Bayesian Inference on Uncertain Kinetic Parameters for the Pyrolysis of Composite Ablators

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Motivation: atmospheric entry

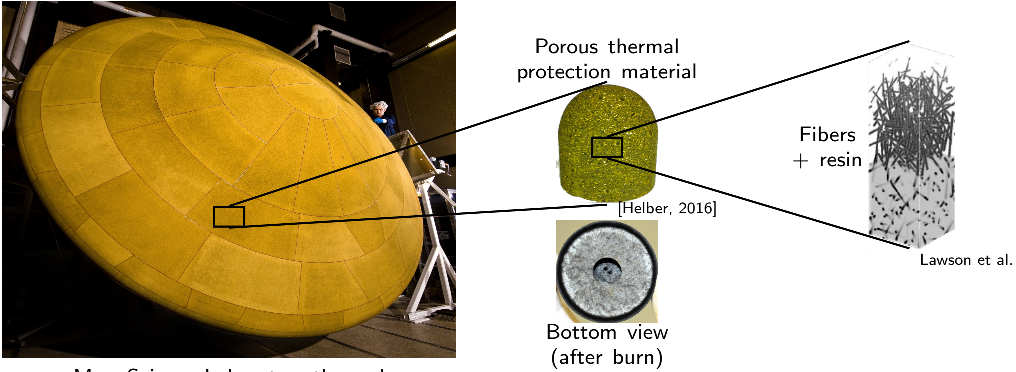
Thermal protection systems (TPS)

Dragon capsule (Space X)

Space debris

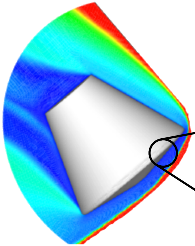
ATV-1 *Jules Verne* (ESA)

Ablative materials for thermal protection systems



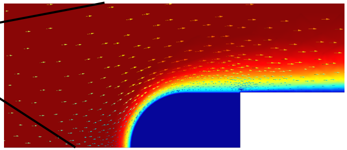
Mars Science Laboratory thermal
protection system (NASA)

Modeling the pyrolysis of ablative thermal protection materials

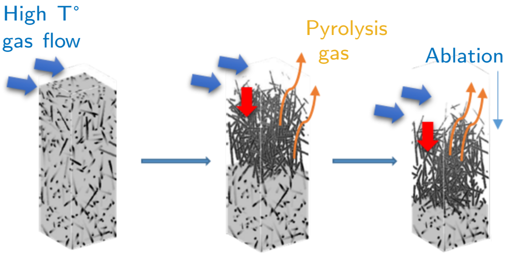


Aerodynamic simulation
(CooLFluiD, VKI)

Aerothermal simulation
(Argo, Cenaero)



[Coheur, 2017]



- CFD codes requires accurate model for ablation [Lachaud, 2014; Schrooyen, 2016], e.g. conservation of mass species

$$\frac{\partial \epsilon_g \langle \rho_i \rangle_g}{\partial t} + \nabla \cdot (\epsilon_g \langle \rho_i \rangle_g \langle u \rangle_g) = \nabla \cdot \langle J_i \rangle + \langle \dot{\omega}_i^{\text{pyro}} \rangle$$

- The governing laws for the pyrolysis gas production $\langle \dot{\omega}_i^{\text{pyro}} \rangle$ must be derived from recent experimental studies and their associated uncertainties must be quantified

