Singular perturbation treatment of the decomposition of ozone
2. Inner and outer solutions, and matching

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We can use singular perturbation theory to obtain approximate solutions to the time evolution of the system. In this lecture, we pursue our analysis of the ozone decomposition model to work out the time dependence implied by these equations to lowest order in the perturbation parameter.

The rate equations we obtained previously were

$$\frac{dx}{d\tau} = -x + \alpha y - (1-\alpha)xy, \tag{1a}$$

$$\epsilon\frac{dy}{d\tau} = x - \alpha y - (1-\alpha)xy. \tag{1b}$$

These equations, in the limit of very small ϵ, govern the evolution on the **slow** time scale, the so-called **outer** solution. On the slow time scale, to lowest order in ϵ, we can replace these equations by

$$\frac{dx}{d\tau} = -x + \alpha y - (1-\alpha)xy, \tag{2a}$$

$$y \approx \frac{x}{\alpha + (1-\alpha)x}. \tag{2b}$$

However, we would have started out with some initial conditions $x = [O_3]/[O_3]_0 = 1$, $y = [O]/[O]_{\mathrm{max,est}} = 0$. The reduced system given above does not pass through this point. (Try substituting $x = 1$ into the equation for y.) So somehow, we need to get from our real initial condition to the conditions represented by the reduced system. We will have to solve a different problem to solve for the dynamics on the fast time scale, i.e. the **inner** solution and then join the two solutions together.

1 The outer solution

Combining the two equations in the system (2), we get

$$\frac{dx}{d\tau} = \frac{-2x^2(1-\alpha)}{\alpha + (1-\alpha)x}.$$

This equation can be solved relatively straightforwardly by separation of variables:

$$dx\,\frac{\alpha + (1-\alpha)x}{-2x^2(1-\alpha)} = d\tau.$$

$$\therefore \int_{x_i}^{x} du \left(-\frac{\alpha}{2(1-\alpha)}u^{-2} - \frac{1}{2}u^{-1}\right) = \int_0^{\tau} dt.$$

Here, I used u and t as dummy integration variables to avoid ambiguity in the expression. I also have a (for now) unknown x_i, which is the value of x at which the outer solution takes over from the inner solution. Evaluating the integrals, we have

$$\left[\frac{\alpha}{2(1-\alpha)}u^{-1} - \frac{1}{2}\ln u\right]_{x_i}^{x} = \tau.$$

$$\therefore \frac{\alpha}{2(1-\alpha)}\left(\frac{1}{x} - \frac{1}{x_i}\right) - \frac{1}{2}\ln\left(\frac{x}{x_i}\right) = \tau.$$

2 The inner solution

To get the inner solution (the fast initial transient), we need to transform our rate equations by stretching out the time variable. Specifically, we choose

$$\tau = \epsilon\theta,$$

where θ is our new "stretched" time, i.e. a measure of time appropriate on the fast time scale. This transformation of time gives the fast-time scale differential equations

$$\frac{dx}{d\theta} = \epsilon \left[-x + \alpha y - (1-\alpha)xy \right],$$
$$\frac{dy}{d\theta} = x - \alpha y - (1-\alpha)xy.$$

If ϵ is small, to lowest order, these equations become

$$\frac{dx}{d\theta} \approx 0, \tag{3a}$$
$$\frac{dy}{d\theta} = x - \alpha y - (1-\alpha)xy. \tag{3b}$$

Thus, x is approximately constant during the transient. Given our initial conditions, the solution for $x(t)$ is therefore

$$x(t) \approx 1.$$

Equation (3b) therefore becomes

$$\frac{dy}{d\theta} \approx 1 - y.$$

This equation is easy to solve by separation of variables. The solution is

$$y = 1 - e^{-\theta}.$$

3 Matching

To lowest order in ϵ, we have the following:

- On the fast time scale, $x \approx 1$ and $y = 1 - e^{-\theta}$, with $\theta = \tau/\epsilon$.
- On the slow time scale,

  $$y = y_{\mathcal{S}}(x) \approx \frac{x}{\alpha + (1-\alpha)x}$$

  and

  $$\frac{\alpha}{2(1-\alpha)} \left(\frac{1}{x} - \frac{1}{x_i} \right) - \frac{1}{2} \ln \left(\frac{x}{x_i} \right) = \tau.$$

Note that, in the slow solution, if we set $x = x_i$, $\tau = 0$. x_i is therefore the initial condition for the slow solution. This should match the large-θ asymptotics of the fast solution. Since x is approximately independent of θ on the fast time scale, this means that we must have $x_i = 1$. But if we make this choice, do the values of y match up? As $\theta \to \infty$, $y \to 1$. If we substitute $x = x_i = 1$ into $y_{\mathcal{S}}(x)$, we get $y = 1$, so the outer solution matches the inner solution automatically.

We can go just a bit further and generate a global solution for y, i.e. one solution that governs the time evolution on both time scales. The rule is the following:

$$\left\{ \begin{array}{c} \text{global} \\ \text{solution} \end{array} \right\} = \left\{ \begin{array}{c} \text{fast} \\ \text{solution} \end{array} \right\} + \left\{ \begin{array}{c} \text{slow} \\ \text{solution} \end{array} \right\} - \left\{ \begin{array}{c} \text{common} \\ \text{part} \end{array} \right\}.$$

In this case, the "common part" is $y = 1$, which is both the limit of the fast solution as $\theta \to \infty$ and the initial value of y for the slow solution. Thus we have

$$\begin{aligned} y(\tau) &\approx \left(1 - e^{-\tau/\epsilon}\right) + \frac{x(\tau)}{\alpha + (1-\alpha)x(\tau)} - 1 \\ &= \frac{x(\tau)}{\alpha + (1-\alpha)x(\tau)} - e^{-\tau/\epsilon}, \end{aligned}$$

where $x(\tau)$ is found by solving

$$\frac{\alpha}{2(1-\alpha)}\left(\frac{1}{x} - 1\right) - \frac{1}{2}\ln(x) = \tau.$$