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Optimal operation of a divided-wall column with local operating condition changes

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Abstract. The aim of this paper is optimal operation of a Divided-Wall Column (DWC) based on Self-Optimizing Control (SOC). By now, the proposed SOC methods have been based on linearization of the process. The novelty of this paper is to overcome this shortcoming of the local optimality of SOC. Theoretically, changes in optimal sensitivity matrix from nominal design, due to changes in the operating condition, make SOC deviate from steady state optimality. These deviations from optimal operation, in already available SOC structures, have to be counteracted by the optimization layer in the control structure hierarchy which involves solving a large nonlinear optimization problem online. The proposed method in this paper solves this problem by modeling the optimal sensitivity matrix with Takagi-Sugeno fuzzy inference. This fuzzy inference system is tuned offline. The proposed method is dynamically validated and compared with conventional SOC. The results showed that the conventional SOC had a high value of loss and deviated from the optimal operation. However, in the same operating condition, the proposed method with the aid of Takagi-Sugeno fuzzy inference system, which involves online calculation of the weighted average of some linear functions, imposed a small loss, made DWC track an optimal trajectory, and removed the need for solving the large nonlinear optimization problem online.

1. Introduction

Optimal operation of the plants has a growing demand nowadays. The price of energy, environmental regulations and competitions make the process plants operate as close as possible to the optimal operation. Generally, steady state operation takes the largest amount of operating cost. So, noticeable economic benefits can be achieved by optimal steady state operation [1]. A control structure that yields nice transient responses and tight control by keeping the selected controlled variables at their specified setpoints may be useless if it provides a non-economical steady state performance. Moreover, operation at a pre-designed nominally optimal point may not necessarily be actually optimal, due to real-time disturbances, measurement errors, and uncertainties.

On the other hand, process intensification makes new processes with more complex multivariable systems which require a suitable control structure for the expected operating condition. The Divided-Wall Column (DWC) is an important example of process intensification [2]. It is an implementation of the topology of fully thermally coupled Petlyuk column [3], as shown in Figure 1. DWC can reduce up to 30% in the capital invested and up to 40% in the energy costs [4]. Reduced mixing loss via reduction in remixing effect, which happens usually in conventional distillation trains, can make considerable savings [5, 6]. The value of saving is dependent on feed composition,

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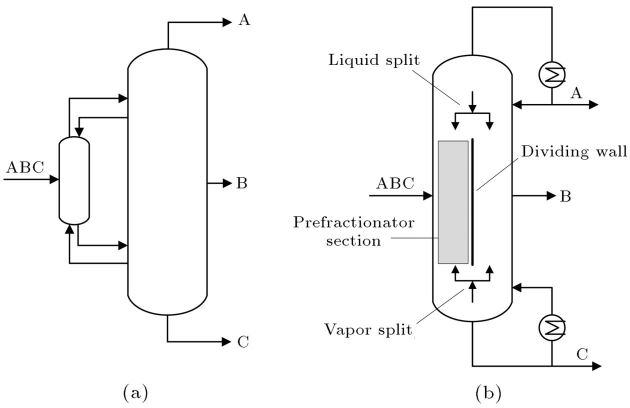

Figure 1. Separation of ternary mixture with (a) Petlyuk configuration, and (b) divided-wall column.

relative volatility, and product purity specification and can be higher in the case of separation of mixtures with more components [7]. In this way, DWC overcomes the usual problem of trade-off between the operation cost and the investment costs when reducing operating cost at the expense of higher investment costs [8]. Also, DWC reduces space requirements by 40% compared to the conventional distillation columns [9].

However, in spite of all these clear advantages, the practical use of DWC at industrial scale is still limited to only a few companies [10], because DWCs have the coupling effect of various phenomena such as mass and energy flows of vapor and liquid which meet above and below the wall and transfer heat across the dividing wall [11]. It makes DWC a comparatively complex multivariable system [12], and understanding its operability and controllability is still a growing matter [4]. Moreover, real-time disturbances in a DWC with fixed vapor and liquid split fraction may move the system to a region where the solution to the optimization problem (optimum operation) is located on a sharp peak (sharp optimum) and the system may be unstable or at least unable to obtain reasonable energy saving [13]. Thus, it seems difficult to achieve the potential energy savings in a DWC without a good control strategy compared to conventional approaches. Control structure design generally classifies problems into two classes. In the first class, all the optimization degrees of freedom are used to satisfy active constraints for all expected disturbances at the optimal solution, while in the second class, which is the focus of this work, one or more optimization degrees of freedom are unconstrained. In the second type of problem, choosing the Controlled Variable (CV) is a very important step in the control structure design in order to obtain optimal operation in practice. Traditionally, controlled variables have been selected based on intuition and process knowledge. Skogestad [14] presented a method for selecting Self-Optimizing Controlled (SOC) variable in the form of some function of the measured variables in such a way that keeps this controlled variable constant, or slowly varying, making the process operate close to economically optimal steady state operation in the presence of disturbances and implementation errors.

In other words, SOC structure design aims to remove or at least decrease the need for solving a nonlinear optimization problem online by converting the optimization problem into a feedback problem. By now, SOC design has been based on linearization of the process model around the nominal operating point. The first approach for SOC design was the maximum gain rule [15] with local consideration of process model. Halvorsen et al. [16] presented the exact local method with the worst-case loss based on the linear model around the nominal operating point and quadratic expansion of the objective function which leads to nonlinear optimization problem. This work was reformulated as a quadratic optimization problem with linear constraints by Alstad et al. [17] which is easier to solve numerically; also, Yelchuru and Skogestad [18] proposed a simpler and more practical calculation. For local linear combination of measurements, Kariwala et al. [19] proposed another method and minimized average loss for local SOC. Alstad and Skogestad [20] devised null space method wherein combination matrix was located in the left null space of local optimal sensitivity matrix. However, null space method holds its optimality for small deviations from the nominal optimum (small magnitude of the disturbance) and is globally optimum in cases wherein the optimal sensitivity matrix, $\mathbf{F}$, is not dependent on the operating point (disturbances) or, in other words, for a system with a quadratic cost objective function and linear model equations [20].

So, in a complex multivariable process with varying operating conditions, the local consideration of process makes SOC design deviate from nominal optimal steady-state operation. This could be counteracted with solving a nonlinear optimization online in optimization layer which is located above the SOC in control structure hierarchy. But, this causes the main role of SOC in removing or decreasing the need for solving large nonlinear optimization problem online become violated. Moreover, this deviation from local optimal design becomes more severe in a more complex multivariable system such as DWC.

With the local consideration of DWC, Arjomand and Fanaei [21] designed a SOC structure with the maximum gain rule [15] which was based on the conventional individual measurement. In the other work, Arjomand and Fanaei [1] developed a SOC structure with the exact local method [16] and it was shown that it was possible to have better self-optimizing properties by controlling linear combinations of measurements than by controlling conventional individual measurements in control structure of a DWC. However, the proposed SOC structure of Arjomand and Fanaei [1] for DWC has the weakness of local optimality problem. The current work presents a novel method for solving the shortcoming of local optimality of SOC through modelling $\mathbf{F}$ with Takagi-Sugeno (T-S) fuzzy inference system in the null space method [20]. In other words, our main concern in this paper is to extend the self-optimizing property of the control structure for a DWC to large variation in operating condition where optimal sensitivity matrix changes from nominal design.

