# Supporting Information

**Criteria for unique steady state for enzymatic depectinization of bael (*Aegle marmelos*) juice in a continuous stirred tank reactor**

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## A. Theory of Contraction Mapping

Let $f: X \rightarrow X$ represent a mapping from set X to itself. Then, a point $x \in X$ is referred to as a fixed point (steady state) of *f*, if $f(x)=x$. As a corollary of the intermediate value theorem[1], it follows that if $[a,b]$ is a closed interval, then any continuous function $f$ has at least one fixed point. The requisite criterion that decides whether there is a unique fixed point is given by contraction mapping theorem. In this context, contraction mapping theorem (also known as Banach's fixed-point theorem) may be stated as [2,3]

*Theorem:* In a complete metric space, *f* is a map such that

$$d\left(f(x), f(x')\right) \leq c\, d(x, x') \tag{A.1}$$

where, d is metric and physically it signifies the difference between two functions and is defined as $d(u,v)=|u-v|$. c is a real valued constant ($0 \leq c < 1$). If Eq. (A.1) is valid then $f(x)$ has unique fixed point (steady state). Moreover, for any $x_0 \in X$, the sequence of iterates $x_0, f(x_0), f(f(x_0)),...$ converges to the fixed point of *f*. Now, a Taylor series expansion of $f(x)$ about $x_0$ gives

$$f(x)=f(x_0)+(x-x_0)f'(x_0)+\frac{(x-x_0)^2}{2!}f''(x_0)+..... \tag{A.2}$$

Using two dummy variables *u* and *v* such that $u,v \in x$ and using Taylor series expansion as Eq. (A.2), the following expression is obtained.

$$f(u)-f(v)=(u-v)f'(v) \tag{A.3}$$

Now, $d\left(f\left(u\right),f\left(v\right)\right)=\left|f\left(u\right)-f\left(v\right)\right|=\left|f'\left(v\right)\right|\left|u-v\right|=z\,d(u,v)$ (A.4)

where, $z=\left|f'\left(v\right)\right|$

Thus, considering Eqs. (A.1) and (A.4) together, to satisfy the condition of existence of a unique steady state, z should be always less than 1, i.e., $z_{\max}<1$.

**References**


1 W. Rudin, *Principles of Mathematical Analysis*, McGraw-Hill, 1976.

2 S. Pushpavanam, *Mathematical Methods in Chemical Engineering*, PHI Learning, 1998.

3 V. I. Istratescu, *Fixed Point Theory: An Introduction*, Springer Netherlands, 2001.


**B. Analysis of unique steady state for non-ideal CSTR**

The schematic of the non-ideal CSTR is depicted in Fig. 6 in the main manuscript. The associated variables are also defined in the main manuscript.

Performing a material balance of reactant A at junction Q yields the following equation

$$C_{A0}v_b + C_{As}v_s = C_A\left(v_b + v_s\right) \quad \text{(B.1)}$$

The above equation may be expressed in terms of $C_A$ as

$$C_A = F\,C_{A0} + \left(1 - F\right)C_{As} \quad \text{(B.2)}$$

where, $E = V_s / V$ and $F = v_b / v_0$ . $E$ is the volume fraction of the reaction zone, while $F$ is the fraction of volumetric flow rate bypassing the zone of reaction.

Assuming steady state operation, a substrate balance at steady state results in the following relation

$$v_s C_{A0} - v_s C_{As} - V_s \frac{v_{max} C_{As}}{K_M + C_{As}} = 0 \quad \text{(B.3)}$$

Eq. (B.3) may be rearranged as

$$Y = \frac{1 + \beta Y}{1 + \beta Y + D} = f(Y) \quad \text{(B.4)}$$

where, $x = \frac{C_A}{C_{A0}}$ , $Y = \frac{C_{As}}{C_{A0}} = \frac{x - F}{1 - F}$, $D = \frac{\alpha E}{1 - F}$

$\alpha$ and $\beta$ are already defined in the main manuscript as $\alpha = \frac{V v_{\max}}{K_M v_0}$, $\beta = \frac{C_{A0}}{K_M}$.

Now, $0 \le Y \le 1, \quad 0 \le f(Y) \le 1$

Also, $$z_Y = \frac{df(Y)}{dY} = \frac{\beta D}{(1 + D + \beta Y)^2} \quad \text{(B.5)}$$

Applying the principle of contraction mapping (similar to the approach followed for ideal reactor), the condition for unique steady state is

$$\beta D < (1 + D)^2 \quad \text{(B.6)}$$

Eq. (B.6) may be expressed in terms of residence time of the non-ideal CSTR ($\tau_{NI}$) and other reactor and kinetic parameters as

$$\tau_{NI} > \left(\frac{1-F}{E}\right)\left(\frac{C_{A0} - 2K_M + \sqrt{C_{A0}K_M\left(\frac{C_{A0}}{K_M} - 4\right)}}{2v_{\max}}\right) \quad \text{(B.7)}$$

Thus, the critical residence time for a non-ideal CSTR is given as

$$\tau_{crit,NI} = \left(\frac{1-F}{E}\right)\left(\frac{C_{A0} - 2K_M + \sqrt{C_{A0}K_M\left(\frac{C_{A0}}{K_M} - 4\right)}}{2v_{\max}}\right) \quad \text{(B.8)}$$