Dynamic Simulation of a Low-Temperature Rectification Column as Part of an IGCC Power Plant

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1 Introduction

IGCC plants (Integrated Gasification Combined Cycle) offer the opportunity to utilize fossil energy sources, like coal or heavy refinery residues, to satisfy increasing energy demand while considering strict environmental constraints [1]. Such a plant consists of a combined power cycle, a fuel gasifier with downstream fuel gas conditioning and an air separation unit (ASU), where the oxygen required for gasification is produced. Using this concept efficiencies of up to 50% can be achieved. Compared to conventional coal-fired plants the use of an IGCC plant provides considerable potential for CO₂ reduction.

First operational experiences with demonstration plants built in USA and Europe indicate the existence of significant potential for development to achieve a level of automation that is common in plant design. This challenge results in the novel linkage of different plants such as gasifier, air separation unit and gas turbine. Large amounts of different feedback complicate the prediction of operational behavior and plant trips and require the application of a dynamic plant simulation.

A matter of particular interest is the coupled air-side integration between gas turbine and air separation unit (fig. 1). By linking of these two components undesired fluctuations of mass flow can occur within the system during changing load demands. These fluctuations are due to the different responses of each of the coupled system components. Therefore for failure-free joint operation of air separation unit and gas turbine including a further air compressor new control concepts are required, which can be designed and tested with the help of a dynamic simulation model.

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The cryogenic rectification column, as the core of the air separation unit, strongly affects the system's transient behavior. In the following sections both a dynamic model of such a column and some simulation results are presented.

2 Model of the Rectification Column

The above-mentioned low-temperature rectification column is a typical double column for cryogenic air separation. Both columns, working on different pressure levels, are linked via material flows through the piping as well as thermally connected via a coupling heat exchanger (often called condenser-reboiler).

The following assumptions form the basis of the simulation model [2]:

- model of theoretic tray,
- neglect of vapor holdup in component balances,
- air as ternary mixture of nitrogen, oxygen and argon (thermal and caloric state variables are calculated with help of the Bender equation of state [3] (equation 6))
- neglect of heat losses of the column.

The mapping of interactions between rectification column and upstream components requires that the pressure dynamics of the column be taken into account. Therefore in addition to the consideration of material balances (equation 1 and 2) and the energy balance (equation 3) the momentum balance (equation 4) for vapor phase and a weir equation (equation 5) have to be part of the model.

$$\frac{dm_i}{dt} = \dot{m}_{i-1}^V + \dot{m}_{i+1}^L - \dot{m}_i^V - \dot{m}_i^L + \dot{m}_i^F$$
 (1)

$$\frac{dx_{k,i}}{dt} = \frac{1}{m_i} \left(\dot{m}_{i-1}^V y_{k,i-1} + \dot{m}_{i+1}^L x_{k,i+1} - \dot{m}_i^V y_{k,i} - \dot{m}_i^L x_{k,i} + \dot{m}_{k,i}^F + x_{k,i} \frac{dm_i}{dt} \right)$$
(2)

$$\frac{du_i}{dt} = \frac{1}{m_i} \left(\dot{m}_{i-1}^V h_{i-1}^V + \dot{m}_{i+1}^L h_{i+1}^L - \dot{m}_i^V h_i^V - \dot{m}_i^L h_i^L + \dot{m}_i^F h_i^F + \dot{Q}_i + u_i \frac{dm_i}{dt} \right)$$
(3)

$$\frac{d\dot{m}_{i}^{V}}{dt} = \frac{A_{o}}{V_{i}^{V}} \left(-\Delta p_{V,i} A_{o} + (p_{i} - p_{i+1}) A_{o} - m_{i}^{V} g + \frac{\dot{m}_{i-1}^{V^{2}}}{\rho_{i-1}^{V} A_{o}} - \frac{\dot{m}_{i}^{V^{2}}}{\rho_{i}^{V} A_{o}} \right)$$
(4)

$$0 = f\left(\dot{m}_i^L, h_i^{cL}\right) \tag{5}$$

$$0 = \overrightarrow{f}(T_i, p_i, \rho_i, x_{k,i}, y_{k,i}, u_i, h_i)$$

$$(6)$$

The transient behavior of the condenser-reboiler is described by a model of Gregorig [4]. This approach takes into account that thermal energy is only transported from the lower column to the upper column by a propulsive temperature difference. Moreover the ability to store energy in the heat-transferring wall is included in the model. The differential equation for the calculation of the wall temperature is

$$\frac{dT_W}{dt} = \frac{1}{c_W m_W} \left(\dot{Q}_C - \dot{Q}_R \right) \tag{7}$$

For the heat transferred from the top of the lower column to the wall \dot{Q}_C and accordingly for the heat fed from the wall to the bottom of the upper column \dot{Q}_R applies

$$\dot{Q}_C = \alpha_C^* A_W \left(T_i - T_W \right) \tag{8}$$

$$\dot{Q}_R = \alpha_R^* A_W \left(T_W - T_{j+1} \right) \tag{9}$$

Model equations are implemented in a Matlab/Simulink-based simulation environment (Fluid Network Initialization Toolbox [5]; developed by Siemens Power Generation) and numerically solved with suitable algorithms.

