Process simulation, optimization, and control of cryogenic Air Separation Units with frequent load changes

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Zhejiang University of Technology

3 campuses
21 colleges
30,000 undergraduates
2,300 postgraduates
2,800 faculties
Process simulation, optimization, and control of cryogenic Air Separation Units with frequent load changes

Background

Process simulation and analysis

Process optimization with load changes

Automatic load control system

Background

Standard Dry Air Composition

<table>
<thead>
<tr>
<th>Component</th>
<th>Chemical Symbol</th>
<th>% by Volume</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>N₂</td>
<td>78.08%</td>
</tr>
<tr>
<td>Oxygen</td>
<td>O₂</td>
<td>20.95%</td>
</tr>
<tr>
<td>Argon</td>
<td>Ar</td>
<td>0.95%</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>CO₂</td>
<td>0.039</td>
</tr>
<tr>
<td>Neon</td>
<td>Ne</td>
<td>0.0018%</td>
</tr>
<tr>
<td>Helium</td>
<td>He</td>
<td>0.0005%</td>
</tr>
<tr>
<td>Krypton</td>
<td>Kr</td>
<td>0.0001%</td>
</tr>
<tr>
<td>Xenon</td>
<td>Xe</td>
<td>8.7 x 10⁻⁶%</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>H₂</td>
<td>0.00005%</td>
</tr>
</tbody>
</table>

Air separation technology

Cryogenic air separation units
- Cryogenic distillation
- Large volumes of gaseous product
- High purity product
- Liquid product
- Connected to Plant

Most effective to get high production rates

<table>
<thead>
<tr>
<th>Separation Technology</th>
<th>Products</th>
<th>Purity</th>
<th>Product rate</th>
<th>Delivery pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cryogenic distillation</td>
<td>GOX/GAN/GAR</td>
<td>Oxygen&gt;99.2%</td>
<td>Large (10000 m³/h)</td>
<td>Low (0.5-0.6 MPa)</td>
</tr>
<tr>
<td>selective adsorption</td>
<td>GDI GAN</td>
<td>Oxygen&gt;95%</td>
<td>Medium (3000-6000 m³/h)</td>
<td>Medium (1-5 MPa)</td>
</tr>
<tr>
<td>differential permeation through membranes</td>
<td>GOX</td>
<td>Oxygen&gt;99%</td>
<td>Small (800 m³/h)</td>
<td>High (10-20 MPa)</td>
</tr>
</tbody>
</table>
Background

- Filtering air
- Compressing air
- Removing contaminants
- Cooling air
- Cryogenic distillation
- Products

Industrial Internal compressed air separation unit

Heat integration

Background

- Automatic Load Control

Gas pipeline network of BaoSteel, China
- Gas products are supplied by the pipeline network with changing demand.
- Release when pressure exceeds the upper limits
Background

1. Purity constrains should be maintained.
2. Fast ramp response can decrease energy consumption.

Characteristics & Challenge

- Precise model
- Robust algorithm
- Profitable optimization
- Rapid response
Process simulation, optimization, and control of cryogenic Air Separation Units with frequent load changes

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**Process simulation**

Simulation structure of internally compressed ASU process

- 37 equipments
- 7461 variables
- 7134 equations
- 327 independent variables

<table>
<thead>
<tr>
<th>NAME</th>
<th>GAS</th>
<th>LIN</th>
<th>GOX</th>
<th>LOX</th>
<th>GAR</th>
<th>LAR</th>
</tr>
</thead>
<tbody>
<tr>
<td>O2</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ar</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N2</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Nominal flowrate
- Maximum flowrate
- Minimum flowrate

Specifications of products

- 3 Gasous products
- 9 Feed and recycle flowrates
- 40 Pressure and pressure drops
- 10 Equipment efficiencies
- 15 Energy losses
- 9 Feed compositions
- 227 Equipment parameters
- 12 temperatures

The model should be easily converged at:

- 70%~110% product flowrates
- Specified product purities
- Varied equipment efficiencies
Process simulation

internally compressed ASU process

Problem & strategy

Problems
• Only several operation points of the plant can be solved with good initial guess.
• The simulation model is not precise enough to describe the characteristics of the ASUs.

Difficulties
• Complicated model with more equations is difficult to solve.
• Highly integrated flowsheet results in a narrow feasible region.
• Traditional Newton algorithm heavily relies on good initials.

Strategy
• Develop an algorithm with wide range convergence to solve nonlinear model.
Homotopy method

- Overcome the dependence on a good initial guess

\[ f(x) = 0 \]

\[ h(x,t) = t \times f(x) + (1-t) \times g(x) = 0 \]

- Solution path

- How to determine a homotopy parameter?

- How to guarantee the convergency of deformed problem family?

