Microreactor Engineering

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Homogenous Reactions in Microreactors

Alternative Boundary Conditions

In Affiliation With:

MBI

Microproducts Breakthrough Institute

PTT - LOA

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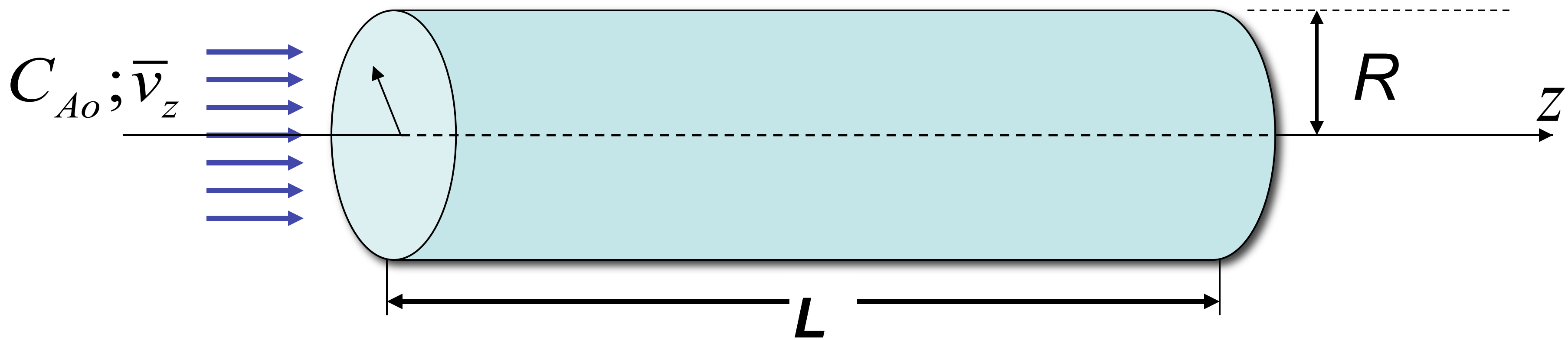
Summary for Homogenous Reaction in Microreactors:

$$A \overset{k}{\Longrightarrow} B \qquad -\frac{dC_A}{dt} = kC_A \left[\frac{mol}{m^3 s}\right]$$

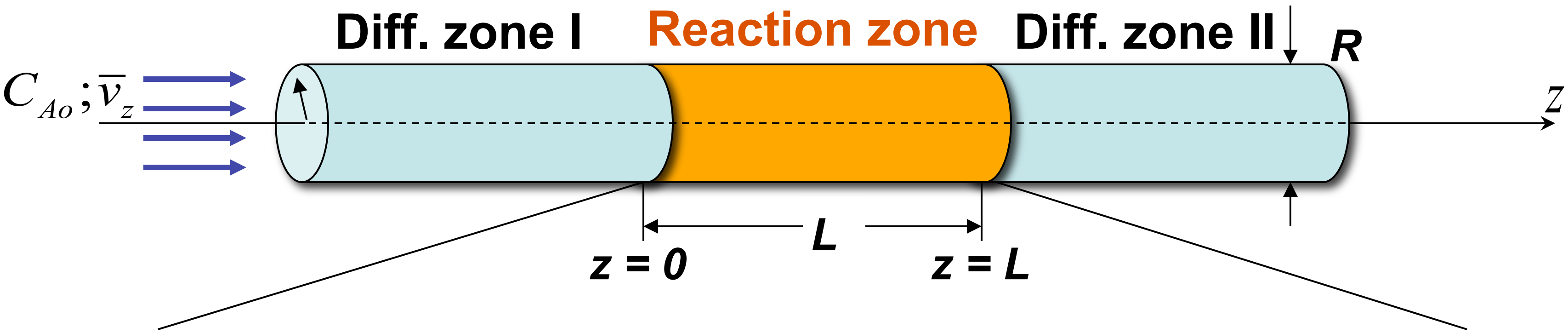


$$\boxed{-v_z(r)\frac{\partial C_A(z,r)}{\partial z} + D_A \frac{\partial^2 C_A(z,r)}{\partial z^2} + D_A \frac{\partial^2 C_A(z,r)}{\partial r^2} + \frac{D_A}{r}\frac{\partial C_A(z,r)}{\partial r} - kC_A = 0}$$

