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SA

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- (VCM)  
- (EDC) :

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Power law

Langmuir-Hinshelwood [ ] Godínez-Cabanes [ ]  
 [ ] BOS [ ]

( )

: Power law

Power Law

$$(r_{C_2H_2}) = K_i (p_{C_2H_2})^a (p_{H_2})^b \quad ( )$$

Power law

( )

:C. Godínez-A, L. Cabanes

$$(-r_{C_2H_2}) = k_1 (p_{C_2H_2})^{m_1} (p_{H_2})^{m_2} \quad ( )$$

SA

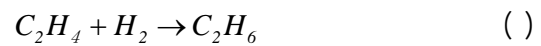
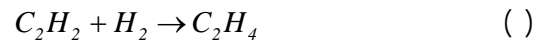
$$(-r_{C_2H_6}) = k_2 (p_{C_2H_4})^{m_3} (p_{H_2})^{m_4} \quad ( )$$

front-end

$$(-r_{C_2H_2}) = \frac{K_1 (p_{C_2H_2})^{m_1} (p_{H_2})^{m_2}}{(p_{CO})^{m_3}} \quad ( )$$

$$(-r_{C_2H_6}) = \frac{K_2 (p_{C_2H_4})^{m_4} (p_{H_2})^{m_5}}{(p_{CO})^{m_6}} \quad ( )$$

:Langmuir-Hinshelwood



Langmuir-

Hinshelwood

SA

$$f = \sum_{i=1}^n \sum_{j=1}^l [C_{ij,ind} - C_{ij,sim}]^2 \quad ( )$$

-                      j                      i                      C<sub>ij</sub>

Hysys                      Hysys

MATLAB

Hysys                      MATLAB

MATLAB

C-                      31C

Simulated

(SA) Annealing

Minimize  $f(x)$  subject to  $G_i(x)$ ,  $i = 1, \dots, m_e$

$G_i(x) \leq 0$ ,  $i = m_e+1, \dots, m$

:

$$r_1 = \frac{K_1 \times e^{-E_1/T} \times [C_2 H_2]^{X_1} \times [H_2]^{Y_1}}{(1 + A_1 [H_2] + B_1 [C_2 H_2] + C_1 [C_2 H_4])^{Z_1}} \quad ( )$$

$$r_2 = \frac{K_1 \times e^{-E_2/T} \times [C_2 H_4]^{X_2} \times [H_2]^{Y_2}}{(1 + A_2 [H_2] + B_2 [C_2 H_2] + C_2 [C_2 H_4])^{Z_2}} \quad ( )$$

:

Bos

Langmuir-Hinshelwood

:

$$r_{C_2H_2} = \frac{k_1 P_{C_2H_2} P_{H_2}}{(1 + k_2 P_{C_2H_2} + k_3 P_{H_2} + k_4 P_{C_2H_2} P_{H_2})} \quad ( )$$

$$r_{C_2H_6} = \frac{k_5 P_{C_2H_4} P_{H_2}}{(1 + k_6 P_{C_2H_2} + k_7 P_{C_2H_4})^3} \quad ( )$$

:

$$K_i = A_i \exp\left(\frac{E_i}{RT}\right) \quad ( )$$

p (mol/sec/m<sup>3</sup>)                      r

E (Pa)

T (Pa m<sup>3</sup>/mol K)                      R (J/mol)

m<sub>1</sub>, m<sub>2</sub> (m<sup>6</sup>/mol kgcat s)                      A (K)

m<sub>3</sub>, m<sub>4</sub>, m<sub>5</sub>, m<sub>6</sub> a, b

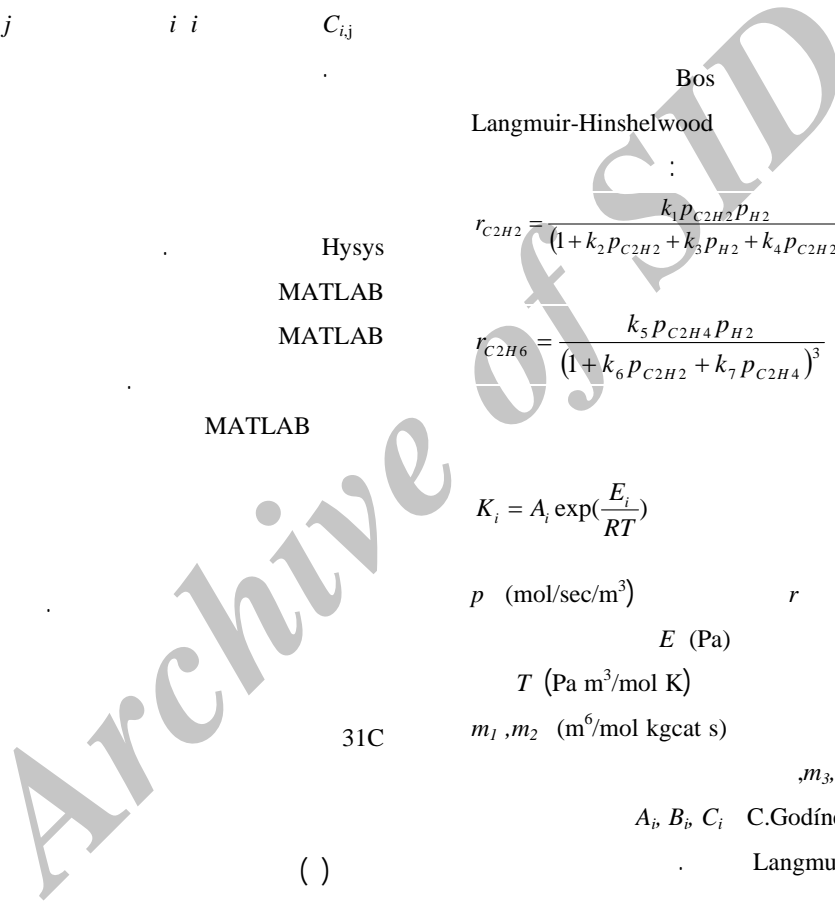
A<sub>i</sub>, B<sub>i</sub>, C<sub>i</sub> C.Godínez-A.L.Cabanes