The T-S fuzzy model can represent nonlinear system by decomposing the whole input space into several fuzzy sets and representing each output space with a linear equation. Such a model is capable of approximating a wide class of nonlinear systems. For the reason that it employs linear model in the consequent part, conventional linear system theory can be applied for system analysis and synthesis accordingly. And hence, the T-S fuzzy models are becoming powerful engineering tools for modelling and control of complex systems.

This paper is organized as follows. The next section describes mathematical formulation of null space method and the basics of T-S fuzzy inference system. Section 3 will review the general structure of a plantwide multilayer control structure and will present the proposed multilayer control structure with fuzzy system. Section 4 will design control structure for the studied DWC which is followed by results and discussions in Section 5 and, finally, conclusion in Section 6.

2. Preliminaries

2.1. Mathematical formulation

To quantify "acceptable operation" or close to optimal steady state operation, a scalar cost function J is considered which should be minimized for optimal operation. The (economic) cost mainly depends on the steady-state behavior, which is a good assumption for most continuous plants in the process industry.

Generally, the original independent variable $\mathbf{u}_0$ is divided into the constrained variable $\mathbf{u}'$ which is used to satisfy active constraints $f'(\mathbf{x},\mathbf{u},\mathbf{d}) = 0$ and the remaining unconstrained variable $\mathbf{u}(\mathbf{u}_0 = \{\mathbf{u}',\mathbf{u}\})$. It is assumed that any optimally "active constraint" has been implemented so that $\mathbf{u}_0$ includes only the remaining unconstrained steady-state degrees of freedom. Finally, the objective is to achieve optimal steady-state operation, where the degrees of freedom $\mathbf{u}$ are selected such that the scalar cost function $J(\mathbf{u},\mathbf{d})$ is minimized in the "reduced space" optimization problem with respect to the unconstraint degrees of freedom for any expected disturbance $\mathbf{d}$ by solving the following problem.

$$\min_{x,u} J(\mathbf{x},\mathbf{u},\mathbf{d}),$$

Subject to:

$$f(\mathbf{x},\mathbf{u},\mathbf{d}) = 0,$$

$$g(\mathbf{x},\mathbf{u},\mathbf{d}) \leq 0,$$

$$\mathbf{x} \in R^{n_x},\ \mathbf{u} \in R^{n_u}, \mathbf{d} \in R^{n_d}, \tag{1}$$

where $\mathbf{x}$, $\mathbf{u}$, and $\mathbf{d}$ are the states, inputs, and disturbances, respectively; f is the set of equality constraints corresponding to the model equation; g is the set of inequality constraints that limits the operation. The objective of SOC is to find an optimal measurement combination:

$$\mathbf{c} = \mathbf{H}\mathbf{y}, \tag{2}$$

such that a constant setpoint, $\mathbf{c}_s$, policy, in which $\mathbf{u}$ is adjusted to keep $\mathbf{c}$ constant on $\mathbf{c}_s$, yields near optimal operation in accordance with Eq. (1) where:

$$\mathbf{c}_s = \mathbf{H}\mathbf{y}^{\text{opt}}. \tag{3}$$

To quantify the difference between alternative choices of $\mathbf{c}$, the loss is defined as the difference between the actual cost and the optimal cost:

$$L = J(\mathbf{u},\mathbf{d}) - J(\mathbf{u}^{\text{opt}},\mathbf{d}), \tag{4}$$

where for a given $\mathbf{d}$, solving Eq. (1) gives $\mathbf{u}^{\text{opt}}(\mathbf{d})$. In the reduced space after implementing active constraints and elimination of the states using model equation:

$$\mathbf{y} = f_y(\mathbf{u},\mathbf{d}), \tag{5}$$

and in a local linearized model around nominal operating point (*), the measured variables are:

$$\mathbf{y} = \mathbf{G}^y\mathbf{u} - \mathbf{G}_d^y\mathbf{d}, \tag{6}$$

where $\mathbf{G}^y = \left(\frac{\partial f_y}{\partial \mathbf{u}}\right)^{*T}$ and $\mathbf{G}_d^y = \left(\frac{\partial f_y}{\partial \mathbf{d}}\right)^{*T}$. The controlled variable $\mathbf{c}$ is the selected function of $\mathbf{y}$:

$$\mathbf{c} = h(y), \tag{7}$$

where the function h is free to choose. By substituting Eq. (5) into Eq. (7) the following equation is obtained:

$$\mathbf{c} = h\left[f_y(\mathbf{u},\mathbf{d})\right] = f_c(\mathbf{u},\mathbf{d}). \tag{8}$$

And the linearized model in the reduced space is expressed as follows:

$$\mathbf{c} = \mathbf{G}\mathbf{u} - \mathbf{G}_d\mathbf{d}, \tag{9}$$

where $\mathbf{G} = \left(\frac{\partial f_c}{\partial \mathbf{u}}\right)^{*T}$ and $\mathbf{G}_d = \left(\frac{\partial f_c}{\partial \mathbf{d}}\right)^{*T}$.

2.2. Null space

The null space method [20] deals with the optimal selection of linear measurement combinations as the controlled variables, $\mathbf{c} = \mathbf{Hy}$, for quadratic approximation of Eq. (1) with the second-order Taylor expansion of the cost function $J(\mathbf{u}, \mathbf{d})$:

$$\min \begin{bmatrix} \mathbf{u} \\ \mathbf{d} \end{bmatrix}^T \begin{bmatrix} \mathbf{J_{uu}} & \mathbf{J_{ud}} \\ \mathbf{J_{du}} & \mathbf{J_{dd}} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{D} \end{bmatrix}, \tag{10}$$

where $\mathbf{J_{uu}} = \frac{\partial^2 J}{\partial \mathbf{u}^2}$, $\mathbf{J_{ud}} = \mathbf{J_{du}^T} = \frac{\partial^2 J}{\partial \mathbf{u} \partial \mathbf{d}}$, and $\mathbf{J_{dd}} = \frac{\partial^2 J}{\partial \mathbf{d}^2}$.

Considering that n_u is the number of independent unconstrained free variable $\mathbf{u}$, n_d is the number of independent disturbance $\mathbf{d}$, and n_y is the number of measurement $\mathbf{y}$. If $n_y \geq n_u + n_d$, it is possible with the null space method [20] to select combination matrix $\mathbf{H}$ in the left null space of $\mathbf{F}$, or:

$$\mathbf{H} = \text{null}(\mathbf{F}^T), \tag{11}$$

such that its optimal value is independent of $\mathbf{d}$ where $\mathbf{F}$ is optimal sensitivity matrix evaluated with the following definition:

$$\mathbf{F} = \frac{\partial \mathbf{y}^{\text{opt}}}{\partial \mathbf{d}^T}. \tag{12}$$

Also $\mathbf{F}$ could be calculated from linearized local model [17]:

$$\mathbf{F} = -\left(\mathbf{G}^y \mathbf{J}_{\mathbf{uu}}^{-1} \mathbf{J_{ud}} - \mathbf{G}_{\mathbf{d}}^y\right). \tag{13}$$

With this choice for $\mathbf{H}$, fixing $\mathbf{c}$ (at its nominal optimal value) will lead to zero loss as long as $\mathbf{F}$ does not change [20].