Homotopy method

Determine \( t \) by load change

\[ f(x, \alpha(t)) = 0 \]

\[ f(\bar{X}, \bar{X}) = 0 \]

- Variables changed

- Relative change

- \( t = 0 \) Base Point

- \( t = 1 \) Target Point

- Relative location of calculated point between base and target point

\[ \alpha = [\alpha_1, \alpha_2, \cdots, \alpha_k]^T = \begin{bmatrix} \frac{X_1 - \bar{X}_{1,lp}}{X_{1,lp}} & \frac{X_2 - \bar{X}_{2,lp}}{X_{2,lp}} & \cdots & \frac{X_k - \bar{X}_{k,lp}}{X_{k,lp}} \end{bmatrix} \]

- Load vector

- Homotopy parameter

- \( t \) relative location of calculated point between base and target point
Homotopy method

Homotopy path of load change simulation:
From $f(x, \alpha_{bp}) = 0$ to $f(x, \alpha_{tp}) = 0$

Search $\alpha_i$ to get homotopy solution

Backtracking Strategy

Keep going ahead until there is no way.
Or go back and choose a new way

Homotopy-based Backtracking Method (HBM)
Program architecture

External Data

HBM (OOMF script) → SOLVER → Results

AOS NLA

Aspen Plus®

Implementation structure of HBM in AspenPlus®

Program flowchart of HBM

Process analysis

Nonlinearity from:
1. Integrate heat exchanger
2. High purity distillation column

Plant data
Process analysis

Base point \( P_{C2}=0.135 \text{ MPa(a)} \)
Target point \( P_{C2}=0.14 \text{ MPa(a)} \)

\[ \alpha = \frac{P_{C2} - P_{C2,ap}}{t_{C2,ap}} \quad t = \frac{P_{C2} - P_{C2,ap}}{P_{C2,ap} - P_{C2,3p}} \]

Vapor composition profiles at condition from \( P_{C2}=0.1384 \text{ MPa(a)} \)
to \( P_{C2}=0.1385 \text{ MPa(a)} \)
Step: 10 Pa

Effect of \( P_{C2} \) on \( y_{O2,C701} \) and \( y_{Ar,C702} \)
Process analysis

Effect of Pcz on C701&C702 with thermal-couple condenser

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Process optimization with load changes

Optimally change load in response to demand, ALC should:
- Reach target product condition accurately and rapidly;
- Maintain product purity;
- Operate equipment safely;
- Minimize compression cost of air feeds;

\[
\begin{align*}
\min & \quad k_1 F_{\text{HPO}} + k_2 M + k_3 T
\\
s.t. & \quad f(\mathbf{X}_{\text{fix}}, \mathbf{X}_{\text{exp}}, \mathbf{X}_{\text{pred}}, \mathbf{X}_{\text{oper}}, \mathbf{X}_{\text{cal}}, \mathbf{p}_{\text{purity}}) = 0
\\
\mathbf{X}_{\text{pred}} & \in \{ F_{\text{GOX}}, F_{\text{GAN}}, F_{\text{LOX}} \}
\\
\mathbf{X}_{\text{purity}} & \leq \mathbf{X}_{\text{purity}} \leq \mathbf{X}_{\text{purity}}^U
\\
\mathbf{X}_{\text{oper}} & \leq \mathbf{X}_{\text{oper}} \leq \mathbf{X}_{\text{oper}}^L
\\
\end{align*}
\]

\( X_{\text{pred}} \): product slate
\( X_{\text{purity}} \): calculated purity
\( X_{\text{oper}} \): control variables
\( X_{\text{fix}} \): fixed parameters
\( X_{\text{exp}} \): experiential variables
\( X_{\text{cal}} \): calculated variables

Algorithm

\[
\begin{align*}
\min & \quad k_1 F_{\text{HPO}} + k_2 M + k_3 T
\\
s.t. & \quad f(\mathbf{X}_{\text{fix}}, \mathbf{X}_{\text{exp}}, \mathbf{X}_{\text{pred}}, \mathbf{X}_{\text{oper}}, \mathbf{X}_{\text{cal}}, \mathbf{p}_{\text{purity}}) = 0
\\
\mathbf{X}_{\text{pred}} & \in \{ F_{\text{GOX}}, F_{\text{GAN}}, F_{\text{LOX}} \}
\\
\mathbf{X}_{\text{purity}} & \leq \mathbf{X}_{\text{purity}} \leq \mathbf{X}_{\text{purity}}^U
\\
\mathbf{X}_{\text{oper}} & \leq \mathbf{X}_{\text{oper}} \leq \mathbf{X}_{\text{oper}}^L
\\
\mathbf{X}_{\text{oper}}(t) & \leq \mathbf{X}_{\text{oper}} \leq \mathbf{X}_{\text{oper}}(t)
\\
\mathbf{X}_{\text{oper}}(t) & = \mathbf{X}_{\text{oper}} + t \times (\mathbf{X}_{\text{oper}} - \mathbf{X}_{\text{oper}}^L)
\\
\mathbf{X}_{\text{oper}}(t) & = \mathbf{X}_{\text{oper}} + t \times (\mathbf{X}_{\text{oper}} - \mathbf{X}_{\text{oper}}^L)
\\
t & = 0 \quad \text{Base point: Simulation}
\\
t & = 1 \quad \text{Homotopy family:}
\\
\text{Extend the lower and the upper bound gradually}

