Resolution of Stiff Differential Systems in Biogeochemical Modeling using Some Advanced Numerical Schemes

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1. Motivation and Objectives

Microbial activity plays a key role in modifying the physical and (geo)chemical conditions of natural and industrial environments. This is crucial for applications like geothermal energy, hydrogen storage, and water treatment, as part of the energy transition. For this reason, it is essential to integrate biogeochemical models of bacterial activity into porous media flow simulators. These models take into account phenomena such as the consumption of substrates contributing to the growth of organisms and their decline through biodegradation.

Challenges:

- Microbial activity models involve stiff differential equations.
- Numerical methods must be robust across a wide range of parameters, especially when coupled with porous media flow models.
- Ensuring positivity of concentrations.

2. Bacterial Reactions in the Subsurface

We focus on sulfate-reducing bacteria (SRB), modeled by the simplified reaction:

$$SO_4^{2-} + 5\,H_2 + \text{SRB} \longrightarrow H_2S + 4\,H_2O + \text{more SRB}$$

This describes the consumption of hydrogen and sulfate, the production of water and hydrogen sulfide (toxic and corrosive), and the growth of SRB.

3. Physical Model

We use a simplified model [1] to describe the reaction kinetics:

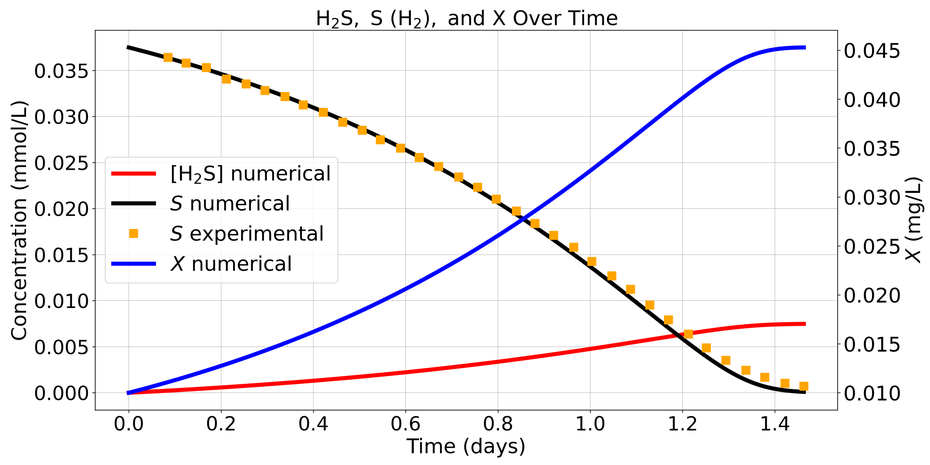
$$\frac{dS}{dt} = -\gamma_S f(S,A) X,$$
$$\frac{dA}{dt} = -\gamma_A f(S,A) X,$$
$$\frac{dX}{dt} = Y f(S,A) X - bX$$

- S : molar concentration of substrate *[mmol/L]*
- A: molar concentration of electron acceptor *[mmol/L]*
- X: biomass concentration *[mg/L]*
- $f(S,A) = \frac{\mu}{Y} \frac{S}{\tau_S + S} \frac{A}{\tau_A + A}$: dual Monod reaction rate
- $\tau > 0$ half-saturation *[mmol/L]*
- $Y > 0$ yield coefficient *[mg/mmol]*
- $\gamma > 0$ stoichiometric coefficient *[adim]*
- $b > 0$ decay rate *[1/day]*
- $\mu > 0$ growth rate *[1/day]*

Reference: [1] de Blanc, P.C. (1998), *Development and Demonstration of a Biodegradation Model for Non-Aqueous Phase Liquids in Groundwater*, PhD Dissertation, University of Texas at Austin.

4. Model Configuration and Initial Conditions

- We use the same kinetic parameters studied by Robinson and Tiedje [2] and we also use their experimental hydrogen data for model validation.
- SRB (sulfate-reducing bacteria) consumes sulfate ions and H_2 to produce water and H_2S, the latter of which is both toxic and highly corrosive to metals and concrete.