The optimal sensitivity matrix, $\mathbf{F}$, may be computed from Eq. (13). However, in practice, it is usually easier to obtain $\mathbf{F}$, numerically. In other words, for practical use, it is more reliable to obtain $\mathbf{F}$, numerically, from its definition in Eq. (12), instead of deriving an analytical expression from Eq. (13) [18]. Moreover, providing analytical expression of $\mathbf{F}$ for the entire operation space in a complex of nonlinear chemical plants from explicit representation of the model equations is even a more difficult problem to be solved, but is readily to be solved numerically through fuzzy modelling.

2.3. Takagi-Sugeno fuzzy inference system

Fuzzy sets are characterized by membership functions or degree of truth of v in $\mathbf{A}$ that map R to the membership space:

$$\mathbf{A} = \{(v, \mu(v)) \,|v \in R\}. \tag{14}$$

The membership function is described by an arbitrary curve suitable from the point of view of simplicity, convenience, speed, and efficiency. When the membership space contains only 0 and 1, $\mathbf{A}$ is nonfuzzy and μ is a characteristic function of non-fuzzy set. The range of the membership functions is a subset of the nonnegative real numbers. In this paper, Gaussian membership functions is regarded as follows:

$$\mu(v) = \exp\left[-\frac{1}{2}\left(\frac{v-\alpha}{\sigma}\right)\right], \tag{15}$$

where α is the center of the membership function and σ is a constant related to the spread of membership function.

Structure of a Takagi-Sugeno fuzzy inference system is shown in Figure 2. It is a model that maps characteristics of input data to input membership functions, input membership functions to rules, rules to output crisp functions, and output crisp functions to a single-valued output [22]. Generally, the process of formulating the mapping from a given input to an output using fuzzy logic is called the fuzzy inference.

In T-S fuzzy systems, the relationships between variables are represented by the means of fuzzy if-then rules as follows:

$$\text{Rule}_i: \text{ If } v_1 \text{ is } \mathbf{A}_i^1 \text{ and } v_2 \text{ is } \mathbf{A}_i^2 \ \ldots\ v_n \text{ is } \mathbf{A}_i^n$$

$$\text{Then } \ z_i = \xi_i(v_1, v_2, ..., v_n), \tag{16}$$

where $\mathbf{v} = [v_1, v_2, ..., v_n]^T$ is the vector of input

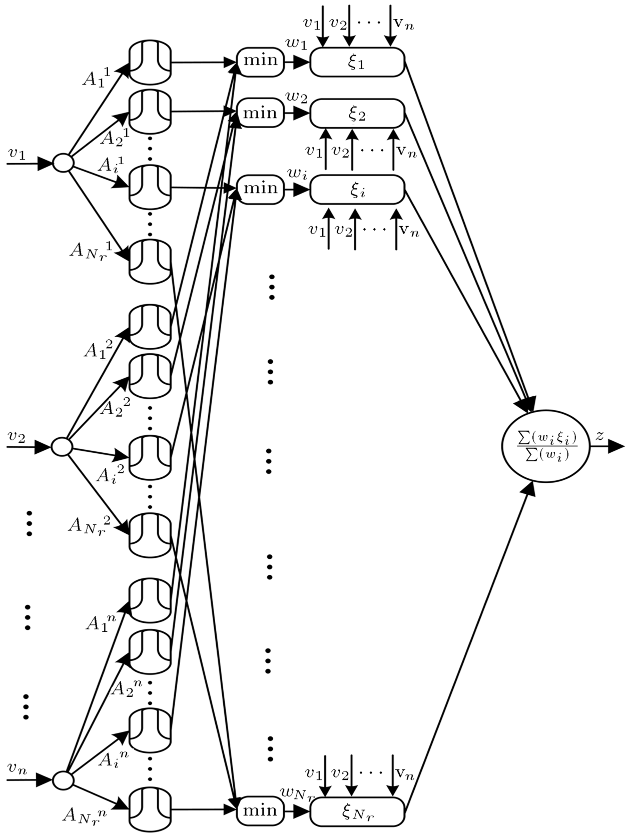

Figure 2. Structure of T-S fuzzy model.

variables, $\mathbf{A}_i^j (1 \leq j \leq n)$ represents fuzzy set, z_i is the output of rule i, and ξ_i is a crisp function of rule i. In the first-order sugeno model, a linear combination of input variables is considered as the consequent crisp function as follows:

$$\xi_i (v_1, v_2, ..., v_n) = b_i^0 + b_i^1 v_1 + b_i^2 v_2 + ... + b_i^n v_n. \quad (17)$$

As such, each rule can be considered as a local linear model that will fuse with others to produce an overall nonlinear output z. Given the input vector $\mathbf{v} = [v_1, v_2, ..., v_n]^{\mathbf{T}}$, the model output z is the weighted average of the individual rule outputs $z_i (1 \leq i \leq N_r)$ according to the following formula:

$$z = \frac{\sum_{i=1}^{N_r} w_i z_i}{\sum_{i=1}^{N_r} w_i}, \quad (18)$$

where N_r is the number of rules, and w_i is the firing strength of rule i calculated as follows:

$$w_i = \mathbf{\Pi}_{j=1}^{n} \mu_i^j (v_j), \quad (19)$$

where Π denotes the fuzzy MIN operator and μ_i^j is the membership function corresponding to fuzzy set $\mathbf{A}_i^j$.

2.3.1. Parameter tuning

One of the most successful fuzzy system identification methodologies within the realm of soft computing is genetic fuzzy system where Genetic Algorithm (GA) is considered to learn the components of a fuzzy rule-based system [23]. A genetic fuzzy system is basically a fuzzy system augmented by a learning process based on a GA and has been coined by a hybridization between GA and fuzzy rule-based system [24]. Genetic learning processes can cover different levels of complexity according to the structural changes produced by the algorithm, from parameter optimization to the highest level of complexity of learning the rule set of a rule-based system [25]. Owing to the fact that T-S type fuzzy system has a linear consequent part, using the least square with GA has also combined the advantages of both algorithms to enhance its search capability; also, the optima can be located more quickly [26].

The T-S fuzzy system parameters are automatically tuned from numerical information (input-output data sets from nonlinear model). An input variable is changed instantly and, at the same time, the behavior of the output variables is collected. Then, the same procedure is performed for the other input variables and finally a data set for identification of the fuzzy models is obtained by offline calculation in nonlinear model. Subsequently, the identification data set is divided into training data set and test data set with random method [22]. The training data set is used for tuning model parameters and these models are then validated through the test data.

In brief, the GA starts with a community of chromosomes known as the initial population. In contrast with classical algorithm which generates a single point at each iteration, GA generates a population of points at each iteration. Then, the chromosomes are passed to the objective function. As the aim is to minimize the error between the output of fuzzy model and output data, the Mean of Squared Error (MSE) is used as evaluation function.

Among the chromosomes in the population, some of them will be arbitrarily selected. This selection component in the GA guides the algorithm to the solution. One approach used in this work, to guide the selection procedure, is stochastic uniform selection function. This reproduction population will then be mated through crossover component. Crossover is the process of creating one or more offsprings from the current population. In this work, arithmetic crossover is used. The last component of GA is mutation. Mutation rules apply random changes to individual to form the next generation. This process is performed to prevent the algorithm from sticking at local minimum by introducing traits not existing in the original population. Gaussian mutation is applied in this work. The so called selection, crossover, and mutation are the three main types of rules at each step to create the next generation from current population. In this work, we use MATLAB software to implement genetic algorithm. For more information about genetic algorithm one can refer to MATLAB software user's guide.

