structures for the subsequent control design phase.

It is non-trivial how to best utilize the full flexibility and potential of the OPR as there are many degrees of freedom, both in process and control design. In this paper we will address this issue and give examples on how to improve the performance by proper choices in

the process design and control phase.

## 2. THE PROCESS: THE OPEN PLATE REACTOR

The OPR consists of a number of reactor plates, in which the reactants mix and react. On each side of a reactor plate there is a cooling plate, through which cold water is circulated. It is possible to have several independent cooling plates mounted on each reactor plate, where each cooling zone has a individually controlled inlet temperature. This improves the possibility for accurate temperature control. In this paper a simple first order exothermic reaction is considered.

$$A + B \rightarrow C + D + \text{heat} \tag{1}$$

In Figure 1, a schematic figure of the first rows of a reactor plate is shown. The reactant $A$ flows into the reactor from the upper left inlet. Between the inlet and the outlet, the reactants are forced by inserts to flow in horizontal channels in alternating directions. The inserts are specifically designed to enhance the mixing and at the same time the heat transfer capacity. The concept relies on an open and flexible reactor configuration. The type of inserts and the number of rows in the reactor plate, which determines the residence time, can be adjusted, based on the type and rate of the chosen reaction. The reactant $B$ can be added through multiple inlet ports distributed along the reactor, also known as side streams, typically in the beginning and in the middle of the reactor. Temperature sensors can be mounted inside the reactor, specifically before and after each inlet port. To acquire accurate measurements of the temperature profile along the flow direction of the reactor, as many as 10 temperature sensors may be used. There can also be other sensors, such as pressure or conductivity sensors. The signals from the internal sensors are then used in the control system for emergency supervision and process control.

To summarize, the main novelty of the OPR is the ability to combine high heat transfer capacity with improved micro-mixing conditions, which has been a limitation for the previous use of heat exchangers as chemical reactors. Further, the additional inlet ports and cooling zones enable significantly improved temperature control of the reactor, thus increasing the performance of the reactor. The spatially distributed inlet ports and cooling zones can be seen as additional actuators and degrees of freedom for the controller to be able to use the full potential of the OPR.

## 3. OBJECTIVES

Before deciding upon a process design, it is important to clearly define the objectives of the production; what are the most important variables in the production? It may be the production rate, product quality, production safety, production cost and so on. The focus will

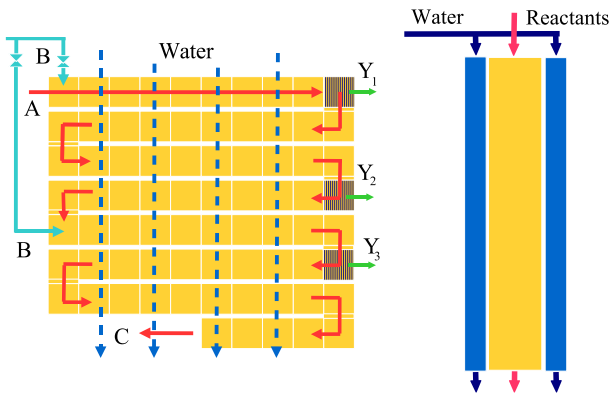


**Fig. 1** Left: A schematic of a few rows of a reactor plate. Reactant $A$ enters at top left and reactant $B$ is added at multiple inlet ports along the reactor. $Y_1$, $Y_2$ and $Y_3$ are internal temperature sensors used for process control and supervision. The cooling water flows from top to bottom in separate cooling plates. Right: The plate reactor seen from the side, with the reactor part in the middle and cooling plates on each side.

depend on the produced chemicals in each case and the market demand for this product.

In general for the OPR, there are two main priorities; the conversion of the reaction and the safety of the operation. The conversion $\gamma$ is defined as the number of moles of reactant $A$ that have reacted per mole of $A$ being fed to the reactor. The conversion is favoured of high reactor temperatures, but this may lead to safety issues due to the exothermic reactions.