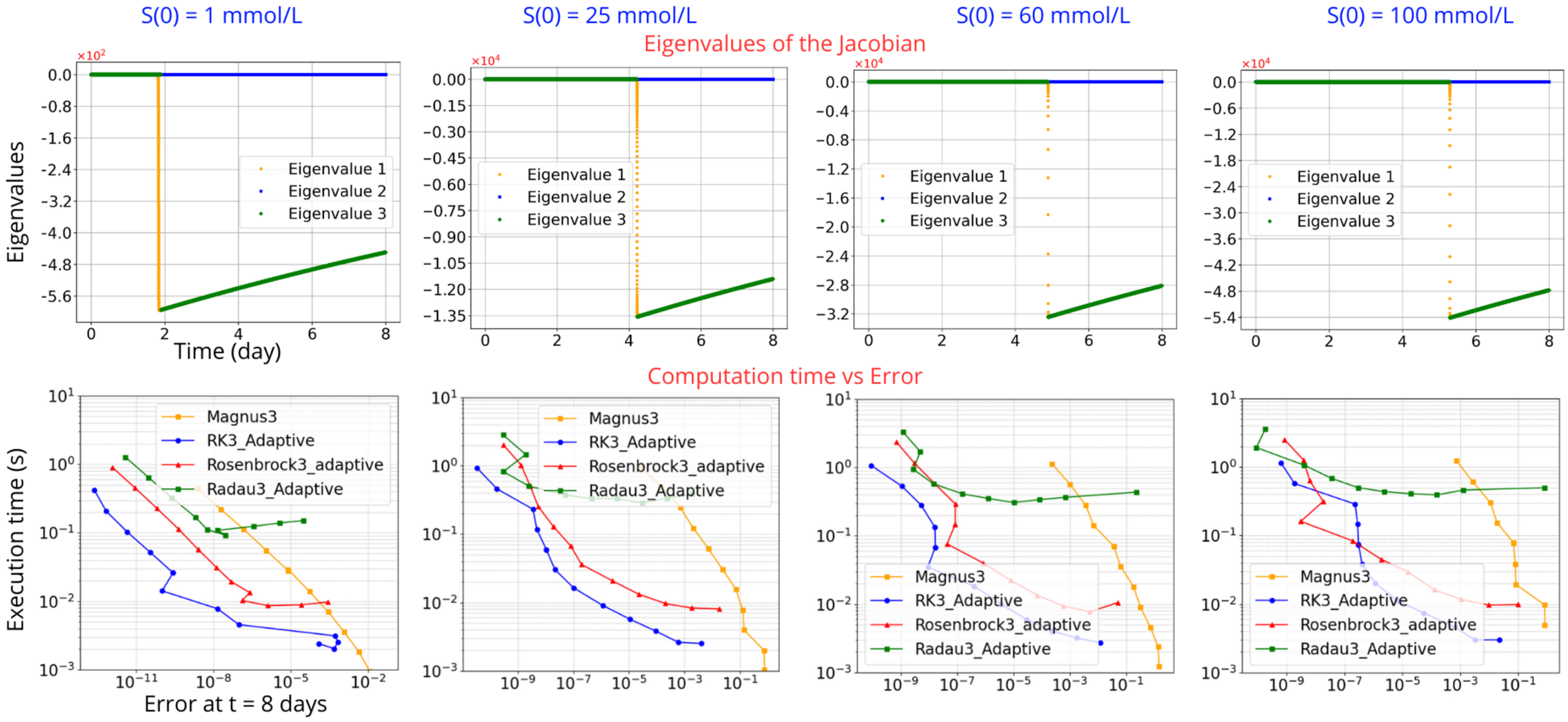


Initial Conditions	$S(0) = 0.0365$ mmol/L	$A(0) = 10$ mmol/L	$X(0) = 0.01$ mg/L
Parameters	$Y = 0.99$ mg/mmol $\tau_A = 0.0001$ mmol/L	$\mu = 2.7$ day^{-1} $b = 0.046$ day^{-1}	$\tau_S = 0.0024$ mmol/L $\gamma_S = 1,\ \gamma_A = 1/5$

Reference: [2] Robinson J.A. and Tiedje J.M. (2005), *Kinetics of substrate depletion by mixed populations*, Appl. Environ. Microbiol.

5. Numerical Performances

- System stiffness: we set $A(0) = 60$ mmol/L and $X(0) = 0.1$ mg, and varied $S(0) \in \{1, 25, 60, 100\}$ mmol/L to study its effect on solver performance.
- **RK4** with very small time step used as a reference solution.
- Numerical methods: **Magnus3** ensures positivity and stability without constraints; **RK3_adaptive** needs small time steps for stability and adapts to preserve positivity; **Radau3_adaptive** and **Rosenbrock3_adaptive** are A-stable, and positivity-adaptive.



6. Conclusion and Perspectives

- Growth of SRB biomass driven by the consumption of H_2, leading to the production of toxic H_2S.
- Increase in initial hydrogen concentration, causing greater system stiffness in our model.
- Preference for Runge-Kutta at low stiffness, Rosenbrock or Radau at high stiffness.
- Evaluating explicit Orthogonal-Runge-Kutta-Chebyshev (ROCKS) method.
- Integrating further biogeochemical processes into the current model.
- Coupling with porous media flow simulators for realistic applications.