Also, the coefficients of the crisp linear functions are constructed with least square estimation method and are dependent on the values of the membership functions in the antecedent part. So, this is quite different from linear model identification wherein the coefficients of the model can be directly calculated from the input variable values. Therefore, in using the least square method, at first, the equations of the output are rearranged to comply with the least square equation as in Appendix A, and the coefficients of the linear equations of fuzzy model can be identified indirectly from the values of input variables and the membership for each rule. The parameter tuning algorithm can be summarized as follows:

1. Generate random initial population;
2. Evaluate objective function for every chromosome.
   - (2-i) Use least square method to define the parameter of linear equations by the desired membership functions parameters;
   - (2-ii) Calculate MSE for every chromosome.
3. Perform selection, crossover, and mutation operation to produce new population;
4. Repeat steps 2 and 3 for a certain number of

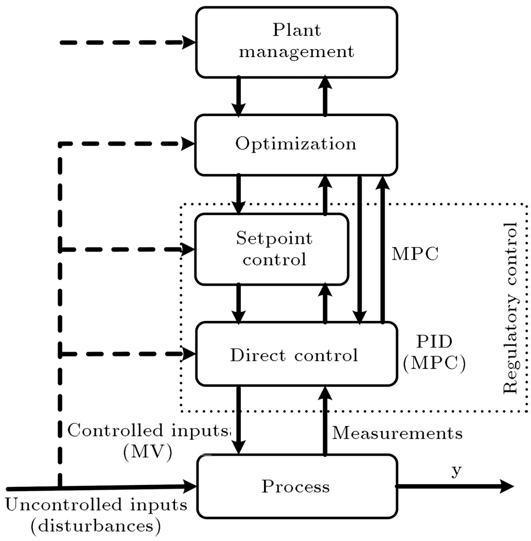

Figure 3. General multilayer control structure [27].

generations to get the best individual which will represent the best fuzzy model.

3. Multilayer control structure

In a complex real chemical plant, a straightforward task of designing and implementing a single centralized control unit is too difficult and, in many cases of complex multivariable processes, is just impossible. Hierarchical multilayer control structure is a solution in such complex situations [27]. The main idea is to decompose the original control task into a sequence of simpler and hierarchically structured subtasks that are handled by dedicated control layers, as shown in Figure 3.

The direct control layer is responsible for safety of dynamic processes in the plant. The main feature of all direct (basic) controllers is direct access to the controlled process (process manipulated variables are outputs of the direct controllers). Algorithms of direct control should be robust and relatively easy, in structure and design method, that is why classic Proportional-Integral-Derivative (PID) algorithms are still dominant. However, rapid development of computer technology made it now possible to apply Model Predictive Control (MPC) also for direct control, when improved control performance is required and cannot be achieved with PIDs [28].

The setpoint control layer keeps high quality of operation. This layer usually does not fully separate the direct control layer from the optimization layer, and some of the setpoints for basic controllers can be assigned and directly transmitted from the optimization layer, as can be seen in Figure 3.

The real process operation is always under uncertainty. A process plant is not isolated from its environment and it undergoes controlled and uncontrolled external influences. One source of the uncertainty is the behavior of disturbances (uncontrolled process inputs). Usually, some parts of these variables are measured or estimated and some others are not. Optimal values of the setpoints are dependent on these disturbance values and vary when their values vary. The optimal operating point is calculated for current values of disturbances, and recalculated after significant changes in these values [27].

Uncertainty makes a single optimization layer usually lead to solutions being only suboptimal setpoints for the real process, with the degree of suboptimality dependent on the level of uncertainty. Therefore, a setpoint optimization at the optimization layer is defined to obtain optimal setpoints of feedback controllers, for current measurements or estimates of the disturbances taken into account in the model which are additionally marked with dashed lines in Figure 3. It performs economic optimization related to the controlled process, which is usually a part of a larger complex plant. The goal is to calculate the process optimal operating point or optimal operating trajectory, i.e. optimal steady-state values of setpoints for current values of disturbance measurements or estimates to be applied for feedback controllers of directly subordinate layers (regulatory layer). So, with decomposing the original centralized control task into a sequence of simpler and hierarchically structured subtasks and assigning a specific task to each layer, which includes feedback information, it copes with the various uncertainties.

3.1. Fuzzy system in multilayer control structure

If a disturbance moves the process far from the nominal point, the local model approximation used for the calculation of self-optimizing CVs by linearization of the nominal operating point and assumption of the quadratic cost function (or approximation of the objective function by the second order Taylor series) may be poor. Therefore, the self-optimizing control task in providing near optimal operation in the case of disturbances which move the process away from the nominal operating point becomes poor. This is usually counteracted by reoptimization of the process with an optimization layer which involves solving a nonlinear optimization online.

Using fuzzy model makes control structure meet changes in operating condition. Figure 4 shows the proposed control structure with fuzzy inference system. In the proposed algorithm, optimal sensitivity matrix is calculated through the T-S fuzzy inference system. The null space receives optimal sensitivity matrix from T-S fuzzy model as well as the selected measurement from plant. The self-optimizing controlled variable is controlled through a controller, which is generally a

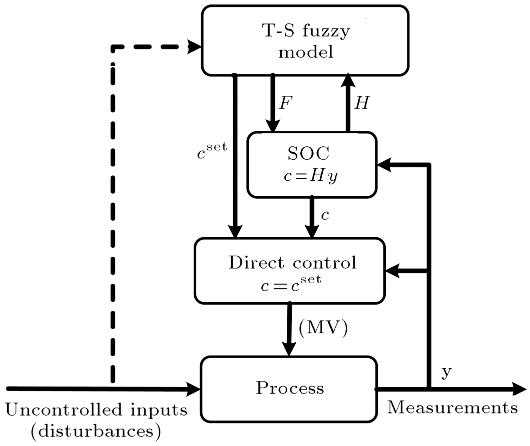

Figure 4. Multilayer control structure with T-S fuzzy inference system.

proportional-integral controller. The setpoint for this controller is calculated with Eq. (3) where $\mathbf{y}^{\mathrm{opt}}$ is, in accordance with the defining Eq. (12), as follows:

$$\mathbf{y}^{\mathrm{opt}} = \int \mathbf{F} d\mathbf{d}. \tag{20}$$

4. Design of control structure

Here, a systematic procedure for control structure design for complete process plants (plantwide control) by Skogestad [29] is followed.

4.1. Process details

In this paper, separation of 1 kmol/s mixture of benzene/toluene/o-xylene with the relative volatility of 7.1/2.2/1 is studied. The design of DWC in this paper is based on the results of optimal steady-state design of Ling and Luyben [30]. Feed enters the DWC at the temperature of 358K and with the concentration of 30/30/40 mol% B/T/X. Physical property package used for this simulation is Chao-Seader in the Aspen simulator. DWC is simulated using two absorbers, single stripper, and a rectifier column as [30,31]. There are 24 stages in prefractionation and also in sidestream section, 9 stages in rectifier section, and 13 stages in stripper section. Feed enters at stage 12 and sidestream withdraws at stage 44. Product purities are 99 mol%, condenser pressure is 0.37 atm, tray pressure drop is 0.0068 atm, and the reflux ratio is 2.85.