It is also important to have a high production rate, that is, the number of moles of desired product formed per unit time. However, it is non-trivial how to choose operating conditions so that both conversion and production rate is maximized. In fact, to improve production rate the flow rate $q$ may be increased, which leads to reduced residence time. This may decrease the conversion as the chemicals are given less time to mix and react.

## 4. PROCESS DESIGN

In this section we will elaborate on what design choices are the most important for the safety and the conversion and what implications these choices may have on the control design. The process design phase involves many decisions, see e.g. (Froment and Bischoff, 1990) and (Fogler, 1992), and this list is limited to design variables that are important from a control point of view. The main focus is on the number and locations of the inlet ports and cooling zones as they can be seen as spatially distributed actuators that may significantly improve the conditions for control of the reactor.

- The nominal production rate and residence time

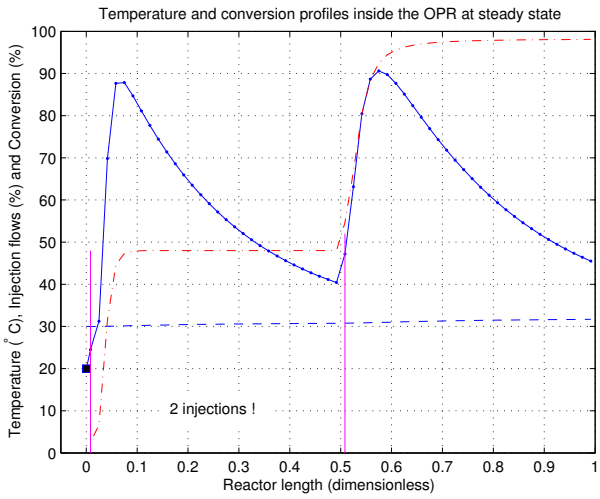


**Fig. 2** Reactor temperature (solid), cooling temperature (dashed) and conversion (dash-dot) profiles at steady state. The vertical lines indicate the inlet ports for reactant $B$ in terms of location and magnitude. The reactor temperature should be lower than $T_{max} = 90°$C.

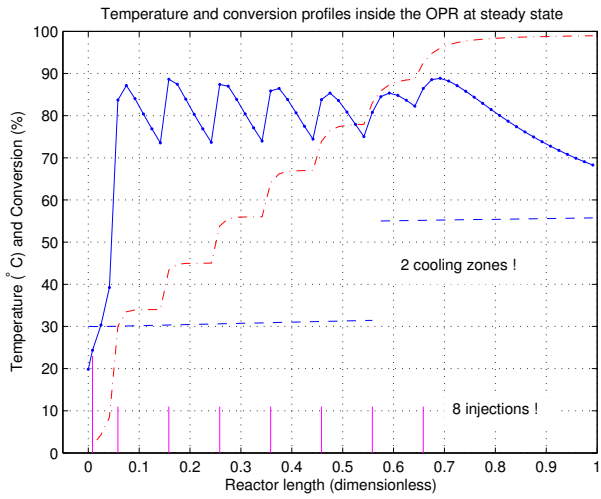


**Fig. 3** Same as Figure 2, but here eight inlet ports are used and two cooling zones, enabling a much more flexible and accurate control of the reactor temperature profile, thus improving productivity by 32% in steady state.

(flow rate and reactor volume)

- The number and location of the reactant inlet ports
- The number and location of cooling zones
- The number and location of sensors
- The desired operating point in terms of
  - Reactor temperature profile
  - Feed flow rates
  - Feed temperatures
  - Feed concentrations
  - Inlet cooling temperatures and flow rates
- Choice of actuator hardware (valves, heat exchangers)

In Figure 2, the temperatures and conversion along the reactor is plotted in steady state. In this figure, the reactant $B$ is added into the main flow of $A$ at two locations, at the inlet and at the mid section of the OPR. In general, there is a maximum allowed reactor temperature for safety reasons, which gives a limitation in production capacity, here $T_{max} = 90°$C.