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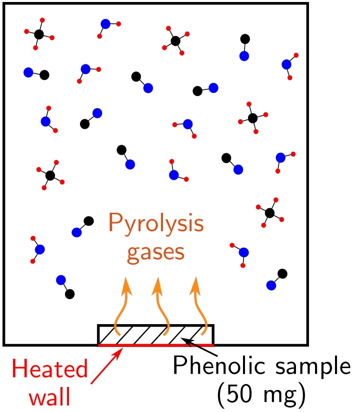
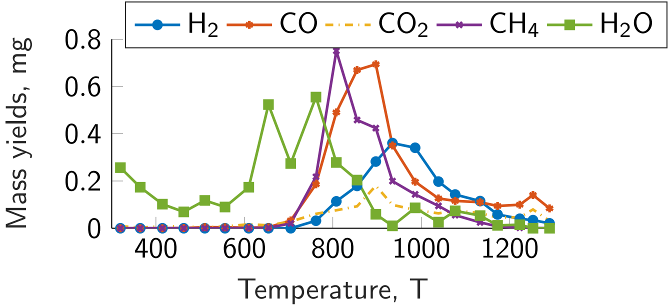
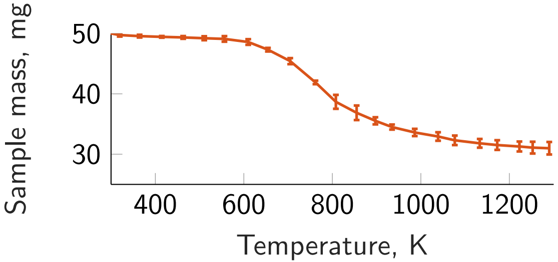
Pyrolysis experiments [Wong et al., 2015]

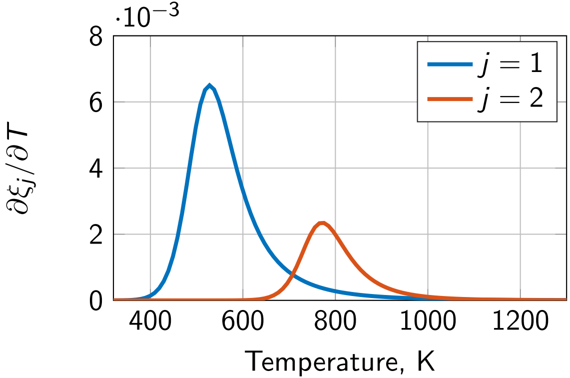






Phenomenological laws for pyrolysis mass loss and gas species production

- Previous pyrolysis experiments showed that the pyrolysis decomposition of ablative materials follows successive reaction rates [Goldstein, 1969; Trick, 1997]



$$\langle \dot{\omega}_i^{\mathrm{pyro}} \rangle = \sum_j^{N_\mathrm{p}} F_{ij} \frac{\partial \xi_j}{\partial T} \tau m_0$$

$$\frac{\partial \xi_j}{\partial T} = (1 - \xi_j)^{n_j} \frac{A_j}{\tau} \exp\left(-\frac{E_j}{\mathcal{R} T} \right)$$

- ξ_j: advancement of reaction of the fictitious resin component j

Phenomenological laws for pyrolysis mass loss and gas species production

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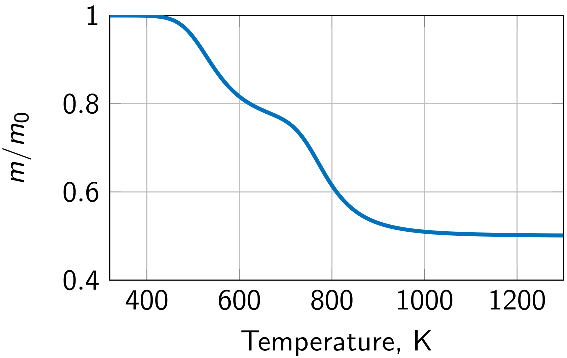

$$m = m_0 - \sum_{j}^{N_p} F_j \xi_j m_0$$

$$\frac{\partial \xi_j}{\partial T} = (1 - \xi_j)^{n_j} \frac{A_j}{\tau} \exp\left(-\frac{E_j}{\mathcal{R} T}\right)$$

- ξ_j: advancement of reaction of the fictitious resin component j

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Mathematical description

- Forward problem: $d_i = \eta(\mathbf{x}_i, \mathbf{p})$

  code output ← d_i ; η → model

- Inverse problem: Find $\mathbf{p}$ knowing the observations d_i^{obs} associated with errors ε_i