$$@z = 0 \quad \frac{\partial C_A(0,r)}{\partial z} = 0; \; or \; C_A(0,r) = C_{Ao} \qquad @r = 0 \quad \frac{\partial C_A(z,0)}{\partial r} = 0;$$

$$@z = L \quad \frac{\partial C_A(L,r)}{\partial z} = 0; \; and \,/\, or \; \bar{C}_A(L) = C_A^* \qquad @r = R \quad \frac{\partial C_A(z,R)}{\partial r} = 0$$

Alternative BC for Homogenous Reaction in Microreactors



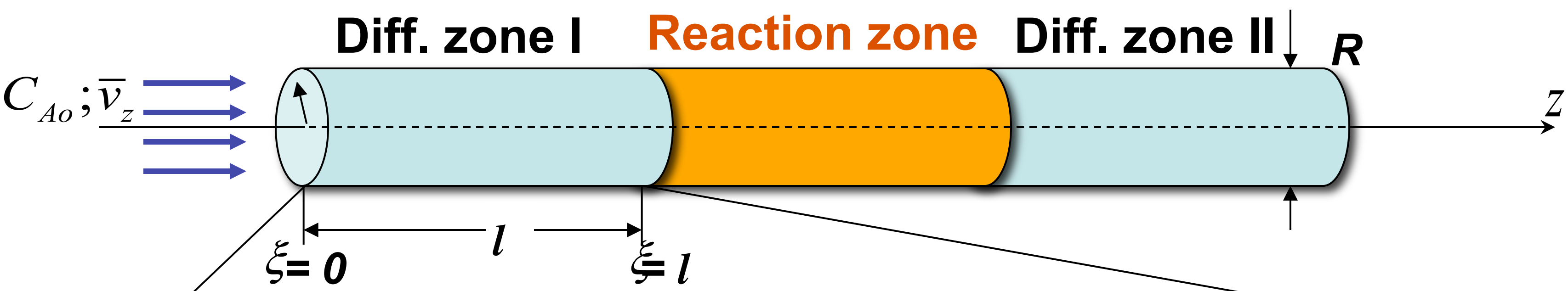
$$\boxed{-v_z(r)\frac{\partial C_A(z,r)}{\partial z} + D_A\frac{\partial^2 C_A(z,r)}{\partial z^2} + D_A\frac{\partial^2 C_A(z,r)}{\partial r^2} + \frac{D_A}{r}\frac{\partial C_A(z,r)}{\partial r} - kC_A = 0}$$

$$@z=0 \quad \frac{\partial C_A^I(l,r)}{\partial \xi} = \frac{\partial C_A(0,r)}{\partial z}; \; C_A^I(l,r) = C_A(0,r) \qquad @r=0 \quad \frac{\partial C_A(z,0)}{\partial r} = 0;$$

$$@z=L \quad \frac{\partial C_A(L,r)}{\partial z} = \frac{\partial C_A^{II}(0,r)}{\partial \eta}; \; C_A(L,r) = C_A^{II}(0,r) \qquad @r=R \quad \frac{\partial C_A(z,R)}{\partial r} = 0$$

$$@any\, z \Rightarrow v_z(r) = \frac{R^2}{4\cdot\mu}\left(\frac{\Delta P}{L}\right)\cdot\left[1-\frac{r^2}{R^2}\right] = 2\bar{v}_z\left[1-\frac{r^2}{R^2}\right]$$

