Surface Kinetics Optimization

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Optimization Method

Physical Simulator

$$\hat{\gamma} = f(\vec{x}, \vec{y}(\vec{x}, \theta); \theta)$$

Objective Loss

$$\min_{\theta} J(\theta) = \sum_{i \in D} \left(\frac{\hat{\gamma}_i - \gamma_{exp,i}}{\gamma_{exp,i}} \right)^2$$

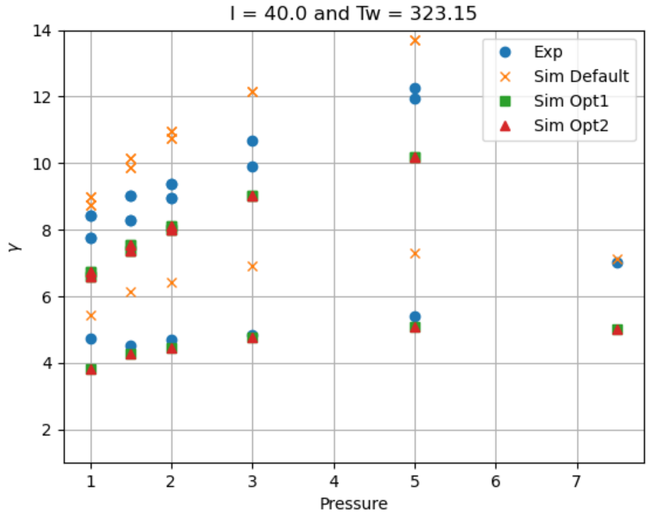
Optimization Problem

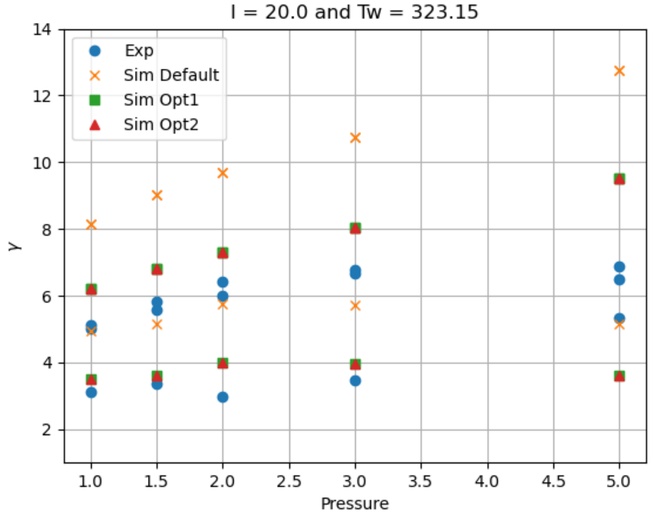
- Model based methods
- Model free methods
- Gradient-based Methods