$$d_i^{\text{obs}} = \eta(\mathbf{x}_i, \mathbf{p}) + \varepsilon_i$$

Deterministic inverse problem
What is the best estimate of $\mathbf{p}$*?*

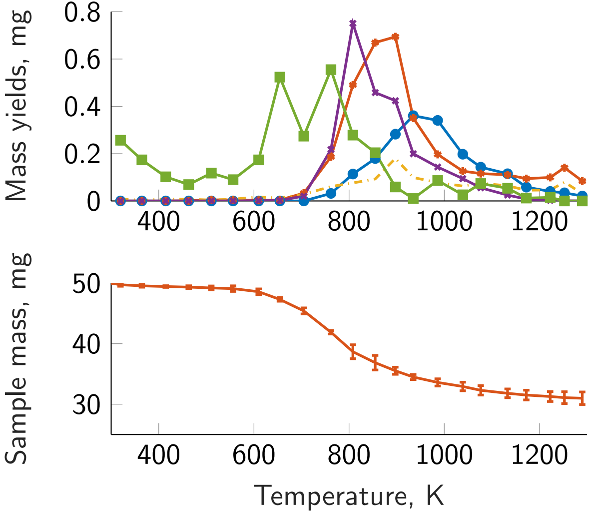
$$\tilde{\mathbf{p}} = \arg\min_{\mathbf{p}\in\mathcal{P}_{\text{ad}}} ||\mathbf{d}^{\text{obs}} - \mathbf{d}||$$

Statistical inverse problem
What is the plausibility about $\mathbf{p}$*?*

$$\pi(\mathbf{p}|\mathbf{d}^{\text{obs}}) = \frac{\pi(\mathbf{d}^{\text{obs}}|\mathbf{p})\pi_0(\mathbf{p})}{\int_{\mathbb{R}^p} \pi(\mathbf{d}^{\text{obs}}|\mathbf{p})\pi_0(\mathbf{p})d\mathbf{p}}$$

Pyrolysis experiments: the forward problem

Experimental observations d_{ik}^{obs}



Code outputs

- Collected mass of species i

$$d_{ik} = \int_{t_{k-1}}^{t_k} \langle \dot{\omega}_i^{\text{pyro}} \rangle |_{T=T_k} dt$$

$$= \sum_j^{N_p} F_{ij} m_0 \left(\xi_j^{(t_f)} - \xi_j^{(t_i)} \right)$$

- Mass of the sample

$$m_k = m_0 - \sum_{i=1}^{n_s} \sum_{l=1}^{k} d_{il}$$

Bayesian inference: the inverse problem

$$\pi(\mathbf{p}|\mathbf{d}) = \frac{\pi(\mathbf{d}|\mathbf{p})\pi_0(\mathbf{p})}{\int_{\mathbb{R}^p} \pi(\mathbf{d}|\mathbf{p})\pi_0(\mathbf{p})d\mathbf{p}} \qquad \text{(Bayes' theorem)}$$

- Choice for the prior $\pi_0(\mathbf{p})$: uniform pdf (bounded support)

- Choice for the likelihood $\pi(\mathbf{d}^{\text{obs}}|\mathbf{p})$

$$\pi(\mathbf{d}^{\text{obs}}|\mathbf{p}) = \frac{1}{\prod_i (2\pi{\sigma_i}^2)^{n/2}} \exp\left(-\sum_{i=1}^{n_s} \sum_{k=1}^{n} \frac{\left[d_{ik}^{\text{obs}} - \eta_i(\mathbf{x}_k, \mathbf{p})\right]^2}{2{\sigma_i}^2} \right)$$

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Metropolis-Hastings algorithm

1. Initialize $\mathbf{p}_0$
2. Iteration i :
   a) Draw a new value $\mathbf{p}^*$ from proposal distribution $J(\cdot|\mathbf{p}_{i-1})$. J specifies $\mathbf{p}^*$ based on previous value $\mathbf{p}_{i-1}$, and $J(\cdot|\mathbf{p}_{i-1})$ should not be interpreted as a conditional density.
   b) Construct acceptance probability

$$\alpha(\mathbf{p}^*|\mathbf{p}_{i-1}) = \min\left(1, \frac{\pi(\mathbf{p}^*|\mathbf{d})J(\cdot|\mathbf{p}_{i-1})}{\pi(\mathbf{p}_{i-1}|\mathbf{d})J(\mathbf{p}_{i-1}|\cdot)}\right) \tag{1}$$

   c) Sample a Uniform(0,1) random variable U. Set

$$\mathbf{p}^i = \begin{cases} \mathbf{p}^*, & \text{if } U \leq \alpha(\mathbf{p}^*|\mathbf{p}_{i-1}) \\ \mathbf{p}^{i-1}, & \text{otherwise} \end{cases} \tag{2}$$

In practice ...