Alternative BC for Homogenous Reaction in Microreactors



$$-v_\xi(r)\frac{\partial C_A^I(\xi,r)}{\partial \xi} + D_A\frac{\partial^2 C_A^I(\xi,r)}{\partial \xi^2} + D_A\frac{\partial^2 C_A^I(\xi,r)}{\partial r^2} + \frac{D_A}{r}\frac{\partial C_A^I(\xi,r)}{\partial r} - \cancel{kC_A} = 0$$

$$@\xi = 0 \quad \frac{\partial C_A^I(0,r)}{\partial \xi} = 0;\; C_A^I(0,r) = C_{Ao}$$

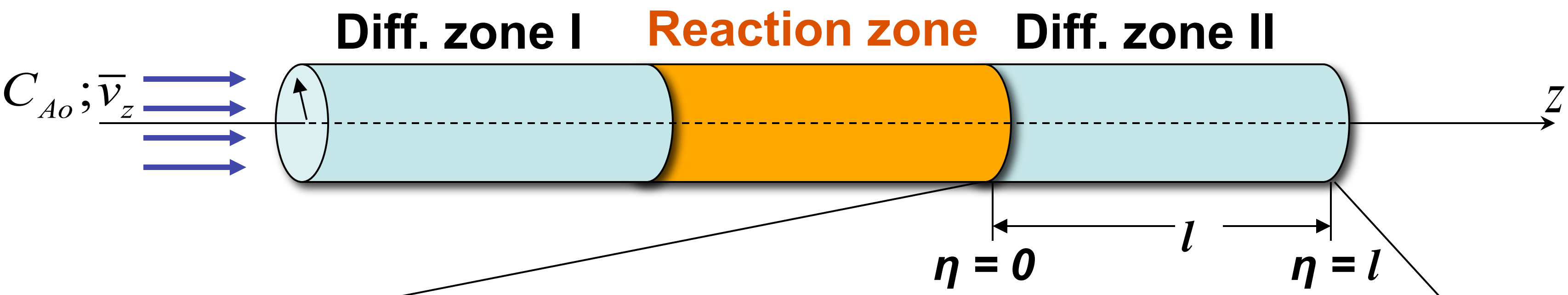
$$@r = 0 \quad \frac{\partial C_A^I(\xi,0)}{\partial r} = 0;$$

$$@\xi = l \quad \frac{\partial C_A^I(l,r)}{\partial \xi} = \frac{\partial C_A(0,r)}{\partial z};\; C_A^I(l,r) = C_A(0,r)$$

$$@r = R \quad \frac{\partial C_A^I(\xi,R)}{\partial r} = 0$$

$$@any\,\xi \Rightarrow v_\xi(r) = \frac{R^2}{4\cdot\mu}\left(\frac{\Delta P}{L}\right)\cdot\left[1-\frac{r^2}{R^2}\right] = 2\bar{v}_z\left[1-\frac{r^2}{R^2}\right]$$

Alternative BC for Homogenous Reaction in Microreactors



$$\boxed{-v_\eta(r)\frac{\partial C_A^{II}(\eta,r)}{\partial \eta} + D_A \frac{\partial^2 C_A^{II}(\eta,r)}{\partial \eta^2} + D_A \frac{\partial^2 C_A^{II}(\eta,r)}{\partial r^2} + \frac{D_A}{r}\frac{\partial C_A^{II}(\eta,r)}{\partial r} = 0}$$

$$@\eta = 0 \quad \frac{\partial C_A^{II}(0,r)}{\partial \eta} = \frac{\partial C_A(L,r)}{\partial z};\ C_A^{II}(0,r) = C_A(L,r) \qquad @r = 0 \quad \frac{\partial C_A^{II}(\eta,0)}{\partial r} = 0;$$

$$@\eta = l \quad \frac{\partial C_A^{II}(l,r)}{\partial \eta} = 0;\ and \quad or\ \bar{C}_A^{II}(l) = C_A^* \qquad @r = R \quad \frac{\partial C_A^{II}(\eta,R)}{\partial r} = 0$$

$$@any\,\eta \Rightarrow v_\eta(r) = \frac{R^2}{4\cdot\mu}\left(\frac{\Delta P}{L}\right)\cdot\left[1 - \frac{r^2}{R^2}\right] = 2\bar{v}_z\left[1 - \frac{r^2}{R^2}\right]$$

