Rare Earth Element SX Systems: *“Are we at steady state yet?”*

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Background

A pilot REE SX plant is monitored for performance during parametric testing. Modeling the system is complicated, since SX systems require long retention times and complex recirculating loops (Baird 1991). After plotting concentrations over time, steady state can be determined by *eye*, but subjective characterization of the data can lead to problems in performance comparisons. Hence, there is a need to find an objective steady state.

Figure 1: Bench scale SX system

Research Goals

Outline modeling criteria for objective determination of steady state concentrations. Fit the model to data with the intention of using calculated steady state concentrations in a mass balance.

Materials and Methods

Data Collection

After making a process parameter change, samples were taken in one hour intervals, at the locations shown in Figure 2, for 43 hours and then assayed via ICP-MS.

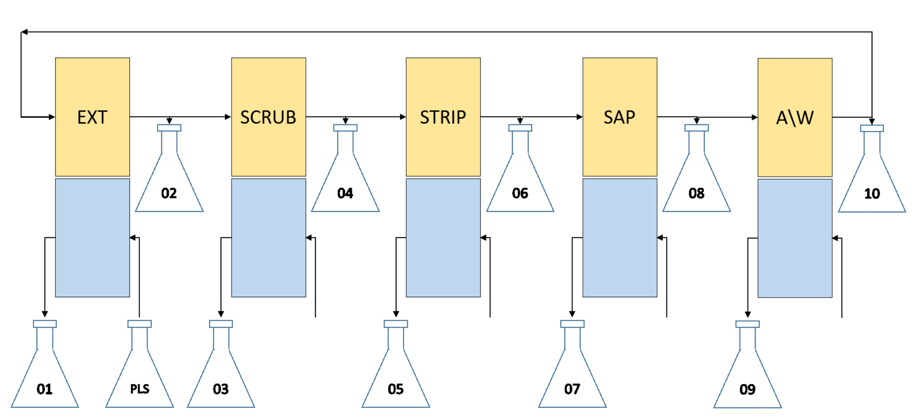


Figure 2: Sampling locations

The Autoregressive Model

An autoregressive (*AR*) time series process is a model where a future state is dependent on the past state (Shumway 2017). An example, which includes the addition of a constant value (μ), and random perturbations (ϵ) is:

$$y_t = \phi y_{t-1} + \mu + \epsilon \qquad (1)$$

If $|\phi| < 1$ the behavior of the model is predictable, as illustrated in Figure 3, and the *steady state* can be calculated as:

$$\frac{\mu}{1-\phi} \qquad (2)$$

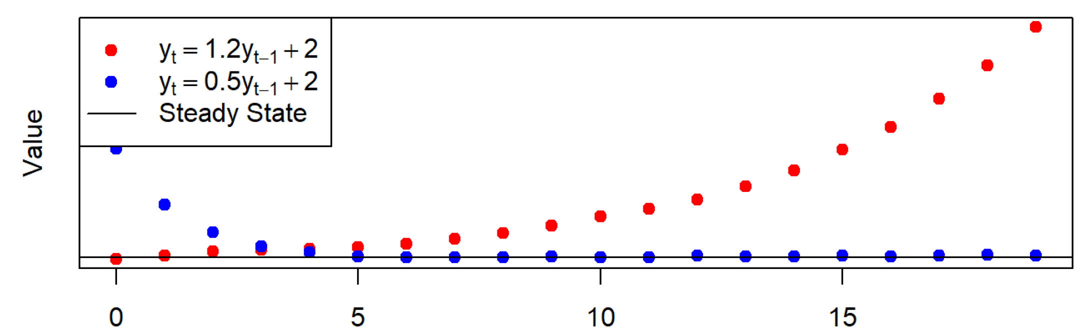
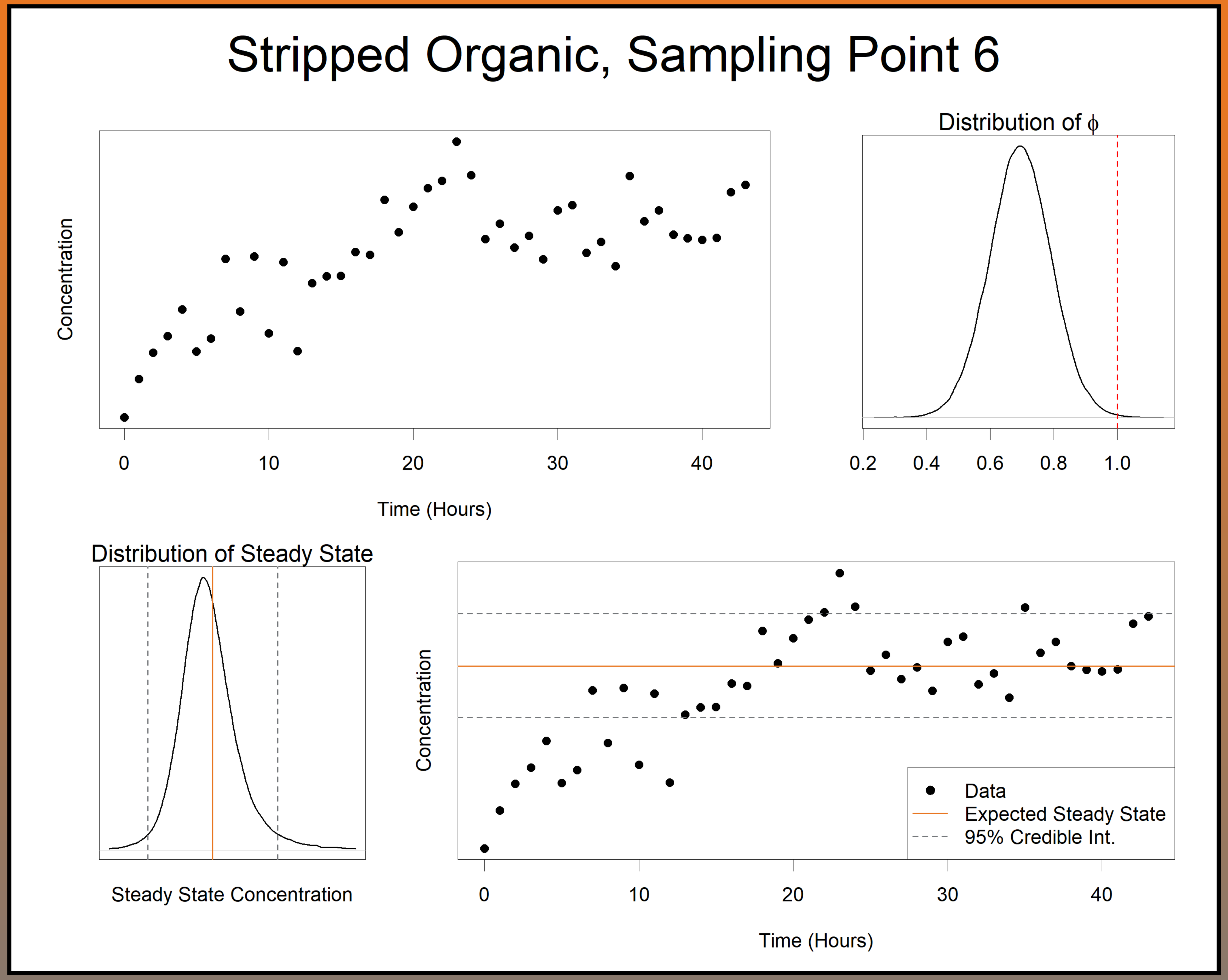


Figure 3: Example autoregressive processes

A **Model** predicting **Steady State** of **Rare Earth Elements** in **SX** systems is proposed and successfully tested on **Real Data**



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Federal Award Number: DE-FE0026927

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Bayesian Inference

Bayesian inference is a statistical method where probability distributions of all unknown model parameters are fully quantified (Hoff 2009).