- Choice for the proposal $J(\mathbf{p}^*|\mathbf{p}_{i-1}) \rightarrow$ random walk metropolis

$$J(\mathbf{p}^*|\mathbf{p}_{i-1}) = \frac{1}{\sqrt{(2\pi)^m \det\Sigma}} \exp\left(-\frac{1}{2}\left(\mathbf{p}^* - \mathbf{p}_{i-1}\right)^{\mathrm{T}} \Sigma^{-1} \left(\mathbf{p}^* - \mathbf{p}_{i-1}\right)\right)$$

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 & \cdots & \rho_{1m}\sigma_1\sigma_m \\ \rho_{21}\sigma_2\sigma_1 & \sigma_2^2 & \rho_{2m}\sigma_2\sigma_m & \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{m1}\sigma_m\sigma_1 & \rho_{m2}\sigma_m\sigma_2 & \cdots & \sigma_m^2 \end{pmatrix}$$

- We assume Σ to be a diagonal matrix

- Using $\log(A)$ and $\log(E)$ values increases the mixing

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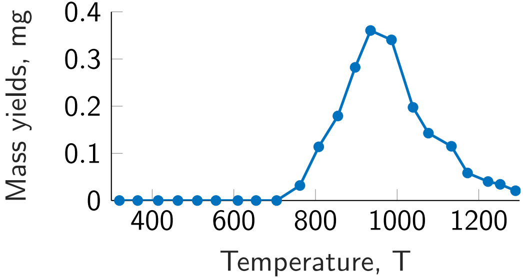
Numerical set-up: one reactant model with one species

- Observable (data) $d^{\text{obs}}_{\text{H}_2 k}$: mass yields of species H_2 at each temperature. $N_\text{p} = 1$.

$$d_{\text{H}_2 k} = F_{\text{H}_2} m_0 \left(\xi^{(k)} - \xi^{(k-1)}\right),$$

$$\frac{\partial \xi^{(k)}}{\partial t} = \left(1 - \xi^{(k)}\right)^n A \exp\left(-\frac{E}{\mathcal{R} T_k}\right),$$