The origin of Characteristic Times

Consider the governing differential equation for a microchannel reactor in which a chemical reaction take place in a catalyst layer at the walls of the microreactor.

$$\boxed{-v_z(r)\frac{\partial C_A(z,r)}{\partial z}+D_A\frac{\partial^2 C_A(z,r)}{\partial z^2}+D_A\frac{\partial^2 C_A(z,r)}{\partial r^2}+\frac{D_A}{r}\frac{\partial C_A(z,r)}{\partial r}-kC_A=0}$$

$$where\ at\ any\, z \Rightarrow v_z\left(r\right)=2\overline{v}_z\left[1-\frac{r^2}{R^2}\right]$$

After the change of variables:

$$r^*=\frac{r}{R};\quad z^*=\frac{z}{L};\quad C_A^*=\frac{C_A}{C_{Ao}}\quad \Rightarrow \quad r=r^*R;\quad z=z^*L;\quad C_A=C_A^*C_{Ao};$$

and all substitutions, one can obtain:

$$-\frac{\overline{v}_z}{L}2\left[1-\left(r^*\right)^2\right]\frac{\partial C_A^*}{\partial z^*}+\frac{D_A}{L^2}\frac{\partial^2 C_A^*}{\partial\left(z^*\right)^2}+\frac{D_A}{R^2}\frac{\partial^2 C_A^*}{\partial\left(r^*\right)^2}+\frac{D_A}{R^2}\frac{1}{r^*}\frac{\partial C_A^*}{\partial r^*}-kC_A^*=0$$

The origin of Characteristic Times

The coefficients in the normalized differential equation represent the characteristic times that we consider earlier:

$$-\left(\frac{\bar{v}_z}{L}\right)2\left[1-\left(r^*\right)^2\right]\frac{\partial C_A^*}{\partial z^*}+\left(\frac{D_A}{L^2}\right)\frac{\partial^2 C_A^*}{\partial\left(z^*\right)^2}+\left(\frac{D_A}{R^2}\right)\left[\frac{\partial^2 C_A^*}{\partial\left(r^*\right)^2}+\frac{1}{r^*}\frac{\partial C_A^*}{\partial r^*}\right]-\left(k\right)C_A^*=0$$

or equivalently:

$$-\frac{1}{\tau_L}2\left[1-\left(r^*\right)^2\right]\frac{\partial C_A^*}{\partial z^*}+\frac{1}{\tau_{D,z}}\frac{\partial^2 C_A^*}{\partial\left(z^*\right)^2}+\frac{1}{\tau_{D,r}}\left[\frac{\partial^2 C_A^*}{\partial\left(r^*\right)^2}+\frac{1}{r^*}\frac{\partial C_A^*}{\partial r^*}\right]-\frac{1}{\tau_A}C_A^*=0$$