It is desirable to operate the reactor so that the reactor temperature is as close as possible to the maximum allowed value for two reasons. First the conversion generally improves for high temperatures as the reaction rate varies exponentially with temperature. Secondly, with large difference between the reactor and cooling water temperature, the heat transfer $Q$ increases. The higher heat transfer capacity, the higher feed concentrations can be used, thus improving the production rate.

In Figure 3, eight inlet ports are used to better distribute the heat released from the reaction. It is then possible to increase the feed concentration with 32% compared to Figure 2 and still comply with the temperature constraint. To further improve the conversion, it is possible to have multiple cooling zones, so that the temperature at the end of the reactor remains high. However, there is a cost associated with each extra inlet port and cooling zone in terms of the additional process equipment needed. The process will also be more complex in terms of maintenance, calibration and safety classification.

The choice of operating point, the number of inlet ports and cooling zones may then be stated as an off-line optimization problem, where the conversion and the production should be maximized while respecting temperature constraints. It is necessary to introduce economic aspects to obtain a reasonable trade-off between improved performance and cost of additional actuators.

$$\max_{\substack{p\in\mathscr{P}\\ u\in\mathscr{U}\\ x\in\mathscr{X}}} \alpha_1\gamma q - \alpha_2(n_{inj}-1) - \alpha_3(n_{cool}-1) \qquad (2)$$

where $\gamma$ and $q$ are the conversion and the flow rate, respectively. $\alpha_1, \alpha_2$ and $\alpha_3$ are cost coefficients and can be seen as weights. $n_{inj}$ and $n_{cool}$ are number of inlet ports and cooling zones. $p$ is the process design vector with physical parameters and variables such as location of the inlet ports and cooling zones. These design choices are constrained in some region $\mathscr{P}$. The

control variables $u$ and the states (temperatures) are also limited in regions $\mathscr{U}$ and $\mathscr{X}$, respectively. In some cases, a desired production rate is given. The feed flow rate $q$ can then be viewed as the gas pedal and the optimization is solely focused on maximizing the conversion.

Eq. 2 will lead to a nonlinear non-convex optimization problem. However, since the number of inlet ports and cooling zones are limited, the optimization can be repeated for each choice of number of actuators.

This optimization is carried out off-line during the construction of the process. However, a similar optimization may be used on-line during production as disturbances and uncertainties may lead the initial off-line optimization to become sub-optimal.

For the OPR it is easy to see that additional inlet ports and cooling zones improve the possibility for accurate control of the reactor temperature. Each extra actuator gives additional degrees of freedom for the controller. This makes it possible to react very quickly on disturbances and uncertainties in order to achieve a product of high quality. On the other hand, it is non-trivial how to utilize these extra degrees of freedom in a suitable manner and that will be further discussed in Section 6.

## 5. UNCERTAINTIES AND DISTURBANCES

The uncertainty can be divided into two parts; parametric uncertainty in the process model and unmodelled dynamics.

Parametric uncertainty covers uncertainty in the reaction kinetics, micro-mixing conditions, heat transfer capacity and heat conduction. This can be seen as structured uncertainty within the process model. For example, if the heat transfer coefficient is overestimated by 10%, this may lead to the maximum temperature being 6°C higher than predicted. For a reaction with dangerous side reactions, such an increase may lead to impurities and even thermal run-aways.

The unmodelled dynamics can be seen as unstructured uncertainty and covers several aspects not included in the process model as more detailed heat transfer, mass transfer, diffusion, dispersion and reaction kinetices. For example if the model has higher dispersion than the actual reactor, the model will underestimate the maximum temperatures, which might lead to dangerous operation.