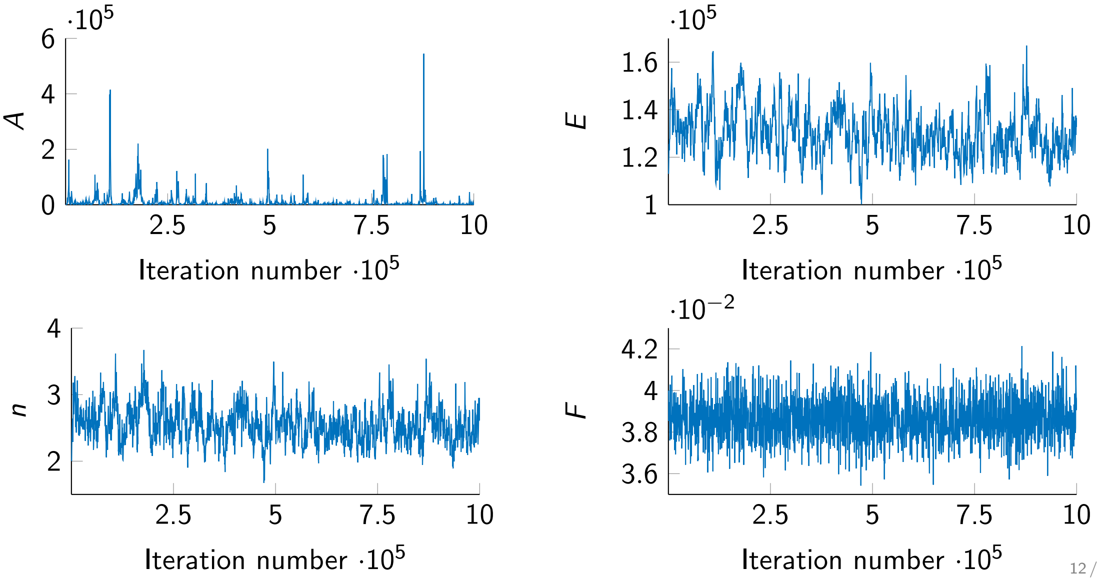
$$\xi^{(0)} = 0.$$



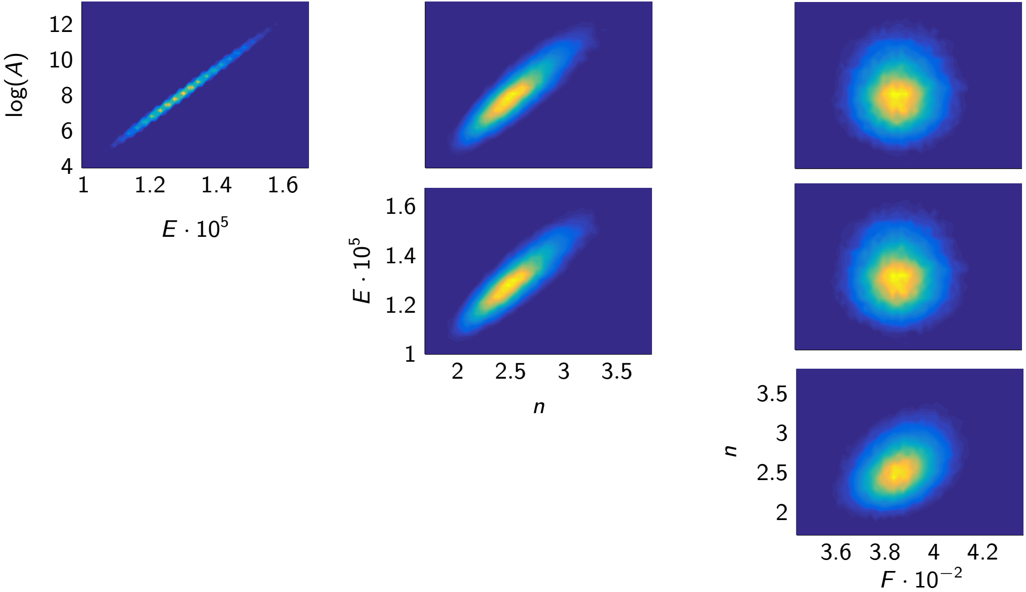
- Simple point-mass model (0D), $k = 1, \dots, n_\text{T}$

- $\mathbf{p} = \{A, E, n, F_{\text{H}_2}\}$

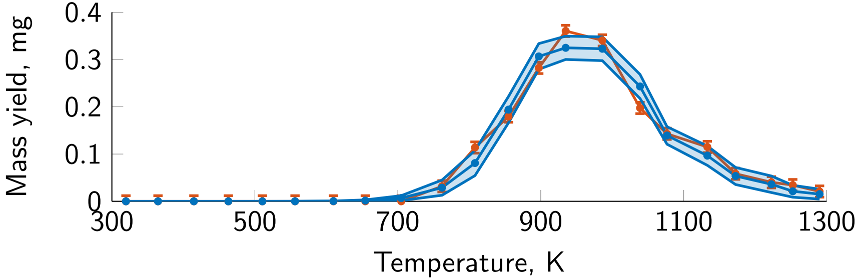
Application to pyrolysis experiments: Markov-Chain

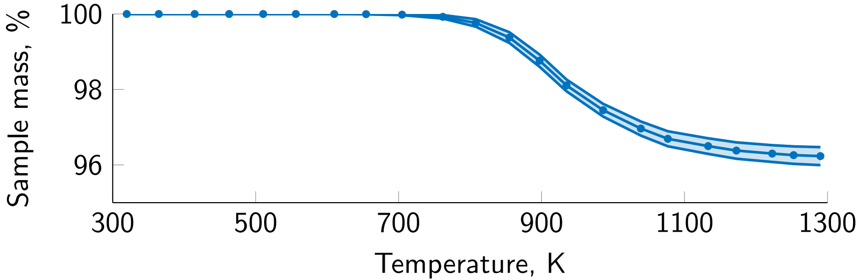


Bivariate posterior PDFs



Posterior predictive checks assuming 1 reactant (4 parameters)