\end{align*}
\]

\( X_{\text{oper}} \): control variables
\( X_{\text{cal}} \): calculated variables

Target problem: Optimization
Algorithm

\[
\min_{X_{\text{max}}} k_1 F_{\text{fract}} + k_2 F_{\text{std}} + k_3 F_{\text{fa}} \\
\text{s.t.: } f(X_{\text{max}}, X_{\text{min}}, X_{\text{std}}, X_{\text{fract}}, X_{\text{oper}}) = 0 \\
X_{\text{min}} \leq X_{\text{purity}} \leq X_{\text{max}} \\
X_{\text{min}}(t) \leq X_{\text{oper}}(t) \\
\]

Homotopy family:
Extend the lower and the upper bound gradually

Solving process of HBM

Feasibility study

Feasibility study of \( X_{\text{purity}} \)

Feasibility study of \( X_{\text{oper}} \)
Feasible product slate

\[
\begin{align*}
\min_{\mathbf{x}_{\text{prod}}} & \quad k_1 F_{\text{IPA}} + k_2 F_{\text{MA}} + k_3 F_{\text{TAD}} \\
\text{s.t.} & \quad f(\mathbf{x}_{\text{ini}}, \mathbf{x}_{\text{prod}}, \mathbf{x}_{\text{prod}}(t), \mathbf{x}_{\text{oper}}, \mathbf{x}_{\text{col}}, \mathbf{x}_{\text{purity}}) = 0 \\
& \quad \mathbf{x}_{\text{purity}} = (F_{\text{GDX}}, F_{\text{GAN}}, F_{\text{LOG}}) \\
& \quad x_{\text{purity}}^L \leq \mathbf{x}_{\text{purity}} \leq x_{\text{purity}}^U \\
& \quad \mathbf{x}_{\text{prod}} = \mathbf{x}_{\text{prod}} + \mathbf{h}(\mathbf{x}_{\text{prod}} - \mathbf{x}_{\text{prod}}')
\end{align*}
\]

729 product slates
404 converged without HBM
531 converged with HBM

• HBM extends the convergence region

Feasible product slate

Optimization results
Plant data
Physical boundary

mass balances on the nitrogen:

\[ F_{\text{AIR}} y_{N2,\text{AIR}} = (F_{\text{LNX}} + F_{\text{GOX}}) y_{N2,O2} + (F_{\text{LIN}} + F_{\text{GAN}}) y_{N2} + F_{wN} y_{N2,wN} + (F_{\text{AR}} + F_{\text{GAR}}) y_{N2,\text{AR}} \]

\[ y_{N2,O2} \approx 0 \quad 1 \geq y_{N2,wN} \geq 0.995 \]

\[ y_{N2,\text{AR}} \approx 0 \quad y_{N2} \approx 1 \]

\[ (F_{\text{LIN}} + F_{\text{GAN}}) \leq F_{\text{AIR}} y_{N2,\text{AIR}} - 0.995 F_{wN} \]

mass balances on the oxygen:

\[ F_{\text{AIR}} y_{O2,\text{AIR}} = (F_{\text{LNX}} + F_{\text{GOX}}) y_{O2,O2} + (F_{\text{LIN}} + F_{\text{GAN}}) y_{O2,N2} + F_{wN} y_{O2,wN} + (F_{\text{AR}} + F_{\text{GAR}}) y_{O2,\text{AR}} \]

\[ y_{O2,\text{AIR}} \approx 0 \quad y_{O2} \approx 1 \]

\[ (F_{\text{LIN}} + F_{\text{GAN}}) \geq F_{\text{AIR}} y_{O2,\text{AIR}} - 0.2% F_{wN} \]

\[ \frac{F_{\text{LIN}} + F_{\text{GAN}}}{F_{\text{LNX}} + F_{\text{GOX}}} \geq \frac{F_{\text{AIR}} y_{O2,\text{AIR}} - 0.2% F_{wN}}{F_{\text{AIR}} y_{N2,\text{AIR}} - 0.995 F_{wN}} = \frac{y_{O2,\text{AIR}} - 0.2% F_{wN}}{F_{\text{AIR}}} \]