External disturbances represent variations in the inlet flows in terms of flow rates, temperatures and concentrations. With sensors and local feedback controllers, the flow rates and temperatures of the reactant flows can be accurately controlled. In general, there is no measurements of the feed concentration available on-line and that may be a cause for input disturbances. For example, an 5% increase in feed concentrations can lead to temperatures being 5°C higher.

To summarize, only the feed concentrations may be seen as unmeasured input disturbances, as the OPR is well equipped with sensors for feedforward control. The reactor and the reactions are very complex to model and therefore uncertainty in the models will require the use of feedback control to safely operate the process.

## 6. THE CONTROL STRATEGY & DESIGN

As seen in Section 5, disturbances and uncertainties will require the use of feedback control to safely operate the OPR. In this section we will elaborate on what input variables to use for feedback control. It is assumed that the process design is fixed and that for simplicity there are two inlet ports for reactant $B$ and one cooling zone. The available input variables for control are the flow rates, the inlet temperatures and the feed concentrations for each of the three inlet flows, $A$, $B$ and the cooling water. In this paper we will investigate the following variables:

- $u_B$, reactant feed distribution
- $T_{cool}$, inlet cooling temperature
- $T_{feed}$, feed temperature
- $c_{feed}$, feed concentration
- $q_{feed}$, feed flow rate

where $u_B$ is defined as the percentage of the total feed flow of $B$ that is added through the first inlet port. The remainder $1 - u_B$ is added through the second inlet port. A high constant cooling flow rate $q_{cool}$ is used to achieve more efficient cooling.

The variables are divided into two sub groups as the first three control variables will influence the temperature profile along the reactor, whereas $c_{feed}$ and $q_{feed}$ will affect the overall heat release inside the OPR direct or indirect, respectively. The control objectives defined in Eq. 2 can be seen as a combination of conversion and production rate. Therefore it is reasonable to discuss what influence the control variables have on either objective.

The feed flow rates $q_{feed}$ and feed concentrations $c_{feed}$ determine how much product that theoretically can be produced per unit time and should therefore be used to control the production rate. The conversion depends on the reactor length, the residence time, the micro-mixing and the reactor temperature, of which only the temperature is left to manipulate on-line. It is therefore critical to optimally control the temperature profile such that the conversion is maximized, see e.g. (Smets *et al.*, 2002). This can be obtained by manipulating $T_{feed}, T_{cool}$ and $u_B$.

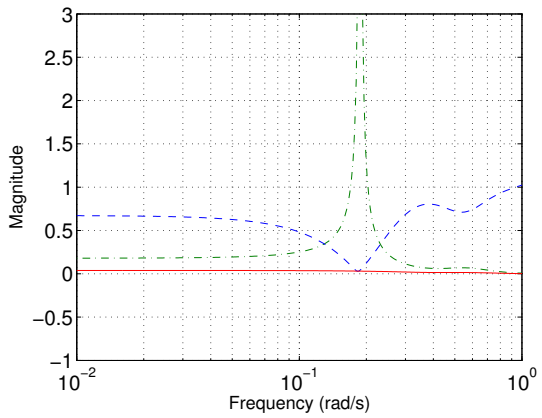


**Fig. 4** The norm of the difference between the RGA matrix $\Lambda$ and suitable pairing matrix, for different control variable selection. Solid line is when $T_{max,1}$ is controlled by $T_{feed}$ and $T_{max,2}$ by $T_{cool}$. Dashed line is when $T_{max,1}$ is controlled by $u_B$ and $T_{max,2}$ by $T_{cool}$. Dash-dot line is when $T_{max,1}$ is controlled by $T_{feed}$ and $T_{max,2}$ by $u_B$.

### 6.1 *Selection of control variables and control structure*

There is trade-off between the number of control variables used and the increased controller complexity this leads to. This choice is very similar to the trade-off in Section 3 between the number of actuators and the additional cost in the process design phase.