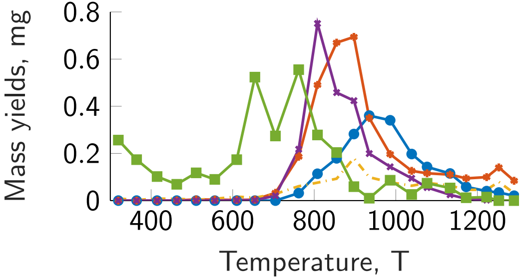
Numerical set-up: 3 reactants model with 5 species

- Observable (data) d_{ik}^{obs} with $i = \{H_2, CO, CO_2, CH_4, H_2O\}$: mass yields at each temperature iteration k. $N_p = 3$.

$$d_{ik} = \sum_{j}^{N_p} F_{ij} m_0 \left(\xi_j^{(k)} - \xi_j^{(k-1)} \right),$$

$$\frac{\partial \xi_j^{(k)}}{\partial t} = \left(1 - \xi_j^{(k)}\right)^{n_j} A_j \exp\left(-\frac{E_j}{\mathcal{R} T_k}\right),$$

$$\xi_j^{(0)} = 0.$$



- Simple point-mass model (0D), $k = 1, \ldots, n_T$

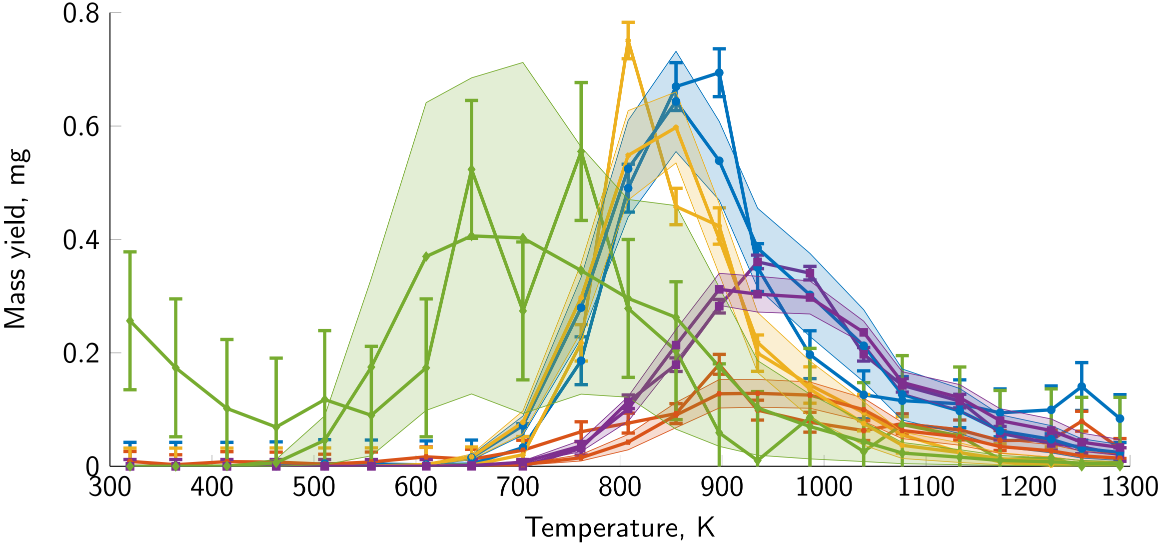
$$\mathbf{p} = \{ \{A_3, E_3, n_3, F_{H_2O,3}, \} \quad \{A_2, E_2, n_2, F_{CO,2}, F_{CH_4,2}, F_{H_2O,2}\}, \quad \{A_1, E_1, n_1, F_{CO,1}, F_{CO_2,1}, F_{H_2,1}\} \}$$

