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SA

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(VCM)

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(EDC)

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Power law

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

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: Power law

Power Law

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

Power law

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:C. Godínez-A, L. Cabanes

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

SA

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

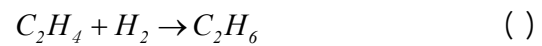
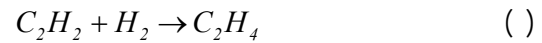
front-end

:

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

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

:Langmuir-Hinshelwood



Langmuir-

Hinshelwood

SA

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

MATLAB

MATLAB

MATLAB

MATLAB

(SA) Annealing

:

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

:

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

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Bos

Langmuir-Hinshelwood

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

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

:

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

:

C-31C

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Simulated

(m)	5
(°C)	182.2
(bar)	6.4

:

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Langmuir-Hinshelwood

C.Godínez-A.L.Cabanes

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

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

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(Holland)

$f(x)$

x

m

$G_i(x)$

(Fitness)

()

(Tournament)



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(K.De.Johng)

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(Richenberg)

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()

(Selection Operator)

:(Roulette Wheel) ()

:(Tournament) ()

(Mating pool)

GA

:(Stochastic) ()

:(Reminder) ()

John Koza
(Genetic programming)

(Mutation)

(Crossover)

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

GA
 : (Single Point) ()

GA
 " " : (Scattered) ()

GA
 : (Intermediate) ()

Blind Watchmakers

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

 GA : (Heuristic) ()

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SA

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Langmuir- Godínez-Cabanes Power law

Bos Hinshelwood

SA

SA

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Rank

tournament selection

:SA (Simulated Annealing)

SA

(Kirk Patrik)

SA []

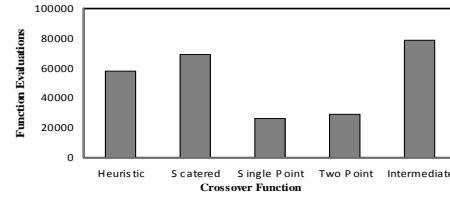
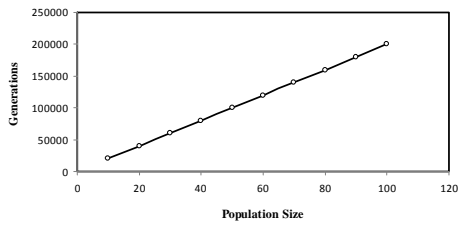
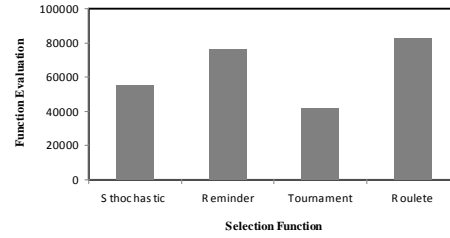
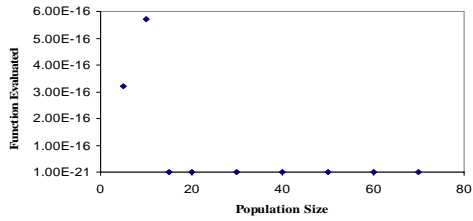
(Annealing)

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Tournament

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SA

() () ()

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Power law

Godínez-Cabanes /

Langmuir-Hinshelwood /

/ Bos /

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

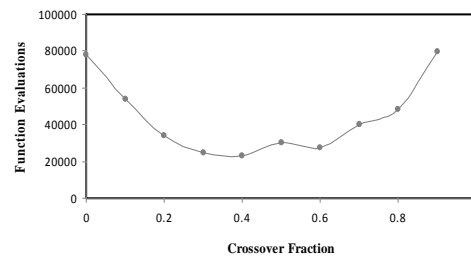
Power law

	GA	SA	
A ₁ (m ⁶ /mol kgcat s)	464.14	10	1.05e3
E ₁ (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 ₁ (m ⁶ /mol kgcat s)	9.88e2	1.44e2	1.51e3
E ₁ (J/mol)	2.94e4	5.83e6	2.96e2
A ₂ (m ⁶ /mol kgcat s)	3.05e4	1.82e2	1.22e2
E ₂ (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 ₁ (m ⁶ /mol kgcat s)	1.96e2	103	31360
E ₁ (J/mol)	1.44e4	104	67.45
A ₂ (m ⁶ /mol kgcat s)	4.17e2	1.09e3	1.05e5
E ₂ (J/mol)	1.04e5	1.022e4	86.71
m ₁	2.54	3	0
m ₂	2.92	3	1
m ₃	1.5	0.5	0
m ₄	4.5	2.28	1
m ₅	0.5	3.004	0.5
m ₆	0.15	0	0
Error%	31.6	33.3	59.31
Duration time(Sec)	30060	19200	

Bos

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

SA

SA

SA

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Tournament

/ / Power law

/ Langmuir-Hinshelwood

Godínez-Cabanes /

/ Bos / /

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Bos

Bos

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