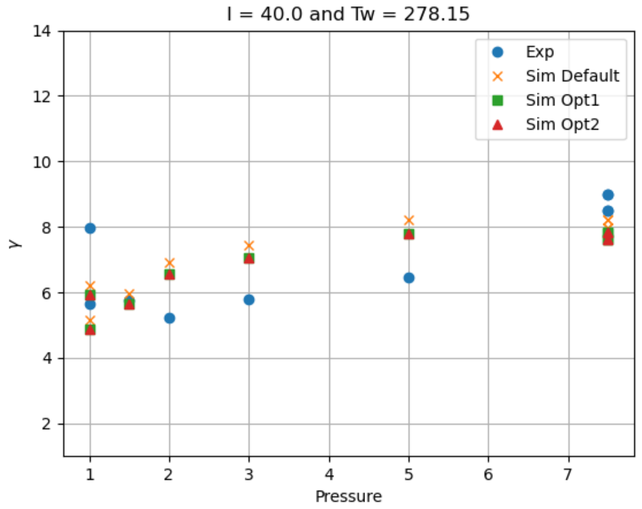
Results

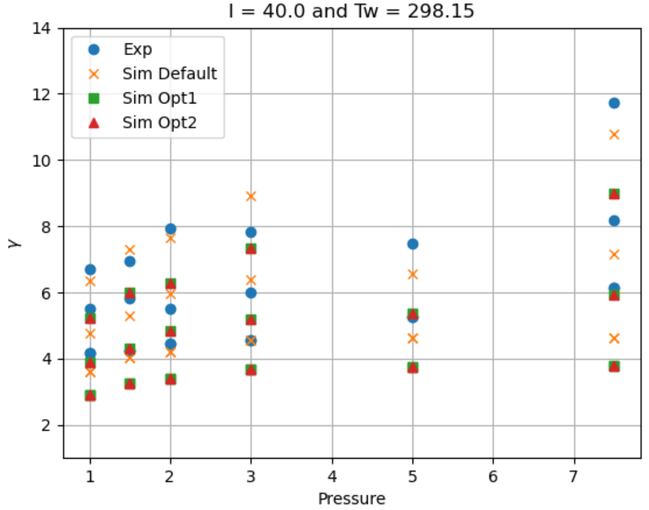
Desorption Frequency

$$\nu_d = A + B \,.\, e^{E/(RT_w)}$$





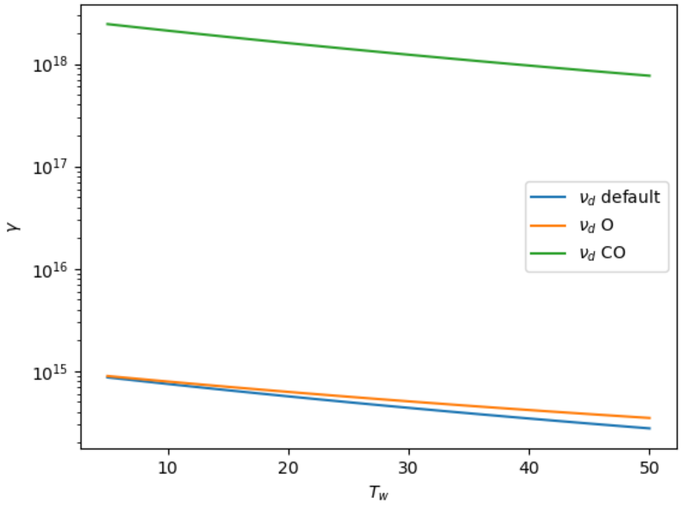




$$\mathscr{L}_{default} = 0.112$$

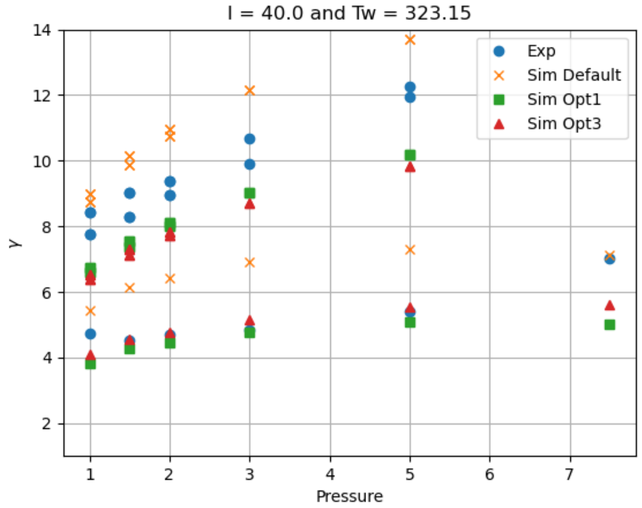
$$\mathscr{L}_{opt1} = 0.4074$$

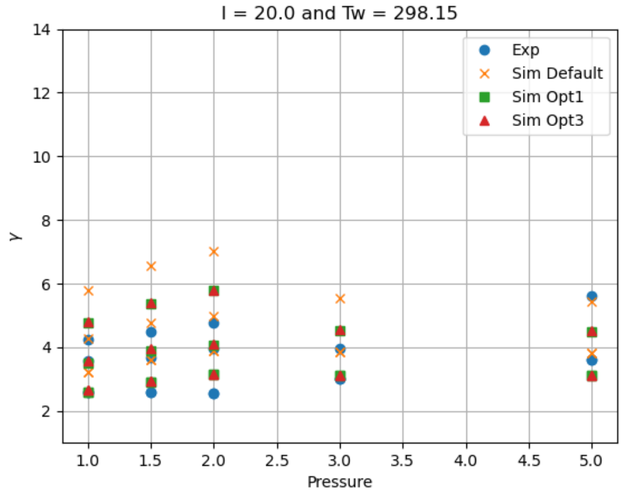
$$\mathscr{L}_{opt2} = 0.4073$$

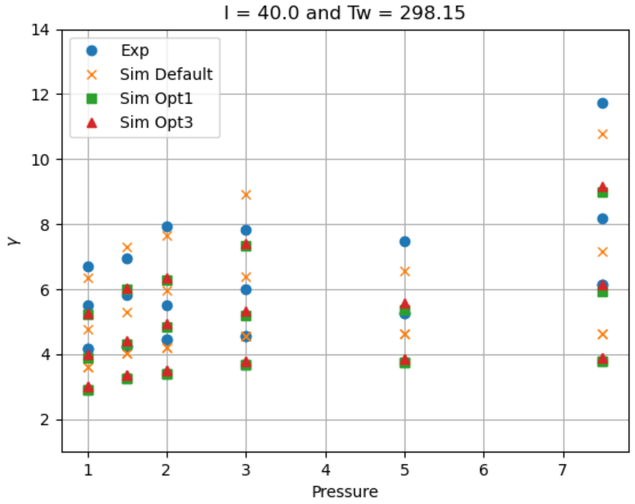


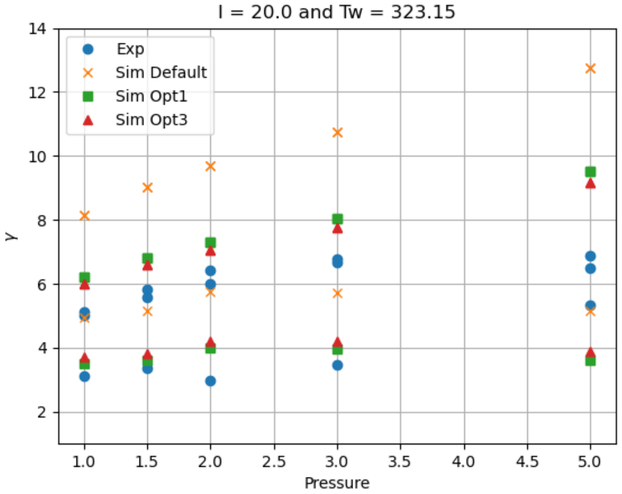
Results

SF CO reactions









$$\mathscr{L}_{default} = 0.112$$

$$\mathscr{L}_{opt1} = 0.4074$$

$$\mathscr{L}_{opt3} = 0.0385$$

Results

SF CO reactions

	$\mathscr{L}_{default,opt1}$	$\mathscr{L}_{opt3}$
$\mathrm{CO(g)} + \mathrm{S}_V \rightarrow \mathrm{CO}_S$	10^{-2}	$1.9 * 10^{-2}$
$\mathrm{O(^3P)} + \mathrm{CO}_F \rightarrow \mathrm{CO_2(g)} + \mathrm{F}_V$	10^{-1}	$5.6 * 10^{-2}$