$R_1 \rightarrow H_2O$

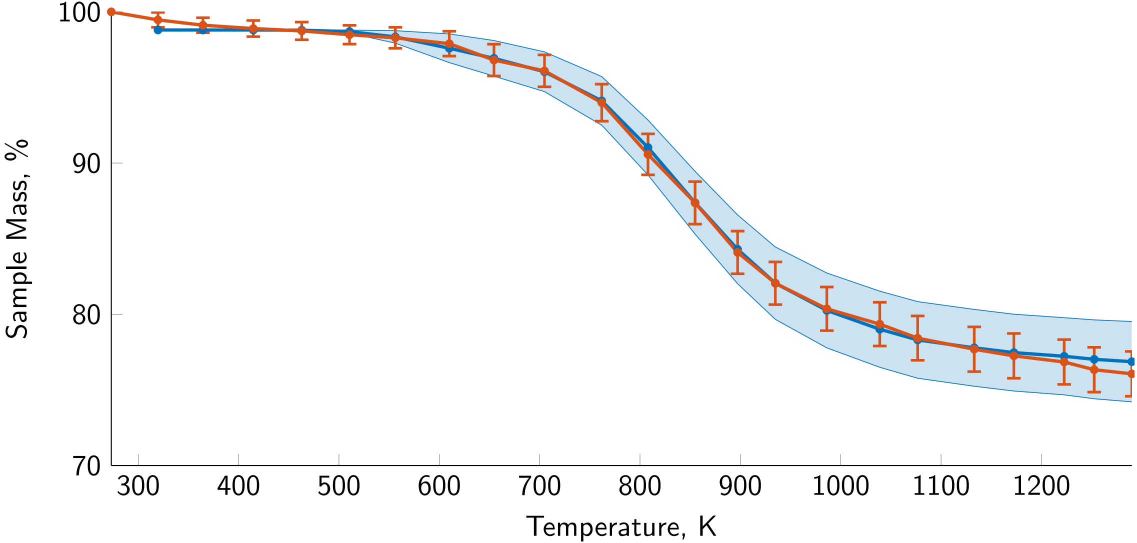
$R_2 \rightarrow CO + CH_4 + H_2O$

$R_3 \rightarrow CO + CO_2 + H_2$

Posterior predictive checks: 3 reactants model with 5 species



Posterior predictive checks: 3 equations, 5 species



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Conclusions and further work

Conclusions:

- Application of a simple model to simulate pyrolysis experiments
- Inference on parameter laws using Bayesian approach
- Efficient method to find kinetic parameters and characterize their uncertainties
- Simulation of mass yields with error bars using the simulated posterior samples. Good agreement with experimental curves.

Further work:

- Improve algorithms to allow the use of more elaborated models. Adaptive MCMC has a high rejection rate. Use Hamiltonian Monte Carlo?
- Inference on reaction mechanisms together with parameter inference [Galagali and Marzouk, 2016]
- Results interpretation and their used in CFD codes

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Additional Information

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Simple model for simulating pyrolysis experiments

For point-mass material, conduction is assumed to be instantaneous and T is uniform inside the material (lumped capacitance model, $\mathrm{Bi} = \frac{L_c h}{k} << 1$).

- $T = T_i = \mathrm{cte}$ in $\Delta t = [0, t_f]$

$$\xi(t) = 1 - \left[(1-n)\left(C_i - A\exp\left(-\frac{E}{RT_i}\right)t\right)\right]^{1/(n-1)}, \quad \text{with } C_i = \frac{(1-\xi(0))^{1-n}}{1-n}$$

- $T_{\text{out}} = \tau t$, τ heating rate

$$\xi(T) = 1 - \left\{(1-n)\left[-\frac{A}{\tau}T\exp\left(\frac{-E}{RT}\right) - \frac{A}{\tau}\frac{E}{R}\mathrm{Ei}\left(-\frac{E}{RT}\right) + C\right]\right\}^{\frac{1}{1-n}}$$

$$C = \frac{(1-\xi_0)^{1-n}}{1-n} + \frac{A}{\tau}T_0\exp\left(\frac{-E}{RT_0}\right) + \mathrm{Ei}\left(\frac{-E}{RT_0}\right)\frac{EA}{\tau}, \quad \text{where } \mathrm{Ei}(x) \equiv \int_{-\infty}^{-x}\frac{\exp(v)}{v}dv$$

For more complex temperature evolution, integration should be performed numerically. When $Bi > 1$ ($L_c, h \nearrow$, or $k \searrow$) more complex model should be used (Argo).