\[ y_{O2,\text{AIR}} \text{ fraction of oxygen in the air} \]
\[ y_{O2} \text{ purity of the oxygen products} \]
\[ y_{O2,N2} \text{ residual fraction of oxygen in the nitrogen products} \]
\[ y_{O2,\text{WN}} \text{ residual fraction of oxygen in the waste nitrogen} \]
\[ y_{O2,\text{AR}} \text{ residual fraction of oxygen in the argon products} \]

\[ \frac{F_{\text{LOX}} + F_{\text{GOX}}}{F_{\text{LIN}} + F_{\text{GAN}}} \geq \frac{F_{\text{AIR}} y_{O2,\text{AIR}} - 0.2% F_{wN}}{F_{\text{AIR}} y_{N2,\text{AIR}} - 0.995 F_{wN}} = \frac{y_{O2,\text{AIR}} - 0.2% F_{wN}}{F_{\text{AIR}}} \]

Physical boundary

Product rate ratio results with HBM

Product rate ratio results without HBM
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Physical boundary

\[
\frac{F_{\text{Gox}} + F_{\text{Gox}}}{F_{\text{Lin}} + F_{\text{Gox}}} = 0.2\% F_{\text{Lin}} \approx 0.48
\]

Product rate ratio of plant data
Automatic Load Change System Design

**Operating-trajectory LPV Model**

\[
y(t) = \alpha_1(w)[\hat{G}_1(q)w(t)] + \cdots + \hat{G}_m(q)w(t) + \cdots + \hat{G}_n(q)w(t) + v(t)
\]

- \(m\) working-points are selected along its operating-trajectory \(w(t)\).
- Linear models are identified using data sets at \(m\) working-points.
- \(\alpha_1(w), \alpha_2(w), \cdots, \alpha_n(w)\) weighting functions are parameterized by cubic splines function, obtained by interpolating the linear models using total data.

The LPV model can model nonlinearities in both gains and time constants.

Weighting functions of the LPV model
Automatic Load Change System Design

Model Predictive Control with Ideal Resting Values

\[
\min J(k) = \sum_{i=0}^{N} \|e(t+i)\|^2 + \sum_{i=0}^{N} \|\Delta u(t+i)\|^2 + \sum_{i=0}^{N} \|r(t+i) - u_i\|^2
\]

s.t.
\[
y^*_i - e(t+i) \leq y(t+i) \leq y^*_i + e(t+i)
\]
\[
\Delta u \leq \Delta u(t+i) \leq \Delta u^*
\]
\[
e(t+i) \geq 0
\]

where \(U_{ss}\) are the ideal resting values (IRVs) for input variables determined by SSO module;

At each sample time \(t\), LPV model is linearized based on the current value of the working-point variable \(w(t)\).

the model between output variable \(y_i\) and input variable \(u_i\) is:

\[
\hat{G}_i(q, w) = \alpha_{ij}(w)\hat{G}_i(q) + \alpha_{ij}(w)\hat{G}_i^2(q) + \cdots + \alpha_{ij}(w)\hat{G}_i^n(q)
\]

Implementation ALC system

Design One MPC controller for whole ASU unit, the controller is comprised of 39 CVs, 14MVs, and 2 DVs.

Using own developed NMPC algorithm, named LPV_NMPC to handle the nonlinear problem.
Implementation ALC system

ALC system Performance evaluated by Nanjing Steel Ltd. China

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Load change range</td>
<td>45% (15000Nm³/h - 24000Nm³/h)</td>
</tr>
<tr>
<td>Max. load change amplitude</td>
<td>30% (6000Nm³/h)</td>
</tr>
<tr>
<td>Average transition speed</td>
<td>4 min / 1% load</td>
</tr>
<tr>
<td>Oxygen in product oxygen (&gt;99.6%)</td>
<td>acceptable and fluctuation &lt; 0.15%</td>
</tr>
<tr>
<td>Oxygen in product nitrogen (&lt;5ppm)</td>
<td>acceptable and fluctuation &lt; 0.3ppm</td>
</tr>
<tr>
<td>Oxygen in product argon (&lt;1ppm)</td>
<td>acceptable and fluctuation &lt; 0.2ppm</td>
</tr>
</tbody>
</table>

First time successful implementation ALC system on native air separation units.

Control performance of ALC system (1 week)

Automatic Load Change Frequency of ASU (Load change amplitude > 1000Nm³/h)
Automatic load control results

![Graph showing automatic load control results]

- Automatic load control results
- 30% automatic load change for ASU (4 hours)

- Oxygen purity 99.94%(v)
- Oxygen residue in rude argon 1.05ppm

- Flue gas flowrate: 23000 Nm³/h
- Duration: 120min
- Final flowrate: 17000 Nm³/h

30% automatic load change for ASU (4 hours)
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