( )                      Langmuir-Hinshelwood

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|       |       |
|-------|-------|
| (m)   | 5     |
| (°C)  | 182.2 |
| (bar) | 6.4   |



[ ]

(Holland)

$f(x)$

$x$

$m$

$G_i(x)$

(Fitness)

( )

(Tournament)



Archive

[ ]

(K.De.Johng)

[ ]

(Richenberg)

( )  
( )

(Selection Operator)

:(Roulette Wheel) ( )

:(Tournament) ( )

(Mating pool)

:(Stochastic) ( )

GA

:(Reminder) ( )

John Koza  
(Genetic programming)

(Mutation)

(Crossover)

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$$Child = Parent2 + ratio \times (Parent2 - Parent1) \quad ( )$$

GA

:(Single Point) ( )

GA

:(Two Points) ( )

" "

:(Scattered) ( )

GA

:(Intermediate) ( )

GA

Blind Watchmakers

$$Child = Parent1 + random \times ratio \times (Parent2 - Parent1) \quad ( )$$

GA

:(Heuristic) ( )

[ ]

SA  
( )

Langmuir- Godínez-Cabanes Power law  
Bos Hinshelwood

SA

SA

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Rank

tournament selection

:SA (Simulated Annealing)

SA

(Kirk Patrik)

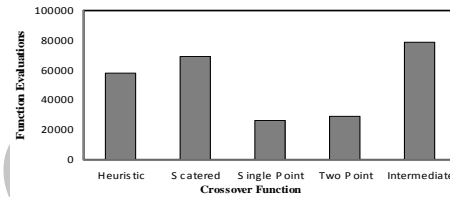
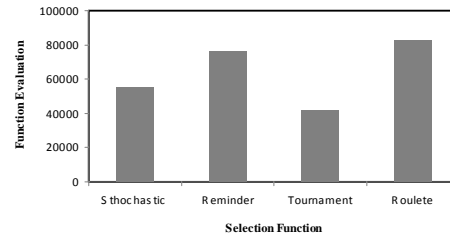
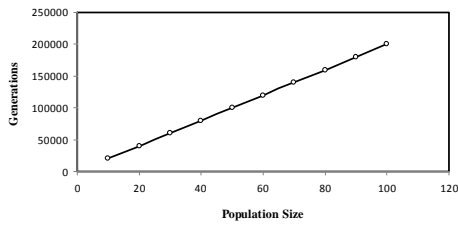
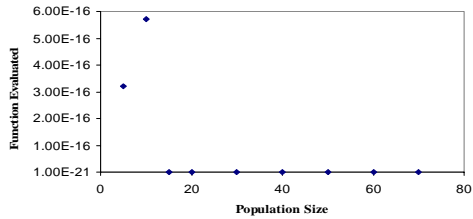
SA [ ]

(Annealing)

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Tournament

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SA

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Power law

Godínez-Cabanes /

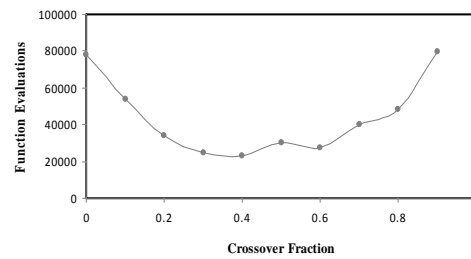
Langmuir-Hinshelwood /

/ Bos /

$$error = \sum \left| \frac{C_{i,j,sim} - C_{i,j,ind}}{C_{i,j,ind}} \right| \quad ( )$$

