Reconfiguration of Production in CSTR Networks: Flexibility of Heterogeneous Setups

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Introduction

- Coupled CSTRs
  Locked mode operation
2D Reactor Network

Cubic autocatalysis

\[ R + 2P_n^{k_n} \rightarrow 3P_n \]

\[ P_n^{d_n} \rightarrow D \]
2D Reactor Network

Cubic autocatalysis

\[ R + 2P_n \xrightarrow{k_n} 3P_n \]

\[ P_n \xrightarrow{d_n} D \]

\[
\frac{dr_{ij}}{dt} = -\sum_{n=1}^{N} k_n r_{ij} p_{ijn}^2 + f(1 - r_{ij}) + g\left(r_{i-1,j} + r_{i+1,j} + r_{i,j-1} + r_{i,j+1} - 4r_{ij}\right)
\]

\[
\frac{dp_{ijn}}{dt} = k_n r_{ij} p_{ijn}^2 - p_{ijn}(f + d_n) + g\left(p_{i-1,j,n} + p_{i+1,j,n} + p_{i,j-1,n} + p_{i,j+1,n} - 4p_{ijn}\right)
\]
Bifurcation Studies: Uniform feed dist*

2 CSTR

4 CSTR

locked

Tatara, et al 2002

Distribution of Feed Flow Rates

- Flow rates sampled from $N(f, \sigma)$
- Observe effect of $\sigma$

Degree of heterogeneity
Resource

$f = 0.002, \sigma = 0.001$
Net Avg Resource

\[ f = 0.002, \sigma = 0.001 \]
Stable Regions

Emergence of stability

$f = 0.005, \sigma = 0$
Resource 0.001

\[ f = 0.005, \sigma = \]

\[ r \]

\[ r \]

\[ g \]
Net Avg Resource $f = 0.005, \sigma = 0.001$
Automated Continuation

1. Identify stable point $p_0$
2. Increment bifurcation parameter
3. Use $p_0$ as initial guess for $p_1$
4. Solve for $p_1$ (LLNL KINSOL)
5. Test stability of $p_1$
6. Repeat 1-5 until unstable
7. Reverse direction
Analysis of Stable Regions

\( \sigma = 0 \)

\( \sigma = 10^{-4} \)

\( \sigma = 10^{-3} \)
Analysis of Stable Regions, $\sigma = 10^{-4}$

$g = 0.0008$

$g = 0.0011$
Analysis of Stable Regions, $\sigma = 10^{-3}$
Analysis of Stable Regions, $\sigma = 10^{-3}$
Conclusions

Heterogeneous network configuration

- Suppression of locked mode
- Emergence of new stable points
  - Increased number of states
  - Increased range of stability wrt bifurcation parm

Network operability and flexibility

- Close proximity of states

Natural systems and evolutionary diversity
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