$\mathrm{CO(g)} + \mathrm{O}_F \rightarrow \mathrm{CO_2(g)} + \mathrm{F}_V$	10^{-1}	$4.3 * 10^{-2}$
$\mathrm{CO}_F + \mathrm{S}_V \rightarrow \mathrm{CO}_S + \mathrm{F}_V$	10^{-2}	$4.5 * 10^{-1}$
$\mathrm{O(^3P)} + \mathrm{CO}_S \rightarrow \mathrm{CO_2(g)} + \mathrm{S}_V$	10^{-2}	$5.78 * 10^{-1}$
$\mathrm{CO(g)} + \mathrm{O}_S \rightarrow \mathrm{CO_2(g)} + \mathrm{S}_V$	10^{-1}	$5.5 * 10^{-2}$
$\mathrm{O}_F + \mathrm{CO}_S \rightarrow \mathrm{CO_2(g)} + \mathrm{F}_V + \mathrm{S}_V$	10^{-1}	$5.59 * 10^{-3}$
$\mathrm{CO}_F + \mathrm{O}_S \rightarrow \mathrm{CO_2(g)} + \mathrm{F}_V + \mathrm{S}_V$	10^{-1}	$1.98 * 10^{-1}$

$$\mathscr{L}_{default} = 0.112$$

$$\mathscr{L}_{opt1} = 0.4074$$

$$\mathscr{L}_{opt3} = 0.0385$$

Error Propagation

Input conditions become RV

$$X = \{X_1, X_2, \ldots, X_n\} \qquad P(X_1, X_2, \ldots, X_n) = \prod_{i=1}^{n} P(X_i)$$