**Power law**

|  | GA     | SA     |        |
|--|--------|--------|--------|
| A <sub>1</sub> (m <sup>6</sup> /mol kgcat s) | 464.14 | 10     | 1.05e3 |
| E <sub>1</sub> (J/mol)                       | 6.39e8 | 5.81e6 | 46     |
| a  | 0.39   | 0.5    | -0.5   |
| b  | 0.4424 | 1      | 1      |
| Error%                                       | 64.4   | 65.8   | 178.68 |
| Duration time(Sec)                           | 13200  | 960    |        |



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**Langmuir-Hinshelwood**

|  | SA     | GA     |        |
|--|--------|--------|--------|
| A <sub>1</sub> (m <sup>6</sup> /mol kgcat s) | 9.88e2 | 1.44e2 | 1.51e3 |
| E <sub>1</sub> (J/mol)                       | 2.94e4 | 5.83e6 | 2.96e2 |
| A <sub>2</sub> (m <sup>6</sup> /mol kgcat s) | 3.05e4 | 1.82e2 | 1.22e2 |
| E <sub>2</sub> (J/mol)                       | 3.3e2  | 8.89e5 | 8.77e7 |
| X!   | 0.59   | 3.95   | 0.5    |
| Y1   | 0.61   | 0.56   | 1      |
| A!   | 10     | 3.18e4 | 1.39e4 |
| B1   | 3.5e2  | 4.67e3 | 8.98e5 |
| C1   | 50     | 5.67e4 | 1.47e3 |
| Z1   | 2.85   | 1.95   | 3      |
| X2   | 0.5    | 0.86   | 1.25   |
| Y2   | 1.19   | 3.07   | 0.75   |
| A2   | 11     | 1.36e4 | 2.58e2 |
| B2   | 3.71e2 | 6.05e3 | 3.55e4 |
| C2   | 5.22e2 | 1.47e4 | 9.78e2 |
| Z2   | 3      | 2.63   | 1      |
| Error%                                       | 21.5   | 25.2   | 85.61  |
| Duration time(Sec)                           | 176400 | 135000 |        |

**Godínez-Cabanes**

|  | SA     | GA      |        |
|--|--------|---------|--------|
| A <sub>1</sub> (m <sup>6</sup> /mol kgcat s) | 1.96e2 | 103     | 31360  |
| E <sub>1</sub> (J/mol)                       | 1.44e4 | 104     | 67.45  |
| A <sub>2</sub> (m <sup>6</sup> /mol kgcat s) | 4.17e2 | 1.09e3  | 1.05e5 |
| E <sub>2</sub> (J/mol)                       | 1.04e5 | 1.022e4 | 86.71  |
| m <sub>1</sub>                               | 2.54   | 3       | 0      |
| m <sub>2</sub>                               | 2.92   | 3       | 1      |
| m <sub>3</sub>                               | 1.5    | 0.5     | 0      |
| m <sub>4</sub>                               | 4.5    | 2.28    | 1      |
| m <sub>5</sub>                               | 0.5    | 3.004   | 0.5    |
| m <sub>6</sub>                               | 0.15   | 0       | 0      |
| Error%                                       | 31.6   | 33.3    | 59.31  |
| Duration time(Sec)                           | 30060  | 19200   |        |

**Bos**

|  | SA      | GA      |          |
|--|---------|---------|----------|
| A <sub>1</sub> (m <sup>6</sup> /mol kgcat s) | 3.356   | 0.634   | 33.39    |
| E <sub>1</sub> (J/mol)                       | 12.26   | 0.371   | 14638    |
| A <sub>2</sub> (m <sup>6</sup> /mol kgcat s) | 1.41e2  | 0.189   | 5.11     |
| E <sub>2</sub> (J/mol)                       | -145.32 | -0.958  | -10.67   |
| A <sub>3</sub> (m <sup>6</sup> /mol kgcat s) | 1.03e4  | 65      | 3379     |
| E <sub>3</sub> (J/mol)                       | -0.98   | -1.021  | 0.0446   |
| A <sub>4</sub> (m <sup>6</sup> /mol kgcat s) | 3.67    | 0.98    | 17262.97 |
| E <sub>4</sub> (J/mol)                       | -5.5e6  | -2.82e4 | 3486.67  |
| A <sub>5</sub> (m <sup>6</sup> /mol kgcat s) | 3.56    | 4.13    | 10.17e-4 |
| E <sub>5</sub> (J/mol)                       | 1.67    | 17      | 40354    |
| A <sub>6</sub> (m <sup>6</sup> /mol kgcat s) | 1.04e4  | 256     | 44.635   |
| E <sub>6</sub> (J/mol)                       | -3.52   | -9      | -33806   |
| A <sub>7</sub> (m <sup>6</sup> /mol kgcat s) | 105     | 17.01   | 0.0316   |
| E <sub>7</sub> (J/mol)                       | 4.56e2  | -34     | -29400   |
| Error%                                       | 0.38    | 2.59e-2 | 27.45    |
| Duration time(Sec)                           | 198020  | 326250  |          |

/ / Power law  
 / / Langmuir-Hinshelwood  
 Godínez-Cabanes /  
 / Bos / /  
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Bos

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