With Bayesian inference we can:

- Inspect the distribution of the value of ϕ, to infer if steady state is predictable.
- Stipulate a prior distribution of ϕ which forces $-1 < \phi < 1$ to ensure Equation (2) is valid for steady state calculations.
- Use algorithms to generate random samples of ϕ and μ, which are simply plugged into Equation (2) to generate a probability distribution of steady state. (Carlin, Gelfand, and Smith 1992) (Hastings 1970)

Figure 4 and Equation (3) illustrate these properties:

$$p(\phi|\text{Data}) \propto p(\text{Data}|\phi)p(\phi) \qquad (3)$$

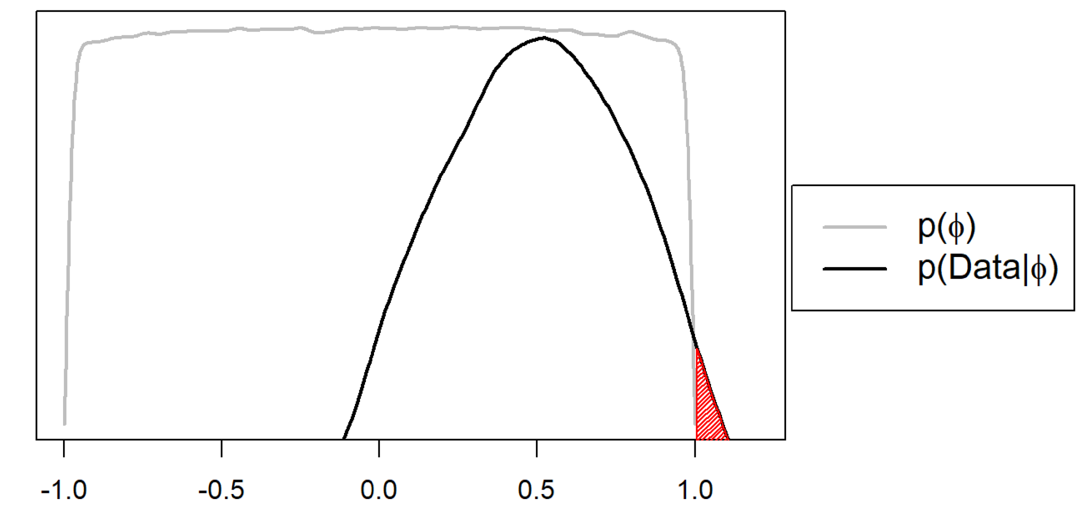

Figure 4: Bounded prior distribution influencing posterior distribution.

Application

The steps for calculating steady state concentrations taken were:

1. Fit a model to the data
2. See if there is any probability $-1 < \phi < 1$. Then, we either:
   a. Keep the model if all samples of ϕ are between -1 and 1
   b. If any samples of ϕ are outside of $(-1, 1)$, refit the model while forcing $-1 < \phi < 1$ with a prior distribution.
   c. Determine the system is not predictable and sample the plant longer.
3. Next, use algorithms to generate random samples of ϕ and μ to plug into Equation (2), producing a probability distribution for what we think steady state is.

Working with sampling point 6, the steps above are implemented. First, the distribution of ϕ is built. The data collected and the distribution of ϕ, given this data, are displayed as the top two plots in the ***Central Figure***. The probability that $|\phi| \geq 1$ is 0.119%. Although the value is small, it is enough where calculation of steady state using equation (2) is not valid.

However, we can be fairly confident that $|\phi| < 1$. So we proceed with refitting the model while forcing $|\phi| < 1$ using a prior distribution. Samples of μ and ϕ are produced and used to calculate the distribution of steady state, shown in the lower two plots of the ***Central Figure***.

Conclusion

- A robust, objective, sensible method for determining steady state concentrations is provided.
- For the observed data, all sampling points had a > 90% chance that $|\phi| < 1$, good evidence the entire system is at steady state and predictable.
- Plotting expected steady state concentration and the 95% credible interval of the steady state distribution with the data produces a plot that makes sense.
- *“All models are wrong but some are useful”* - George Box (Box 1979). This model can be improved to account for conservation of mass between stages, but is a good foundation for future models. Most importantly, the model is useful for objective verification of steady state.

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