4.2. Definition of objective function, degrees of freedom, and optimization

The objective is to minimize reboiler energy consumption. With the constant feed flow rate and pressure, there are 7 dynamic degrees of freedom [32]. However there are two liquid level inventories that need to be controlled and since these levels have no steady-state effect, the number of degrees of freedom for steady-state optimization is 5 [33]. Three product purities are three active constraints maintained by three freedom degrees. So, two unconstrained degrees of freedom, namely vapor and liquid split fraction, are left to minimize energy. The surface plot in Figure 5 shows that how reboiler heat duty changes with these two unconstrained degrees of freedom. At optimum, vapor and liquid split fraction at the bottom and top of the wall is 0.625 and 0.353, and reboiler heat duty is 35.6 MW.

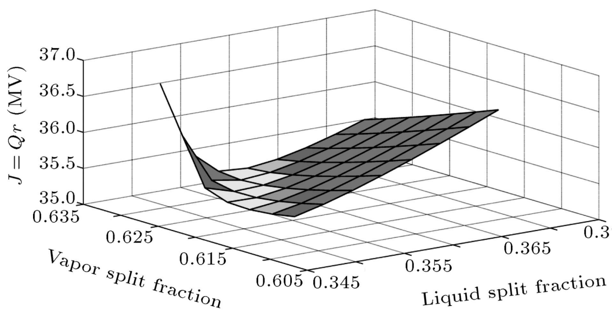

Figure 5. Surface plot for reboiler heat duty as a function of liquid and vapor split fraction.

From practical point of view, it is a more realistic case where the vapor split is not a degree of freedom [34] and it does not change later on during the operation [10]. In this paper, we also consider that the vapor split is not a degree of freedom. Therefore, there is one remaining unconstrained degree of freedom. In addition, active constraints (product composition) and also feed composition are considered as important disturbances.

4.3. Identification of measurements and selection of CVs

It is common in distillation column control to use temperature as measurement. In this work, all of the DWC stage temperatures are selected as candidate measurements. So, it has 70 individual candidate measurements (stages 1 to 24 in prefractionator, 25 to 33 in rectifier, 34 to 57 in sidestream, and 58 to 70 in stripper section).

There are 4 disturbances ($n_d = 4$) and one unconstrained degree of freedom ($n_u = 1$). Based on the null space method in Section 2.2, the minimum number of measurement is $n_y = 5$ ($n_y \geq n_u + n_d$). So, 5 stage temperature measurements must be selected among all 70 individual candidate measurements. To select these 5 stage temperatures among all 70 candidate stage temperatures, the maximum gain rule is used [15]. The maximum gain rule method selects variables with maximum gain of the appropriately scaled steady-state gain matrix $\mathbf{G}_{\mathrm{scl}}$ from inputs ($\mathbf{u}$) to the selected controlled variables ($\mathbf{c}$). It identifies candidate controlled variables that satisfy all of the following requirements [14]:

1. Optimum insensitivity to disturbances;

2. Easy to measure and control so that the implementation error is small;
3. Sensitive to changes in the manipulated variables;
4. Independent selected controlled variables (for cases with two or more controlled variables).

The key part of this procedure is scaling of each q-th input and p-th controlled variable. Each q-th candidate input is scaled with Eq. (21). By this scaling, a unit deviation in each input from its optimal value produce the same effect on the cost function [16].

$$\mathbf{u}_{\mathrm{scl},q} = \frac{1}{\sqrt{[J_{uu}]_{qq}}}. \tag{21}$$

The Hessian matrix is calculated with finite difference and is $J_{uu} = 8327$. The maximum optimal variation due to variation in disturbance ε_p is [16]:

$$\varepsilon_p = \left[\mathbf{G}\mathbf{J}_{uu}^{-1}\mathbf{J}_{ud} - \mathbf{G}_d\right](\mathbf{d}_{\max} - \mathbf{d}^*), \tag{22}$$

where the Hessian matrix is $\mathbf{J}_{ud} = [-995\ 766\ -17922\ 341]$ and the maximum expected magnitude of disturbance is 10% of nominal value. The scaling factor in Eq. (23) is defined to scale controlled variable such that for each p-th controlled variable, the sum of the magnitude of $\boldsymbol{\varepsilon}_\mathbf{p}$ and the implementation error n_p become similar [16]:

$$\mathbf{c}_{\mathrm{scl},\mathbf{p}} = |\boldsymbol{\varepsilon}_\mathbf{p}| + |n_\mathbf{p}|. \tag{23}$$

The implementation or measurement errors are taken to be 0.3 degree Celsius. And finally the scaled gain matrix is:

$$\mathbf{G}_{\mathrm{scl}} = \mathbf{D}_c^{-1}\mathbf{G}\mathbf{D}_u, \tag{24}$$

where $\mathbf{D}_c = \mathrm{diag}\{\mathbf{c}_{\mathrm{scl},p}\}$ and $\mathbf{D}_u = \mathrm{diag}\{\mathbf{u}_{\mathrm{scl},q}\}$ are the diagonal scaling matrices. The first 5 measurements among all 70 candidate measurements with the largest scaled gain with corresponding scaled gains are shown in Table 1. Therefore, the measurement vector is $\mathbf{y} = [T_1\ T_{14}\ T_{15}\ T_{55}\ T_{56}]^T$.

4.4. Design of CV

The sensitivity matrix $\mathbf{F}$ is obtained numerically from nonlinear model by perturbing each of the four disturbances around nominal operating point directly from the defining Eq. (12). The null space method gives the combination matrix $\mathbf{H}$ with Eq. (11) and the corresponding CV with Eq. (2) as follows:

$$c = -454T_{56} - 900T_{14} + 1180T_{15} + T_1 + 309T_{55}. \tag{25}$$

Table 1. The first five individual measurements with the largest scaled gain.

Rank	CV	Scaled gain
1	Temperature on tray no. 56	0.979
2	Temperature on tray no. 14	0.915
3	Temperature on tray no. 15	0.783
4	Temperature on tray no. 1	0.762
5	Temperature on tray no. 55	0.575

4.5. T-S fuzzy modelling

Optimal sensitivity matrix is modeled through the T-S fuzzy inference system. The fuzzy if-then rules represent the relationships between variables as follows:

$$\text{Rule}_i: \text{ If } d_1 \text{ is } \mathbf{A}_i^1 \text{ and } d_2 \text{ is } \mathbf{A}_i^2 \text{ and } d_3 \text{ is } \mathbf{A}_i^3 \text{ and } d_4 \text{ is } \mathbf{A}_i^4 \text{ Then}:$$

$$\xi_i(k,j) = b_i^0(k,j) + b_i^1(k,j)d_1 + b_i^2(k,j)d_2 + b_i^3(k,j)d_3 + b_i^4(k,j)d_4. \tag{26}$$

The fuzzy domain of input space is equally partitioned with three fuzzy sets to avoid redundant information in the form of similarity between fuzzy sets [35]. Recently, attention has been increasingly paid to improve the transparency and interpretability of fuzzy systems. The transparency and compactness of the fuzzy rule base can even be further improved by methods like rule reduction or rule-base simplification [36]. As there are four disturbances (d_1, d_2, d_3, d_4), the inference system consists of 81 rules $(1 \le i \le 81)$ for elements of optimal sensitivity matrix. Optimal sensitivity matrix $\mathbf{F}$ has five rows $(1 \le k \le 5)$ for each measurement and four columns $(1 \le j \le 4)$ for each disturbance, and $\xi_i(k,j)$ is the local linear representation of the corresponding element, $\mathbf{F}(k,j)$, with rule i. The identification data set with 100 elements is divided into training and test data set with 80 and 20 elements, respectively, with random method [22]. The parameters are tuned by tuning algorithm procedure described in Section 2.3.1. The fuzzy models are then validated through the test data and Table 2 demonstrates the validation results of the fuzzy models for the test data set. Small errors in Table 2 show that T-S fuzzy models are close to nonlinear model. Moreover, the performance of the

Table 2. Error quantification for output variables.