*Two inlet ports and one cooling zone* With two inlet ports, there will in general be two temperature maxima, see Figure 2, here denoted $T_{max,1}$ and $T_{max,2}$. To control these two temperatures arbitrarily, it is sufficient to use two of the three control variables $u_B$, $T_{feed}$ and $T_{cool}$. To obtain some insight what variables to choose, the Relative Gain Array number, see e.g. (Skogestad and Postlethwaite, 2005), is plotted in Figure 4. It is defined as the norm of the difference between the RGA matrix and a pairing matrix, e.g. $||\Lambda - [1 \quad 0; \quad 0 \quad 1]||$ when the pairing is diagonal. If there is no or negligible cross-coupling, the pairing can be chosen so that the RGA number becomes zero.

With three control variables, there are six possible combinations. The best three combinations are plotted in Figure 4. It is clear that using $T_{feed}$ to control $T_{max,1}$ and $T_{max,2}$ with $T_{cool}$ leads to the least cross-coupling (solid line). This is expected as the control variables mainly affects the reactor temperature at different spatial coordinates. When the feed distribution $u_B$ is used, more cross-coupling is present as the feed distribution affects both temperature maxima. The peak of the dash-dot line corresponds to large cross-coupling between $u_B$ and $T_{feed}$ for a given frequency, which depends on the flow time between the inlet ports for reactant $B$.

A RGA number around 0.05 indicates that $T_{feed}$ and $T_{cool}$ are the control variables with the least cross-coupling between them. It is then straight forward to implement decentralized control with two PID controllers without the need for decoupling matrices. Figure 5 shows a possible control structure, where PID 1 controls the reactor temperature around the first inlet port by manipulating the feed temperature $T_{feed}$. PID 2 controls the reactor temperature around the second inlet port by manipulating the inlet cooling temperature $T_{cool}$. A similar control structure was used in (Luyben, 2001). The PID controllers send reference signals to local feedback controllers in each sub system, the heat exchanger for pre-heating and the cooling system. The temperature references to each PID may come from the initial process optimization in Eq. 2. If some other combination would have been used, e.g. $u_B$ and $T_{cool}$, there would have been more cross-couplings and decoupling matrices may be necessary. So a wise choice of control variables leads to a simplified controller.

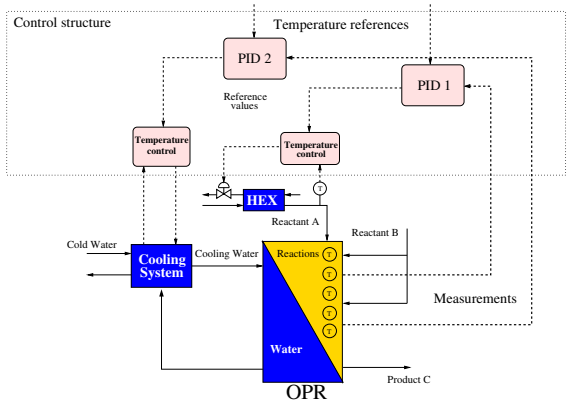


**Fig. 5** Control structure for the OPR, with two PID regulators controlling the reactor temperature. They send reference signals to local feedback controllers for the cooling system and the feed temperature using a cascade structure.

To increase control flexibility, the feed distribution $u_B$ may also be used as a third control variable. However, it is non-trivial how to best extend the control structure to incorporate additional control variables in Figure 5. One alternative is to use $u_B$ to mid-range $T_{feed}$ around some level to reduce unnecessary pre-heating. Another is to use $c_{feed}$ to mid-range $T_{cool}$, so that there is always some margin in $T_{cool}$ to its lower boundary $T_{cool,min}$. It is then possible to use a higher $c_{feed}$, thus increasing the production, if the heat release is less than predicted.

