

CLAIMS

1. A chemical system for an operation exhibiting steady-state gain inversion; the system comprising:
 - a reactor configured to receive a feed stream and produce an outlet stream to form a process; and
 - a control device configured to control the process, wherein the control device receives inputs indicative of an operational parameter and output variables and, in response to the inputs and output variables, provides a steady-state manipulated input configured to control or optimize the process, the control device including:
 - an input disturbance model based on using the steady-state manipulated input as a custom output measurement to determine unmeasured disturbances,
 - a state estimator configured to utilize the custom output measurement to estimate the unmeasured disturbances entering the process and thereby predict a change in the process based on a characterization of the process by the model,
 - a non-linear steady-state target calculator configured to determine the steady-state manipulated input for the process based on the characterization of the process as calculated by the model, and
 - a regulator configured to provide a signal for adjustment of one or more inputs based on the steady-state manipulated input and associated output variables.
2. The chemical system of claim 1, wherein the calculator is configured to determine an optimum range for the steady-state manipulated input.
3. The chemical system of claim 1, wherein the model includes at least one of a fundamental first principles model, an empirical model, an adaptive model, a fuzzy model or a neural network model with dynamics.

4. The chemical system of claim 1, wherein the control device maximizes the output variable that exhibits steady-state gain inversion with respect to the manipulated input (u) through the relationship:

$$y_{1ss} = l(u_{ss}, m)$$

wherein u_{ss} is the steady-state manipulated input, m is the measured disturbances, and y_{1ss} is an output variable that exhibits steady-state gain inversion.

5. The chemical system of claim 1, wherein the control device comprises a nonlinear model predictive control (NMPC) device as a primary controller to address real-time computational needs and a linear model predictive controller (LMPC) or a proportional–integral–derivative (PID) controller for executing one or more moves of the NMPC.

6. The chemical system of claim 1, wherein the control device is configured to estimate the unmeasured disturbances that shift a position of the optimum peak where steady-state gain inversion occurs, the unmeasured disturbances including catalytic aging and associated over/under performance of the reactor.

7. The chemical system of claim 1, wherein the manipulated input includes at least one of a steady-state production rate, a steady-state chloriding effectiveness parameter, or a steady-state ethylene oxide (EO) selectivity.

8. The chemical system of claim 1, wherein the regulator determines a change in the manipulated output to optimize the output variable based on an observation of a gain inversion over a settling time of the control device if the manipulated input to maximize the variable output is within an operational threshold, one or more measured disturbances are steady as based on statistical criteria, the manipulated input is steady or moving towards an optimum steady-state manipulated input, and a new optimum optimized manipulated input is observed after a settling time of the control device.

9. The chemical system of claim 1, wherein the output variable is intermittently maximized by using an output disturbance model along with a high infeasible target for the calculator and the regulator.
10. The chemical system of claim 1, wherein the manipulated input includes at least one of chlorination effectiveness parameter (Z) or ethylene oxide (EO) production rate to control ethylene oxide (EO) selectivity.
11. The chemical system of claim 1, wherein the control device is configured to optimize a selectivity of effluent ethylene oxide (EO) in the reactor.
12. A method for controlling a chemical system through a control device, the method comprising:
- receiving inputs indicative of an operational parameter of a process and a steady-state output variable;
 - implementing an input disturbance model based on using an optimum manipulated steady-state input as a custom output measurement to determine the optimized manipulated input in a presence of both measured and unmeasured disturbances;
 - estimating a state of the process to predict the process based on a characterization of the process by the model;
 - determining an a targeted manipulated input for the process based on the characterization of the process by the modelling and the estimating of the one or more steady-state output variables of the chemical system; and
 - regulating the process based on the targeted manipulated input.
13. The method of claim 12, wherein the regulating of the chemical system based on the optimized manipulated input includes manipulating at least one of a chlorination effectiveness parameter (Z) or an ethylene oxide (EO) production rate to control an ethylene oxide (EO) selectivity.
14. The method of claim 12, wherein the regulating the chemical system based on the optimized manipulated input includes maximizing a steady-state gain inversion

proximate to a value in which sign change indicating a change from a rise in selectivity to a decrease in selectivity occurs.

15. The method of claim 12, wherein the regulating of the chemical system is configured to optimize a selectivity of effluent ethylene oxide (EO) in an epoxidation reactor.