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| Research Article

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Formation of a Discrete Model Mass-Transfer Processes at Distillation Plants

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Abstract: The article addresses the problem of optimizing mass transfer processes within a multi-input, multi-output (MIMO) automatic control system. To improve control accuracy and robustness to external disturbances, a Model Predictive Control (MPC) method is applied. The proposed MPC strategy accounts for the interdependence between control and output variables as well as technological constraints. Numerical simulation results demonstrate enhanced control efficiency compared to traditional methods, including improved control quality, reduced energy consumption, and increased system stability. The findings confirm the feasibility and effectiveness of predictive control in dynamic mass transfer process management.

Keywords: mass transfer, automatic control, MIMO system, predictive control, MPC, optimization, robustness.

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Introduction

Automation of mass transfer processes, such as distillation, is a key challenge in the chemical engineering industry. Modern industrial installations are characterized by a high degree of interrelationship between variables and complex dynamics, requiring the use of advanced control methods. Several authors [1–3] note that classical PID control methods do not provide sufficient efficiency in multi-input, multi-output (MIMO) systems with constraints and interconnected channels.

In recent decades, the management approach based on a predictive model has been actively developing (Model Predictive Control (MPC), which allows one to take into account constraints on inputs and outputs, as well as predict the behavior of a system based on its model [4, 5]. According to studies [6–8], MPC demonstrates high efficiency in controlling dynamic processes, especially in the presence of external disturbances and strong relationships between variables.

Of particular interest is the application of MPC to control of distillation columns, where stability and energy efficiency are critical. Several studies [9, 10] have shown that the implementation of MPC not only improves control accuracy but also reduces energy costs and operational risks.

Methodology and materials.

The proposed approach takes into account interconnected process variables, physicochemical constraints, and a dynamic plant model described by a system of differential equations. The MPC strategy implements online optimization of control actions using a system behavior prediction based on the identified model. Analysis and modeling based on a specific mass exchange process (e.g., an absorption column) demonstrate that the developed controller provides improved control quality, robustness to external disturbances, and adherence to process constraints compared to traditional methods (e.g., PID and LQR).

Mathematical formulation of the MPC problem, a discrete model of mass dynamics of the exchange process is considered in the form:

$$x_{k+1} = A_{xk} + B_{uk}$$

$$y_k = C_{xk} + D_{uk}$$

Where:

$x_k \in R^n$ is the vector of system states (concentrations of components),

$u_k \in R^m$ - vector of control actions (reactant consumption),

$y_k \in R^p$ is the vector of output variables (output concentrations),

A,B,C,D are matrices describing the dynamics of the MIMO system.

MPC minimizes the control functional over the prediction horizon N:

$$J = \sum_{i=0}^{N-1} [(y_{k+i|k} - y_{ref})^T Q (y_{k+i|k} - y_{ref}) + \Delta u_{k+i}^T R \Delta u_{k+i}]$$

Where:

y_{ref} - vector of given values (goals),

$Q \geq 0$, $R > 0$ R - matrices of weights for errors and control efforts,

$\Delta u_{k+i} = u_{k+i} - u_{k+i-1}$ is the increment of the control signal.

State restrictions:

$x_{min} \leq x_{k+i} \leq x_{max}$

Limitations on control actions:

$u_{min} \leq u_{k+I} \leq u_{max}$

Limitations on the speed of control change:

$\Delta u_{min} \leq \Delta u_{k+i} \leq \Delta u_{max}$

At each step k, MPC solves the optimization problem:

$$\min_{\{u_k, u_{k+1}, \ldots, u_{k+N-1}\}} J$$

subject to dynamic equations and all constraints.

The solution to the problem yields an optimal sequence of control actions

$\{u_{k}^*, u_{k+1}^*, \ldots\}$, of which only the first value u_k^* u is used in practice. The cycle then repeats at the next step with updated measurements.

What do the matrices *A, B, C, D* mean in the context of a MIMO system (Multi-Input Multi-Output) and mass transfer processes.

For dynamic systems (including mass transfer processes, such as absorption and distillation columns), a linear model in state space is often used:

$x_{k+1} = Ax_k + Bu_{kx}$

$y_k = Cx_k + Du_k$

This model describes how the internal parameters of the system (state) change under the influence of control actions, and what we observe at the output.

What do the matrices mean:

1. Matrix *A* is the matrix of state dynamics

Size: $n \times n$. Describes how the current state affects the next one, how the current concentration in the column trays affects the concentrations after a time step.