*Additional inlet ports and cooling zones* How should the control system be structured when additional actuators are used? In Figure 3, eight inlet ports and two cooling zones were used resulting in seven local temperature maxima. In a first approach we assume there are three inlet ports and two cooling zones with the inlet temperatures $T_{cool,1}$ and $T_{cool,2}$. This leads to three separate temperature maxima. The second cooling zone improves the conversion by allowing more

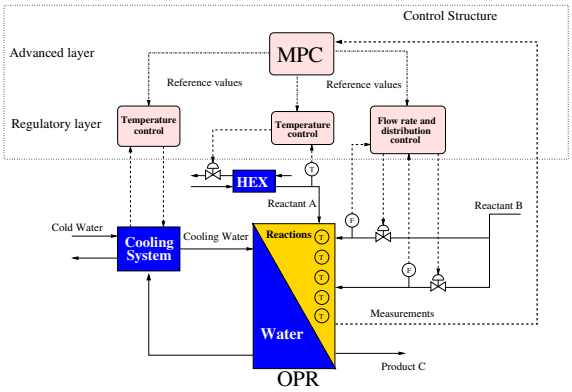


**Fig. 6** Control structure for the OPR with a multivariable MPC. It sends reference signals to local feedback controllers as in a cascade control.

flexible cooling after the final inlet point. It is still possible to control the reactor temperature with $T_{feed}$ and $T_{cool,1}$, but then only two of the maxima can be controlled independently. This may lead to suboptimal performance.

If a third control variable is added, e.g. the reactant feed distribution $u_B$, all three maxima can be independently controlled with feedback. However, there will now be increased cross-couplings between the control variables and the best pairing will be when $T_{feed}$ controls the first, $u_B$ the second and $T_{cool,1}$ the third temperature maximum. The RGA matrix for this pairing is evaluated for $\omega = 0.1$ rad/s and becomes

$$\begin{bmatrix} 0.98+0.02i & 0.04-0.03i & -0.013+0.01i \\ 0.03-0.03i & 0.69+0.00i & 0.28+0.03i \\ -0.01+0.01i & 0.27+0.02i & 0.74-0.037i \end{bmatrix}$$

The RGA number for this pairing at $\omega = 0.1$ rad/s is around 1.3 compared with 0.036 for the case with only two inlet ports and one cooling zone. Note that the main cross-couplings are between $u_B$ and $T_{cool,1}$ as their influence on the reactor is more distributed than $T_{feed}$, which only affects the inlet properties.

A high RGA number indicates that decoupling may be necessary. Therefore, a process design with more actuators to improve the steady-state performance, may also require a more complex controller to achieve the same level of feedback control.

With decoupling matrices, PID controllers may still be able to control the reactor temperature. However, when the temperature constraints are critical and the cross-coupling between the control variables are significant, a multivariable MPC controller may be used, see Figure 6. It is then possible to operate the process closer to the temperature constraints, thus improving the conversion. With a multivariable controller it is also easier to incorporate additional control variables, as more actuators are used in the process design.

## 7. SUMMARY & CONCLUSIONS

The Open Plate reactor is a very flexible process, where the numerous inlet ports and cooling zones are used to accurately control the reactor temperature to improve performance. The process design is often based on optimization of the steady-state performance. For two inlet ports and one cooling zone, it is possible to control the OPR quite easily with two decentralized PID-controllers with a proper choice of control variables.

The performance of the OPR can be significantly improved by including additional inlet ports and cooling zones, so the capacity of the reactor is better utilized. It is non-trivial how to best use these additional degrees of freedom in the feedback control, to be able to compensate for disturbances and model uncertainties. With more actuators it is inevitable that there will be more cross-coupling between the additional control variables.

By using model-based decoupling matrices, PID controllers can still be used. However, when the temperature constraints are critical and the cross-coupling between the control variables are significant, a multivariable MPC controller may be used. With a multivariable controller it is also easier to incorporate additional control variables, as more actuators are used in the process design. MPC has already been used to optimize conversion in the case with two inlet ports and one cooling zone, (Haugwitz *et al.*, 2006). The next step may be to develop routines how to incorporate additional control objectives, such as optimizing the total production.

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