MSE for output variables				
	j			
k	1	2	3	4
1	2.63×10^{-4}	1.70×10^{-3}	8.290×10^{-5}	7.20×10^{-4}
2	4.13×10^{-4}	2.62×10^{-4}	1.31×10^{-4}	2.62×10^{-5}
3	7.32×10^{-4}	2.12×10^{-3}	7.45×10^{-5}	1.65×10^{-4}
4	9.56×10^{-4}	7.68×10^{-4}	1.47×10^{-4}	9.25×10^{-5}
5	1.30×10^{-4}	8.21×10^{-4}	8.05×10^{-4}	1.09×10^{-4}

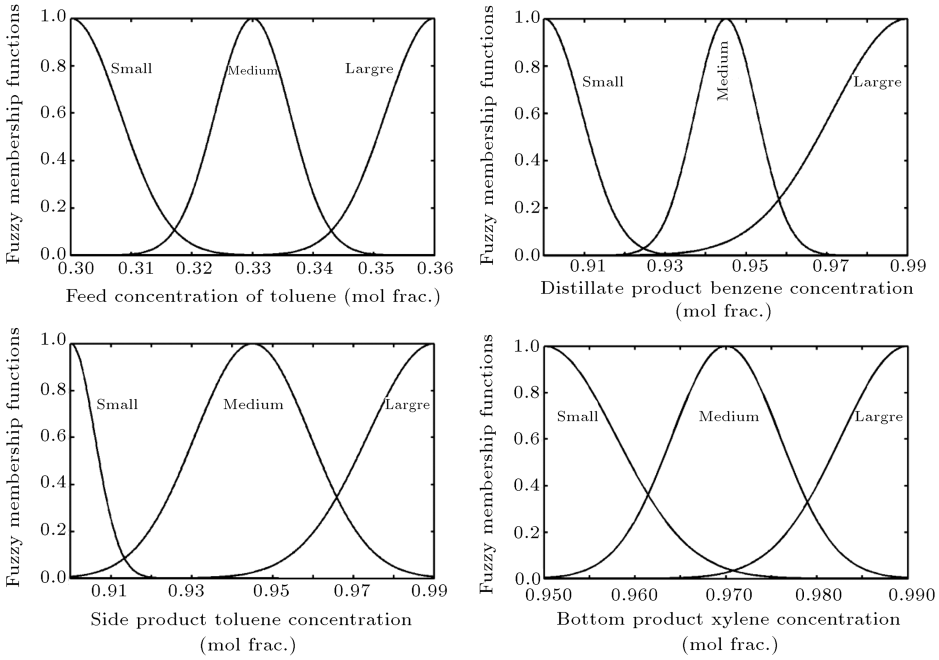

Figure 6. The fuzzy domain partitions of the input space.

tuned T-S fuzzy model will be dynamically evaluated in the control structure of DWC. The fuzzy domain of the input space is as shown in Figure 6.

4.6. Dynamic validation

Proportional-Integral (PI) controller is used in the control structure. Pairing of manipulated variables and controlled variables forms a simple multiloop decentralized structure (DB/L_RSQ_R) which is used frequently in the direct control layer of DWC in literatures such as Kiss and Rewagada [4] and Vandiggelen et al. [37]. In this structure, the concentration of benzene in distillate product, the concentration of toluene in side product, and the concentration of xylene in bottom product are controlled with reflux flow, side stream flow, and reboiler heat duty, respectively. This control structure is shown in Figure 7. The 5 points on column trays in Figure 7 show the locations of the selected tray temperature measurements which are selected with the maximum gain rule in Section 4.3. A 5-minute dead time is added in all composition loops, and level controllers are proportional only with the gain value of 2. PI controllers are tuned with SIMC method [38] and the controller parameters are shown in Table 3.

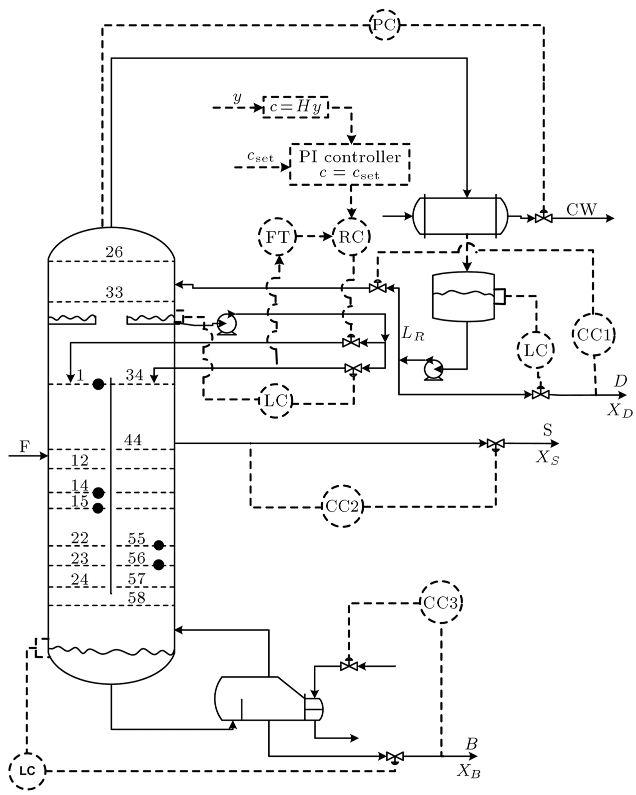

Figure 7. Control structure configuration for divided-wall column.

5. Results and discussions

DWC has a complex multivariable system. Figure 8 shows the effect of changes in liquid split fraction over the wall on reboiler heat duty in different values of feed toluene concentration. It also shows that how the minimum value of reboiler heat duty changes with different values of toluene concentration in the feed (disturbance). A negative 20% change means the toluene is changed from 30 mol% to 24 mol% while the other two feed compositions are changed and kept in the same ratio of 30/40, as base case, to make total add of 100 mol%. Therefore, a simple open loop

Table 3. Controller tuning parameter.