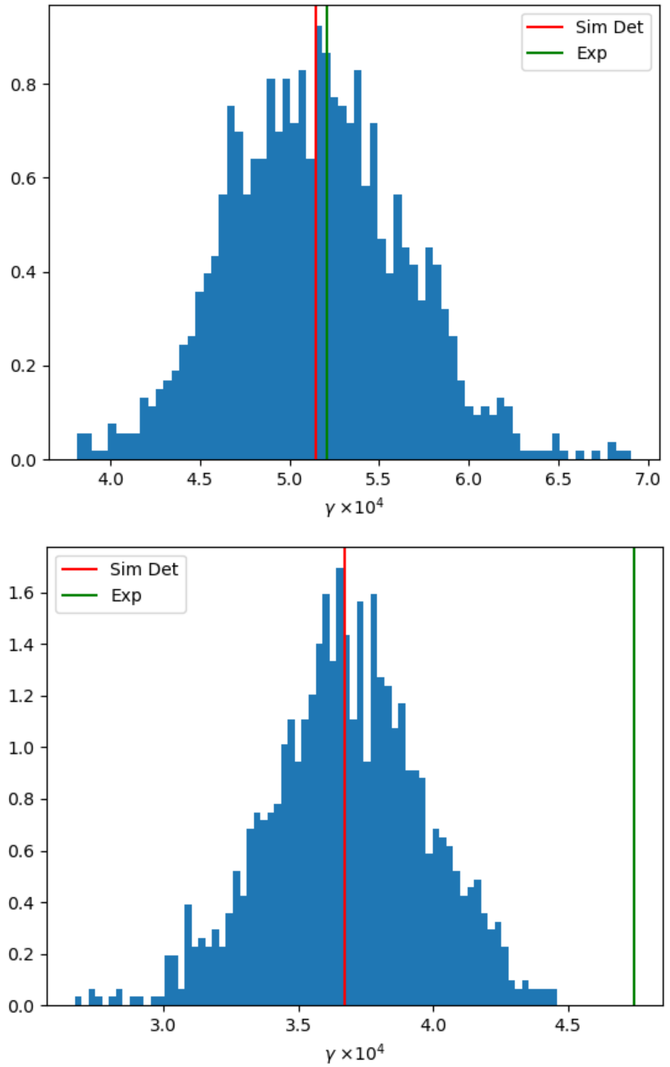
$$\gamma = \tilde{f}(X_1, X_2, \ldots, X_n)$$

$$P(\gamma \,|\, X_1, \ldots, X_n) = \delta(\gamma - \tilde{f}(X_1, X_2, \ldots, X_n))$$

$$P(\gamma) = \int_{x_1} \ldots \int_{x_n} \delta(\gamma - \tilde{f}(x_1, \ldots, x_n)) P(x_1, \ldots, x_n) dx_1 \ldots dx_n$$

