FIRST-ORDER CHEMICAL REACTIONS IMPLEMENTATION IN RUBY

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Contents

1. Theory

Consider a batch reactor hosting a first-order-kinetics chemical reaction of the form $\mathrm{R} \xrightarrow{k} \mathrm{P}$, where R represents the reactant and P the product and k the reaction kinetic coefficient, $\dim k = 1/\mathsf{T}$.

Let t represent the chemical reaction duration, $\dim t = \mathsf{T}$, let $r = r\,[t]$ be R molar concentration and let $p = p\,[t]$ be P molar concentration, $\dim r = \dim p = \mathsf{N}/\mathsf{L}^3$. Consider r_i to be the reactant concentration when $t = 0$. Then, model the reaction kinetics by applying the mass conservation principle to the reactor:

$$r' = -kr \qquad \text{and} \qquad r\,[0] = r_\mathrm{i}\,,$$

where r' represents the reactant accumulation rate, $\dim r' = \mathsf{N}/\mathsf{T}\mathsf{L}^3$.

To find the reactant concentration, solve the differential equation by separating variables and applying the initial condition to have

$$r = r_\mathrm{i} \exp\,[-kt]\ .$$

Choose the set $\{\mathsf{N}, \mathsf{L}, \mathsf{T}\}$ as a dimensional system. Then, non-dimensionalize the model by applying the transformations

$$r_\mathrm{i}\,\Pi_r = r\,, \qquad r_\mathrm{i}\,\Pi_p = p \qquad \text{and} \qquad \Pi_t = kt\,,$$

which yields

$$\Pi_r = \exp\,[-\Pi_t]\ .$$

Next, to calculate the product concentration, apply the stoichiometric [1] condition $\Pi_r + \Pi_p = 1$:

$$\Pi_p = 1 - \exp\,[-\Pi_t]\ .$$

Now, compute the half-life time, $\Pi_{t=0.5}$, defined as the time at which the product concentration equals the half of the reactant concentration:

$$\Pi_{t=0.5} = \ln\,[2]\ .$$

Finally, find the 99.99%-life time, $\Pi_{t=0.9999}$: the time at which the product concentration equals 99.99% of the reactant concentration:

$$\Pi_{t=0.9999} = -\ln\,[1 - 0.9999] = \ln\,[10000]\ . \qquad \square$$

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[1] In dimensional form, the stoichiometric condition is $r + p = r_\mathrm{i}$.

$$E = \frac{-\Delta G}{ZF} - \frac{RT}{ZF} e_n \left(\frac{P_x}{P_y} \right)$$

Appendix A. Notation

A.1. **Maths.**

A.1.1. *Sets.*

- set: set A, $\mathcal{A}$.
- n-dim set: nset nA, $\mathcal{A}^n$.
- n-dim. Euclidean space: espace n, $\mathcal{E}^n$.
- region: region A, $\mathcal{A}$.

A.1.2. *Functions.*

- function value at: vat x, $[x]$.

A.1.3. *Geometric objects.*

- boundary: bound, ∂.
- surface: surf, s.
- volume: vol, v.

A.1.4. *Geometric algebra.*

- magnitude: magn u, $|u|$.
- inner product: iprod, $a \cdot b$.
- outer product: oprod, $a \wedge b$.
- inverse: inv a, a^{-1}.
- unit vector: uvec a, $\hat{a}$.

A.1.5. *Geometric calculus.*

- geometric derivative: gder, ∇.
- Laplace operator (derivative): lder, ∇^2.
- divergence: div, div.
- gradient: grad, grad.
- Laplace operator: lap, lap.

A.1.6. *Calculus.*

- differential operator: dx, d.
- difference operator: Dx, Δ.

A.1.7. *Derivatives.*

- dot derivative: dt a, $\dot{a}$.
- dot dot derivative: ddt a, $\ddot{a}$.
- expanded ordinary derivative: xod at, $\frac{\mathrm{d}a}{\mathrm{d}t}$.
- expanded partial derivative: xpd at, $\frac{\partial a}{\partial t}$.
- indexed ordinary derivative: iod t, d_t.
- indexed partial derivative: ipd t, ∂_t.
- indexed geometric derivative: igder k, ∂_k.
- comma derivative: cder Tt, $T_{,t}$.

A.1.8. *Index notation.*

- basis vector: bvec, γ.
- frame (basis) element: fbvec 1, γ_1.
- reciprocal frame (basis) element: rbvec 1, γ^1.
- frame: frm k, $\{\gamma_k\}$.
- reciprocal frame: rfrm k, $\{\gamma^k\}$.
- metric: met, g.
- metric in frame: fmet 12, g_{12}.
- metric in reciprocal frame: rmet 12, g^{12}.

- up indexed partial derivative: upipd 1, ∂^1.
- down indexed partial derivative: dnipd 1, ∂_1.
- frame (contravariant) components: fvec pos 1, ξ^1.
- reciprocal frame (covariant) components: rvec pos 1, ξ_1.

A.1.9. *Matrices.*

- diagonal: diag, diag.
- signature: sig, sig.

A.1.10. *Brackets.*

- Iverson brackets: iverson k, $[k]_{\mathrm{Iv}}$.

A.2. **Physics.**

A.2.1. *Mechanics.*

- position: pos, ξ.
- pressure: press, p.

A.2.2. *Energy transport.*

- time change rate: rate a, a'.
- flow: flow q, q'.
- flux: flux q, q''.
- thermal energy (heat): then, e.
- mechanical work: work, w.
- internal energy: ien, i.
- accumulation (*e.g.*, internal energy): accu ien, i'.
- thermodynamic temperature: temp, θ.
- specific heat capacity: kshcap, c.
- thermal diffusivity: kthdiff, α.
- thermal conductivity: kthcond, k.
- local film (heat transfer) coefficient (thermal convection): kthconv, f.
- global (average) film coefficient: kavthconv, $\bar{f}$.
- time constant (conduction-convection lumped solution): ktime, τ.
- thermal radiation absorbance: absorb, α.
- thermal radiation reflectance: reflect, ρ.
- thermal radiation transmittance: transm, τ.
- body energy flux distribution function: dbflux, $\check{e}_{\lambda_{\mathrm{body}}}$.
- black-body energy flux: bbflux, e''_{bb}.
- black-body energy flux distribution function: dbbflux, $\check{e}_{\lambda_{\mathrm{bb}}}$.

A.2.3. *Mass transport.*

- n (number of) particles: npart, n.
- mass: mass, m.
- mass density: dens, ρ.
- chemical reaction thermal energy: chthen, r.
- mass concentration: conc, c.
- species mass concentration: sconc A, A.
- chemical reaction kinetic coefficient: kchrcoeff, k.
- life time: lifetime(0.5), $t_{0.5}$.

A.2.4. *Waves.*

- wavelength: wlen, λ.
- wave frequency: wfreq, μ.

A.2.5. *Physical constants.*

- Boltzmann constant: kboltz, k_{b}.
- Stefan-Boltzmann constant: kstef, σ_{sb}.
- Planck constant: kplanck, h_{p}.
- speed of light in vacuum: klight, c_0.
- ideal gas constant: kgas, r_{g}.
- Avogadro's number: kavog, n_{a}.

A.3. **Dimensional analysis.**

- units of a physical quantity: unit q, $\operatorname{unit} q$.
- dimension of a physical quantity: dim q, $\dim q$.
- dimensionless quantity: kdim, Π.
- physical dimension: phdim L, L.
- Biot number: kbiot, Π_{bi}.