Controller	Controlled variables	Manipulated variable	Closed loop time constant, τ_c (min)	k_c (%/%)	τ_I (min)
CC1	x_D	L_R	275	1.7	150
CC2	x_S	S	130	1.5	100
CC3	x_B	Q_R	124	2.4	120
SOC controller	Self-optimize control	Liquid split fraction	412	1.9	100

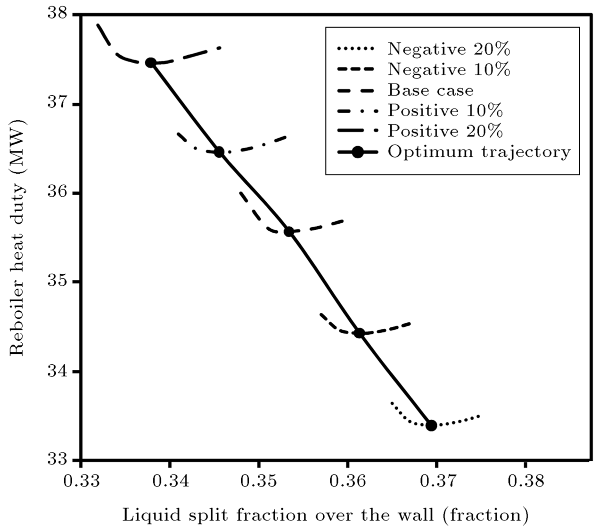

Figure 8. Effect of changes in liquid split fraction over the wall on reboiler heat duty in different feed toluene concentration.

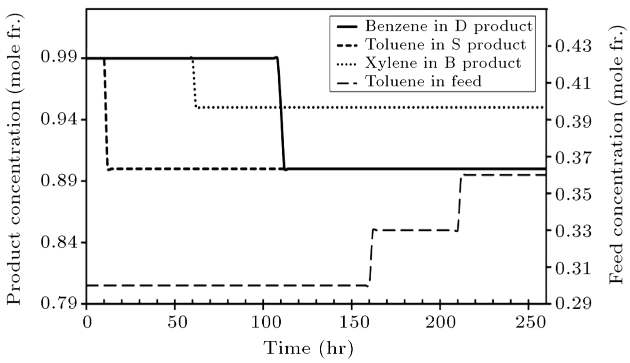

Figure 9. Disturbance trajectory.

feedforward control will lead to suboptimal solution, if it does not lead to an infeasible operation. Since controlling reboiler heat duty in a feedforward fashion on its optima may impose infeasible operation, the reboiler heat duty implemented by control structure goes lower than real optimum reboiler heat duty. So, a more advanced control structure is necessary to provide a stable as well as optimal operation.

To compare the proposed method in this paper with the conventional null space method, two methods are studied in rejecting the same disturbance trajectory entered into the plant, according to Figure 9.

Figure 10 compares dynamic responses of the fuzzy based method, which is proposed in this paper, and conventional null space method. It shows that both methods with the help of low-complexity simple PI controller stabilize the plant, reject the effect of disturbances, and make DWC to produce the product with desired specifications. Here "stabilization" means that the process does not drift too far away from the designed operational point when there are disturbances [29]. Bold flashes in Figure 10 (in CC3 controller output graph) show that the proposed control structure with fuzzy inference system has a lower steady-state reboiler heat duty than that of the conventional control structure. So, it results that the conventional control structure, which is based on local approximation of the nominal operating point, deviates from near optimal operating condition, in comparison with the proposed method based on fuzzy model, and it needs optimization online.

Table 4 shows the loss from the nonlinear model, with Eq. (4), for the conventional null space method. By comparing the values of Table 4 with those of Table 5, it is clear that the proposed method with

Table 4. Nonlinear loss imposed by the conventional null space.

Disturbance	Loss (KW)	Loss (percent of nominal value)
d_1 : decreased toluene mole fraction in S to 0.9	457.6	1.2
d_2 : decreased xylene mole fraction in B to 0.95	1052.7	2.9
d_3 : decreased benzene mole fraction in D to 0.9	1112.8	3.1
d_4 : increased toluene mole fraction in F to 0.33	1279.9	3.5
d_5 : increased toluene mole fraction in F to 0.36	1943.9	5.4

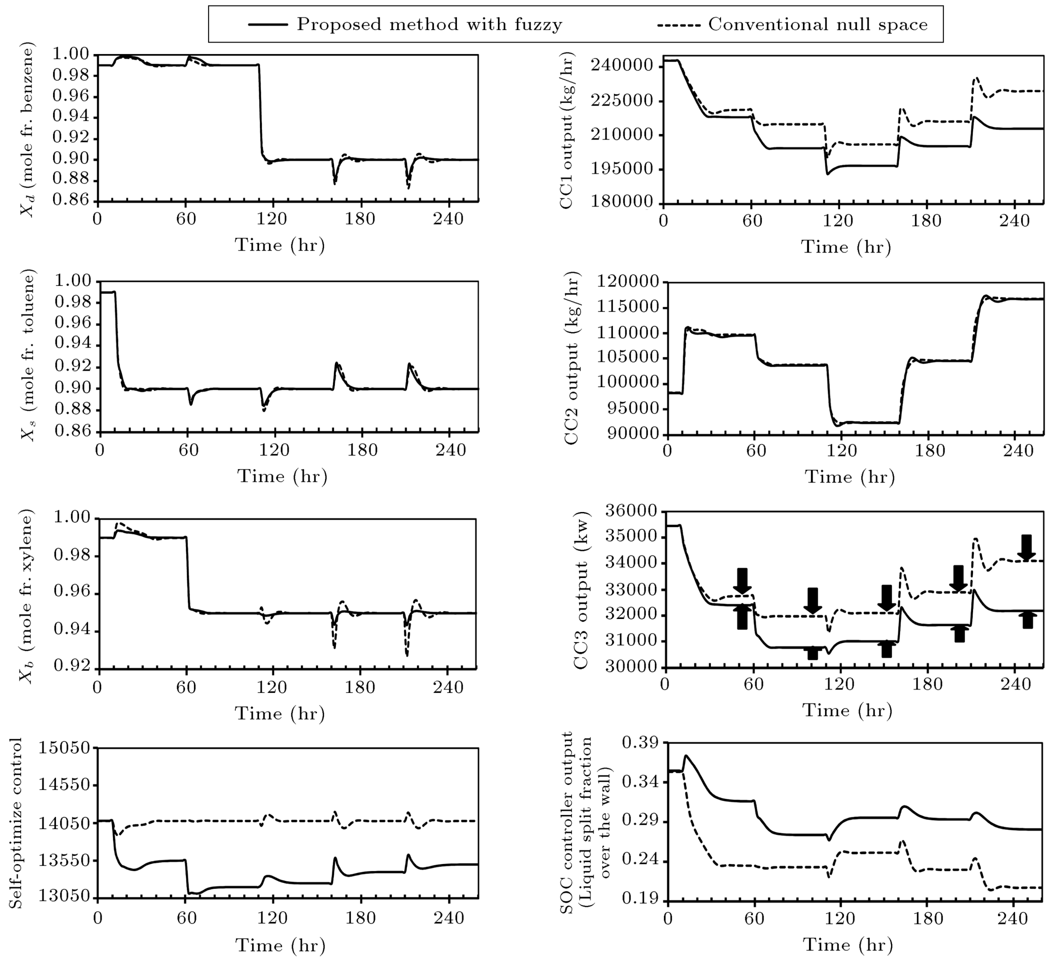

Figure 10. Dynamic responses of the proposed multilayer control structure with fuzzy inference system in comparison with the conventional control structure.