3 Transient Behavior of the Column - Change of Feed Enthalpy

Subject of the experiment presented is the dynamic behavior of the lower part of the double column (so-called pressure column) during the failure of an upstream air cooler and the associated increase of feed enthalpy.

Figure 2 shows the chosen simulation set-up. The pressure column is assumed to be a nine-tray column. The vapor flow that reaches the column's top is totally condensed using a cooling medium at a constant temperature. The outlet mass flows (liquid nitrogen at the top and liquid oxygen at the bottom of the column) are kept constant. The piping, that connects the column and the air-side of the gas turbine is substituted by a throttle with a corresponding drag

coefficient. Hence the column feed (air at approximately dew point temperature) adapts to the pressure difference between the gas turbine's air-side and the column feed tray. The pressure at the air-side is assumed to be constant. Starting from a steady state profile the feed enthalpy is raised by 2% and the system's transient behavior is observed.

The increase of feed enthalpy represents an increase of the heat duty fed to the bottom of the column. Therefore the bottom boils up, in doing so the vapor flows on every tray are elevated almost without any time lag. The additional vapor flow that reaches the top is condensed and leads, as the top product flow (nitrogen) is constant, to an elevated liquid level on the upper tray and a corresponding increase of the liquid flow leaving this tray. By means of a series connection of the trays' liquid side this procedure repeats downwards on every tray (fig. 3) until the additional amount of liquid finally reaches the bottom after 150 seconds and the fluid dynamics of the column has stabilized.

Due to the elevated liquid and vapor flows the purity of the distillate increases (fig. 4). The time constant of this response lies in the magnitude of 1000 s. The initial downtrend that can especially be seen in the lower trays results from the stabilization process of the fluid dynamics described. As nitrogen has a higher heat capacity compared to oxygen temperatures on tray one to eight drop with increasing nitrogen mass fractions.

The temperature in tray nine (top) in contrast has to increase. To condense the additional vapor on the column's top an increase in the condenser's performance is necessary. As the temperature of the cooling medium is kept constant this can only be achieved by an increase in the column's top temperature. At initial constant and later increasing nitrogen mass fraction a temperature increase on the upper tray is only possible by an increase of the pressure according to the phase equilibrium. As the vapor flows are dominated by energy and mass balances all the other trays follow this behavior so that the pressure on every tray rises (fig. 5).

Congruent to the course of the bottom pressure the column feed changes. Since the pressure at the bottom rises but the pressure on the air-side of the gas turbine is constant the feed flow drops (fig 6.). After the bottom pressure becomes stationary, the deviation in feed flow accounts for -0.2%. As the

product flows are constant, this deviation causes a continuous decrease in the bottom liquid level (fig. 6).

4 Conclusions and Outlook

The analysis of our results shows that by the disturbance of feed enthalpy, caused for example by the failure of a cooler not only the temperature, pressure and mass fractions are subjected to dynamic changes but also the column feed flow decreases. As the product flows are constant, this causes a continuous reduction in the bottom liquid level. By using a liquid level controller as is usually installed drying up of the bottom would be prevented.

With the help of the model, the transient behavior of the system, which is difficult to predict, can be studied. Compared to an expansive experiment with a real system the use of the simulation model makes available a variety of variables, which would otherwise be too costly or even not measurable, for the evaluation of the test. Therefore the simulation model presented represents an important tool for the planning and design of novel process options and control concepts.

In the near future it will be necessary to simulate the whole air separation unit connected with several plant components. To reduce calculation time to a tolerable value a reduced model should be applied, which will be our next step. Thereby the special challenge will be to modify existing reduced approaches in such a way, that the pressure dynamics can also be considered.

Symbols used

A	$[m^2]$	Area
A_o	[m²]	Free Area
С	$[J/kg \cdot K]$	Unit-mass heat capacity
g	$[m/s^2]$	Earth gravity
h	[J/kg]	Unit-mass Enthalpy
h^{cL}	[m]	Height of clear Liquid
m	[kg]	Mass
ṁ	[kg/s]	Mass flow
p	[Pa]	Pressure

$\dot{\mathcal{Q}}$	[J/s]	Heat flux
T	[K]	Temperature
t	[s]	Time
u	[J/kg]	Unit-mass internal energy
V	$[m^3]$	Volume
x	[kg/kg]	Mass fraction in liquid phase
У	[kg/kg]	Mass fraction in vapor phase
$lpha^*$	[W/K]	Modified heat transfer coefficient
Δp_V	[Pa]	Pressure drop
ρ	$[kg/m^3]$	Density

Indices

i	Tray i
k	Component k
C	Condenser
V	Vapor
L	Liquid
R	Reboiler
W	Heat exchanger wall
F	Feed

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Figure 1: Coupled air-side integration between gas turbine and air separation unit

Figure 2: Simulated part of the rectification column

Figure 3: Simulated transient behavior – Liquid flows versus time

Figure 4: Simulated transient behavior – Liquid phase nitrogen mass fraction in selected trays versus time

Figure 5: Simulated transient behavior – Pressure in selected trays versus time

Figure 6: Simulated transient behavior – Bottom liquid level and column feed versus time