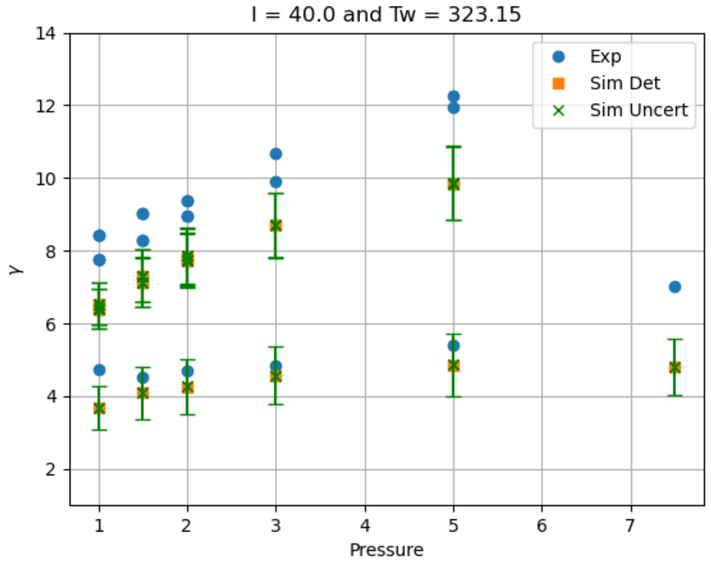
Monte Carlo

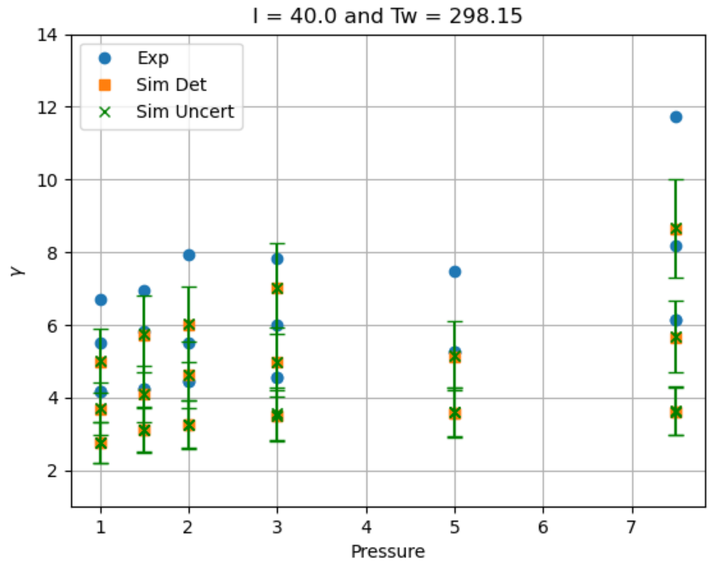
Samping

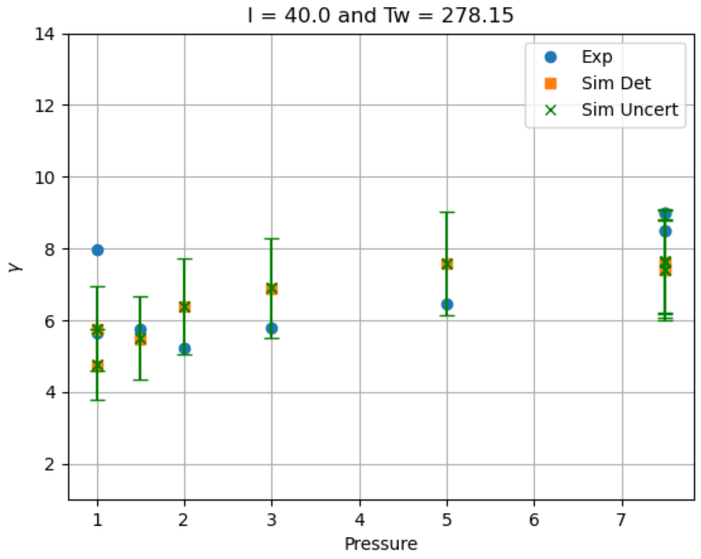


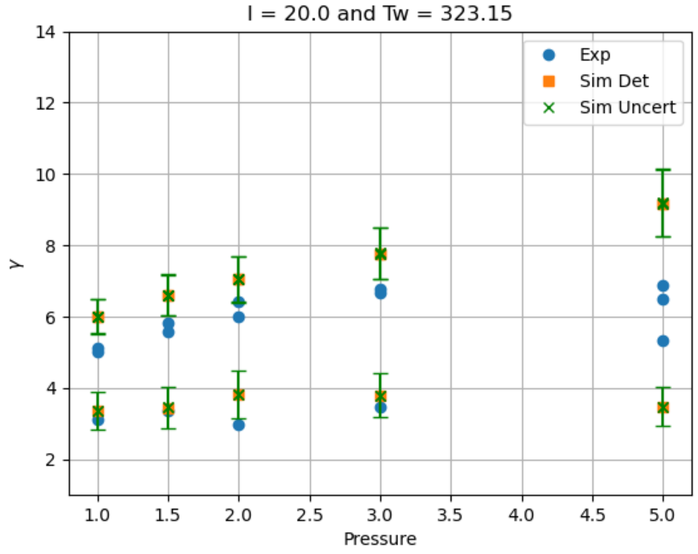
Error Propagation

Results









$$CO : 10\,\%$$
$$CO_2 : 10\,\%$$
$$O : 10\,\%$$
$$O_2 : 10\,\%$$
$$T_w : 1\,\%$$
$$T_{gas} : 1\,\%$$

$$E_i \sim \tilde{\mathcal{N}}(\bar{E}_i, f^2 \,.\, \bar{E}_i^2)$$