Table 5. Nonlinear loss imposed by the proposed control structure with fuzzy model.

Disturbance	Loss (KW)	Loss (percent of nominal value)
d_1 : decreased toluene mole fraction in S to 0.9	8.2	0.023
d_2 : decreased xylene mole fraction in B to 0.95	1.8	0.005
d_3 : decreased benzene mole fraction in D to 0.9	4.7	0.013
d_4 : increased toluene mole fraction in F to 0.33	4.2	0.012
d_5 : increased toluene mole fraction in F to 0.36	7.4	0.020

fuzzy model has reduced the loss to approximately zero, from the practical point of view. This means that fuzzy modelling of optimal sensitivity matrix makes control structure meet changes in operating condition imposed by successive disturbances entered into the plant. To be more precise, the proposed method of self-optimizing control structure with fuzzy inference system works well even for successive and large disturbances where optimal sensitivity matrix changes. Therefore, it results to fewer need to complex and intensive online optimization [29]. The value of loss in Table 5 shows slight variation in loss near zero for the proposed integrated method. This is because of the modelling error of fuzzy inference engine. Increasing the number of input partitions, rules, and number of selected measurements will make less variation, if it is necessary.

The assumption of ignoring the implementation error in the null space method is limiting and may provide a suboptimal solution. In this paper, in selection of measurement with the aid of maximum gain rule, the implementation error has been considered. In future, one can use exact local method [16] which handles implementation error explicitly by the method developed in this paper.

6. Conclusion

This paper proposed a method to solve the problem of local shortcoming of available SOC structure for DWC by modeling optimal sensitivity matrix with Takagi-Sugeno fuzzy inference. This fuzzy inference system was tuned offline by the input-output data from the nonlinear model. Results of the proposed method in this paper were compared with those of the conventional null space method. The results showed that conventional SOC had high value of loss and deviated from optimal operation in case of successive disturbances entered into the plant. So, it required solving a nonlinear optimization problem online for re-optimizing the plant operation. However, in the same operating condition, the proposed method in this paper with the aid of Takagi-Sugeno fuzzy inference system, which involves online calculation of weighted average of some linear function, imposed small loss, made DWC track optimal trajectory, and removed the need for complex and intensive online solving of the large nonlinear optimization problem. In addition to optimal steady-state operation, dynamic simulation showed that the proposed control structure rejected the effect of disturbances and stabilized the plant.

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Nomenclature

$\mathbf{A}_i^j$	Fuzzy set that is characterized by the membership function μ_i^j corresponding to input j of rule i
$b_i^0, b_i^1, ..., b_i^n$	Coefficients of linear crisp consequent function corresponding to n input variables of rule i
$\mathbf{c} = h(\mathbf{y}) = f_c(\mathbf{u}, \mathbf{d})$	Controlled variable (function h free to select)
$\mathbf{c}_s$	Setpoint
$\mathbf{D}_c, \mathbf{D}_u$:	Scaling matrices
$\mathbf{d}$	Disturbances vector with the dimension n_d
$\mathbf{d}_{\max}$	Maximum expected magnitude of disturbance
$\mathbf{F}$	Optimal sensitivity matrix
f	Set of equality constraints corresponding to the model equation
f'	Active constraints (equality constraints) which are satisfied with $\mathbf{u}'$
$\mathbf{G}, \mathbf{G}_d, \mathbf{G}^y, \mathbf{G}_d^y$	Steady-state gain matrices;
$\mathbf{G}_{\text{scl}}$	Scaled steady-state gain matrix
g	Set of inequality constraints
$\mathbf{H}$	Combination matrix
$\mathbf{J}_{uu}, \mathbf{J}_{ud}, \mathbf{J}_{du}, \mathbf{J}_{dd}$	Hessian matrix
J	Scalar cost function
k_c	Proportional gain of PI controller
L	Loss
L_R	Reflux flow (kg/hr)
M	Number of identification data pairs
N_r	Number of the rules
n_p	Implementation error
Q_R	Reboiler heat duty (kW)
R	The set of real numbers
S	Side stream flow (kg/hr)
T	Temperature measurements;
$\mathbf{u}_0 = \{\mathbf{u}', \mathbf{u}\}$	Independent inputs vector
$\mathbf{u}'$	Constrained independent inputs vector to satisfy f'
$\mathbf{u}$	Unconstrained independent inputs vector with the dimension n_u
w_i	Firing strength of rule i
$\mathbf{x}$	States vector with the dimension n_x
x_D	Benzene mole fraction in distillate product
x_S	Toluene mole fraction in side product
x_B	Xylene mole fraction in bottom product
$\mathbf{y} = \mathbf{f_y}(\mathbf{u}, \mathbf{d})$	Measurements vector with the dimension n_y
z	Fuzzy model output

Greek letters

α	Center of the Gaussian membership function
$\varepsilon_{\mathbf{p}}$	Maximum optimal variation due to variation in disturbance
μ	Membership function
$\mathbf{v} = [v_1, v_2, ..., v_n]^T$	Vector of fuzzy model inputs
ξ_i	Crisp consequent linear function of rule i

σ	Spread of the Gaussian membership function
τ_c	Closed loop time constant
τ_I	Integral time constant of PI controller

Superscripts

opt	Optimum
$*$	Nominal value
T	Transpose of a matrix

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Appendix A

Developing the least square to estimate the coefficients of linear function in the T-S fuzzy inference engine

It can be defined that:

$$\lambda_i = w_i / \sum_{i=1}^{N_r} w_i. \tag{A.1}$$

Then, from Eq. (18), the output is:

$$z = \sum_{i=1}^{N_r} \lambda_i z_i. \tag{A.2}$$

According to Eq. (17), a linear combination of input variables is considered as consequent crisp function, so:

$$z = \sum_{i=1}^{N_r} \left(b_i^0 + b_i^1 v_1 + ... + b_i^n v_n\right) \lambda_i. \tag{A.3}$$

Let:

$$\boldsymbol{\theta} = \Big[b_1^0, b_1^1, ..., b_1^n, b_2^0, b_2^1, ..., b_2^n, ..., b_{N_r}^0, b_{N_r}^1, ..., b_{N_r}^n\Big]^T, \tag{A.4}$$

and:

$$\varphi = \Big[\lambda_1, v_1\lambda_1, ..., v_n\lambda_1, \lambda_2, v_1\lambda_2, ..., v_n\lambda_2, ..., \lambda_{N_r}, v_1\lambda_{N_r}, ..., v_n\lambda_{N_r}\Big]^T. \tag{A.5}$$

For M data points:

$$\boldsymbol{\Phi} = \begin{bmatrix} \varphi^T(v_1) \\ \vdots \\ \varphi^T(v_M) \end{bmatrix}. \tag{A.6}$$

Then, the output of fuzzy model can be rearranged as follows:

$$\mathbf{z} = \boldsymbol{\Phi\theta}. \tag{A.7}$$

The input data are mapped into $\boldsymbol{\Phi}$ using inference mechanism and the least square algorithm produces an estimate of the best coefficients, $\boldsymbol{\theta}$.

$$\boldsymbol{\theta} = (\boldsymbol{\Phi}^T\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^T\mathbf{z}. \tag{A.8}$$

So the coefficients of the linear equations of fuzzy model can be identified indirectly from the values of input variables and the membership for each rule.

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