mean resident time

diffusion time in *z*

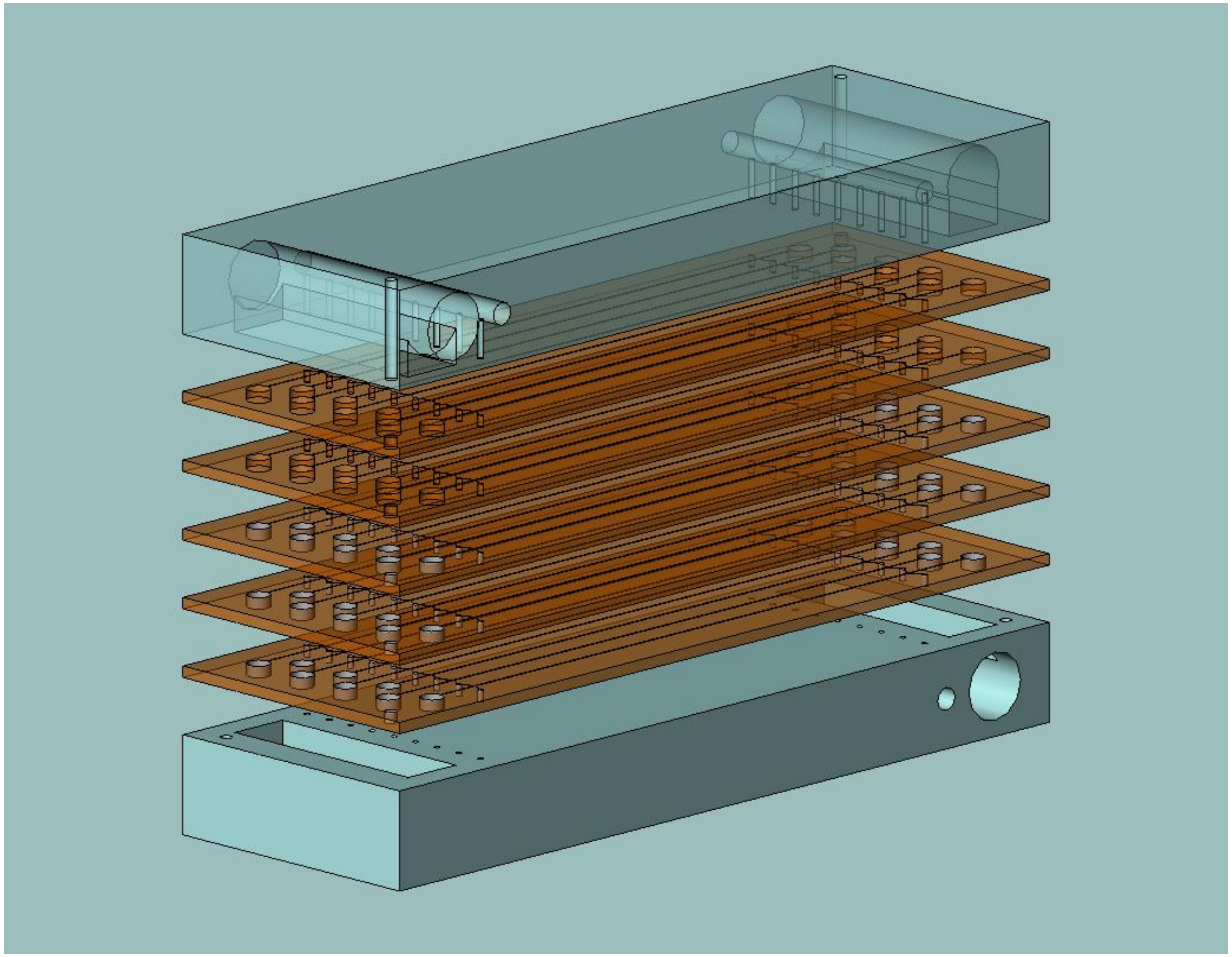
diffusion time in *r*

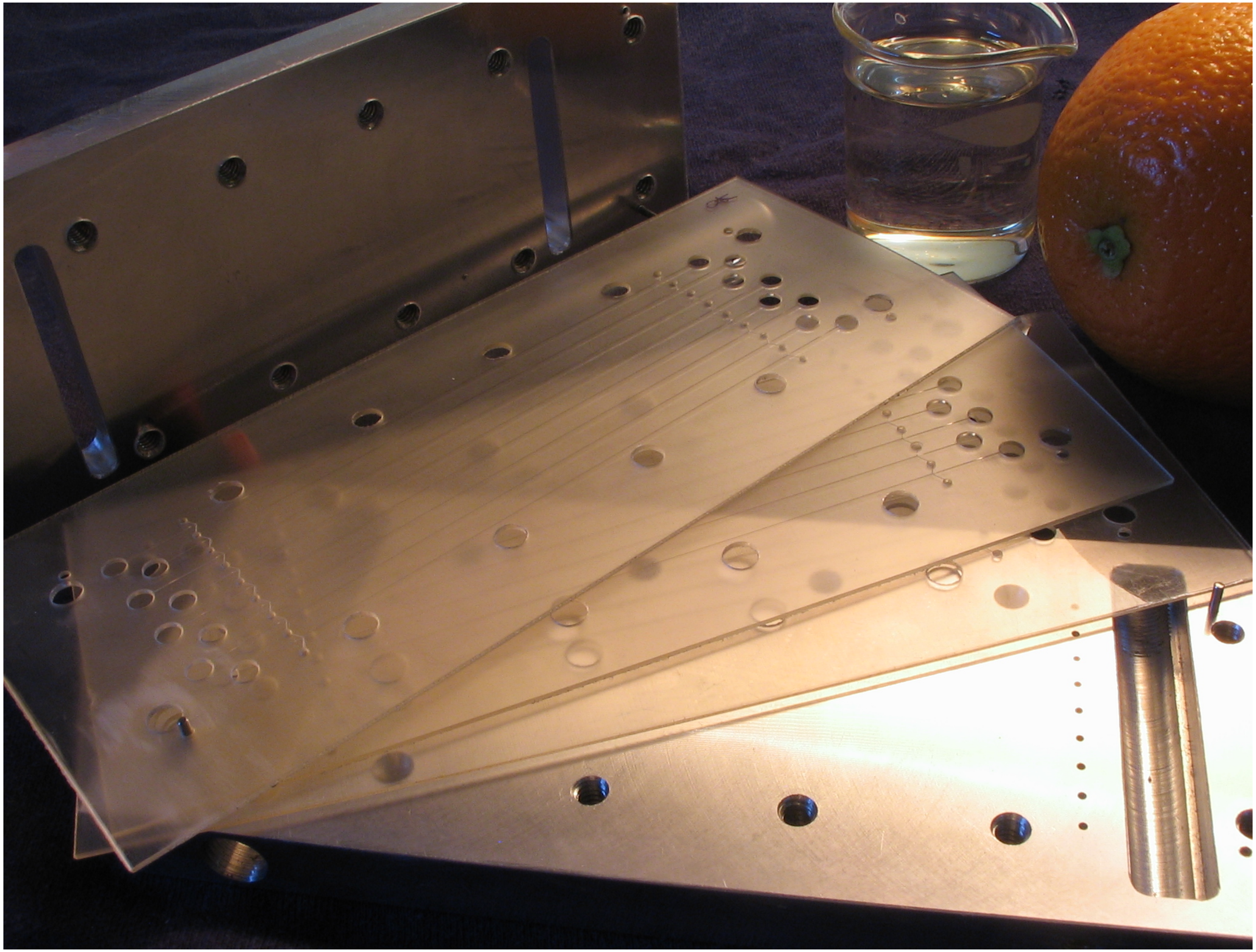
reaction time

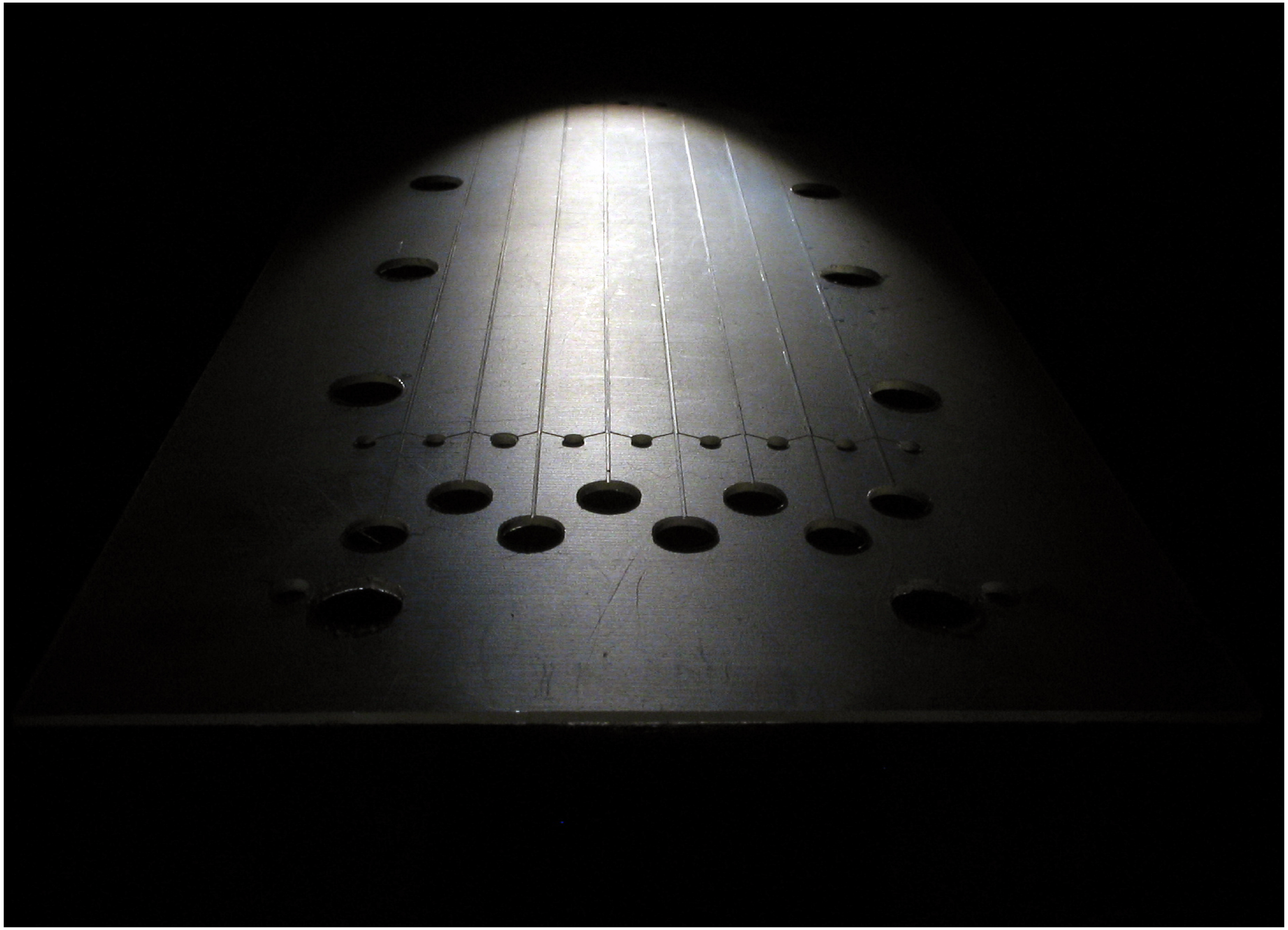
Microreactors For Biodiesel Production

- Tiny parallel channels — 100 microns wide — are embossed into a polymer plate about the size of a credit card.
- Thin streams of alcohol and oil are injected into each channel.
- Because the alcohol and oil molecules are in close contact all along the channel, the chemical reaction that converts them into biodiesel happens ***faster*** than in a large macroscopic vessel.
- Thousands of these microchannels stacked side-by-side create a microreactor the ***size of a suitcase*** that could produce approximately ***0.5 M-Gal*** of biodiesel a year.

Biodiesel Synthesis in Microscale Reactors







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