2. Matrix *B* is the input (control) matrix

Size: $n \times m$. Shows how control actions affect changes in state; changes in solvent flow rate affect concentrations in the system.

3. Matrix *C* is the matrix of observed outputs

Size: $p \times n$. Determines which states we measure as outputs; we only measure the concentration at the column outlet, not at each stage.

4. Matrix *D* - direct transfer of input to output

Size: $p \times m$. Takes into account the influence of the input directly on the output (in the same time step), without accumulation across states.

In many physical systems, *D* often = 0 if there is no instantaneous communication.

Let's imagine a column with 3 plates, in which:

x - concentrations on plates (states),

u - solvent supply (control),

y is the concentration at the outlet (measured output).

Then: *A*: describes how the concentrations on the plates influence each other over a single time step; *B*: shows how changing the solvent feed affects the concentrations on each plate; *C*: shows that we are measuring the concentration on the last plate only (e.g. product yield); *D*: most likely 0 - there is no instantaneous effect of solvent flow on yield.

These matrices define the system's behavior and are used in the MPC predictive model. They can be obtained from physical equations (mass transfer, energy, and substance balances) or through model identification (e.g., through experiments and identification methods such as subspace ID or least squares).

Physical equations that underlie mass transfer process modeling - this is especially important when constructing the *A*, *B*, *C*, and *D* matrices for the MPC controller. Classical material balance equations, which are most often used when developing models for processes such as absorption, distillation, extraction, and others, are also used.

A simple discrete model of an absorption column with *N* plates in which component A is removed from the gas phase to the liquid phase.

Designations:

x_i is the concentration of *A* in the liquid on plate *i*,

y_i is the concentration of A in the gas on plate i,

L, G - liquid and gas flow rates (assumed constant),

V is the volume of each stage,

k_y ,a - mass transfer coefficient and specific surface area,

y_i^* is the equilibrium concentration of gas corresponding to x_i : $y_i^* = f(x_i)$

Dynamic equation for the i-th stage:

For liquid (mass balance):

$$V\frac{\partial x_i}{\partial t} = L(x_{i+1} - x_i) + k_y a(y_i - y_i^*)$$

For gas:

$$V\frac{\partial y_i}{\partial t} = G(y_{i-1} - y_i) + k_y a(y_i - y_i^*)$$

These equations describe the time evolution of component concentrations at each stage depending on flows and mass transfer.

Linearization and transition to matrix form (A, B, C, D)

If the equations are nonlinear ($y_i^* = f(x_i)$ according to Henry's law), they can be linearized around the operating point:

$$\frac{\partial x}{\partial t} = Ax + Bu$$

$$y = Cx + Du$$

Where:

x is the vector of concentrations at the steps,

u is the vector of control actions (solvent consumption L),

y is the output concentration (in the liquid at the last stage).

Matrices A and B are formed on the basis of partial derivatives from linearized equations:

$$Ax = \left.\frac{\partial f}{\partial x}\right|_{x_0,u_0}, B = \left.\frac{\partial f}{\partial u}\right|_{x_0,u_0}$$

We derive physical equations for the object. We linearize them around the operating point. We discretize the equations (for example, using Euler's method).

We form a discrete model in the form:

$$x_{k+1} = Ax_k + Bu_k$$
$$y_k = Cx_k$$

We use it in the MPC controller. Let: x: concentration in the liquid, u: solvent flow rate,

Balance equation: $\frac{\partial x}{\partial t} = -k(x - x^*) + \alpha u$,

When linearized: $A=-k$, $B=\alpha$

After discretization:

$$x_{k+1} = (1 - k\Delta t)x_k + \alpha\Delta t \cdot u_k$$

Results and discussion. Key differences between MPC and classical control methods.

Criterion	Classical control (PID)	Predictive control (MPC)
Accounting for the object model	Not required (or used indirectly)	Requires an exact or approximate model
Predicting the future	Absent	Executed at each step (prediction horizon)
Taking into account restrictions	Not taken into account or implemented externally	They are taken into account directly in the optimization problem
Support for MIMO systems	Limited , often requires decomposition	Supported directly in a single task
Adaptation to dynamics	Poorly adaptive , manual settings	Flexible , easily adaptable to different dynamics
Response speed and accuracy	Depends on the setting, not optimal	As close to optimal as possible
Energy consumption	Often higher due to overshoot	Lower due to optimal resource allocation

Conclusions

MPC is a more flexible and powerful approach than classical methods, especially in complex dynamic systems with multiple interrelated variables and constraints. Its application is particularly suitable for technological processes such as distillation, where high precision, reliability, and energy efficiency are required .

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