Cannabis Brownie Kinetics

```
CBDA \stackrel{k_1}{\rightarrow} CBD \stackrel{k_2}{\rightarrow} THC
THCA \stackrel{k_3}{\rightarrow} THC \stackrel{k_4}{\rightarrow} CBN
or
A \stackrel{k_1}{\rightarrow} B \stackrel{k_2}{\rightarrow} D
C \stackrel{k_3}{\rightarrow} D \stackrel{k_4}{\rightarrow} E
```

Estimated initial 9.1 mM CBDA + 1.1 mM THCA averaged from various strains

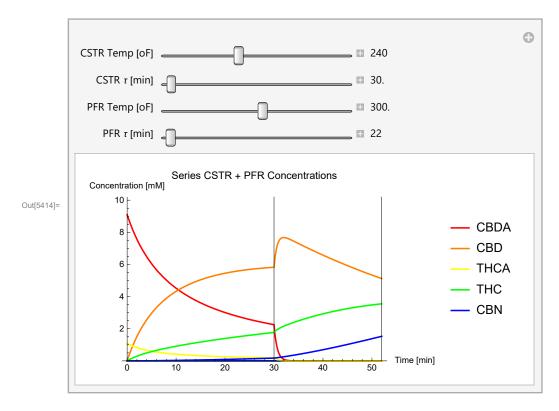
Assumed decarboxylation (k1 & k3) and degradation (k2 & k4) reactions are elementary and follow the Arrhenius equation with constants below

	Rate Constant	A [s ⁻¹]	E _a [kJ/mol]
Out[5335]=	k1	$\textbf{1.9}\times\textbf{10}^{12}$	112
	k2	950.	52
	k3	$1. \times 10^9$	86
	k4	$\textbf{1.2}\times\textbf{10}^{6}$	77

```
ln[5382] = ca0 = 9.1; (*mM CBDA*)
      cb0 = 0; (*mM CBD*)
      cc0 = 1.1; (*mM THCA*)
      cd0 = 0; (*mM THC*)
      ce0 = 0; (*mM CBN*)
                      ca0
      cacstr := -
                 1 + 60 t k1cstr
                 cb0 + 60 t k1cstr cacstr
      cbcstr :=
                      1 + 60 t k2cstr
      cccstr := -
                 1 + 60 t k3cstr
                 cd0 + 60 t k2cstr cbcstr + 60 t k3cstr cccstr
                                1 + 60 t k4cstr
      cecstr := ca0 + cb0 + cc0 + cd0 + ce0 - cacstr - cbcstr - cccstr - cdcstr;
```

```
ca0
1 + 60 taucstr k1cstr
ca0new := ----
cb0new := \frac{\text{cb0} + 60 \text{ taucstr k1cstr ca0new}}{1 + 60 \text{ taucstr k2cstr}}
                  1 + 60 taucstr k3cstr
 cd0new:=(cd0+60 taucstr k2cstr cb0new+60 taucstr k3cstr cc0new)/(1+60 taucstr k4cstr);
 ce0new := ca0 + cb0 + cc0 + cd0 + ce0 - ca0new - cb0new - cc0new - cd0new;
capfr := ca0new Exp[-60 (t - taucstr) k1pfr];
 cbpfr :=
     \frac{\text{k1pfr}}{\text{k2pfr}-\text{k1pfr}} \operatorname{capfr} + \frac{\text{cb0new} \left(\text{k2pfr}-\text{k1pfr}\right) - \text{k1pfr} \operatorname{ca0new}}{\text{k2pfr}-\text{k1pfr}} \operatorname{Exp} \left[-60 \left(\text{t-taucstr}\right) \operatorname{k2pfr}\right];
ccpfr := cc0new Exp[-60 (t - taucstr) k3pfr]
        varb := \frac{\text{k2pfr} \left(\text{cb0new} \left(\text{k2pfr} - \text{k1pfr}\right) - \text{k1pfr} \text{ca0new}\right)}{\text{k1pfr} \left(\text{cb0new} \left(\text{k2pfr} - \text{k1pfr}\right)\right)};
        varc := k3pfr cc0new;
cdpfr := \frac{1}{k4pfr - k1pfr} vara \left( Exp[-60 (t - taucstr) k1pfr] - Exp[-60 (t - taucstr) k4pfr] \right) +
       \frac{1}{k4pfr-k2pfr} \ varb \ \left( Exp \left[ -60 \ \left( t-taucstr \right) \ k2pfr \right] - Exp \left[ -60 \ \left( t-taucstr \right) \ k4pfr \right] \right) + \\
       \frac{1}{k4pfr-k3pfr} varc \left(Exp[-60 (t-taucstr) k3pfr]-Exp[-60 (t-taucstr) k4pfr]\right) +
       cd0new Exp[-60 (t - taucstr) k4pfr];
cepfr := ca0 + cb0 + cc0 + cd0 + ce0 - capfr - cbpfr - ccpfr - cdpfr;
k1cstr := 1.9 * 10^{12} Exp \left[ \frac{-112}{8.314 * 10^{-3} \frac{tempcstr+459.67}{100}} \right];
k2cstr := 9.5 * 10^{2} Exp \left[ \frac{-52}{8.314 * 10^{-3} \frac{tempcstr + 459.67}{9.75}} \right];
k3cstr := 1.0 * 10^9 \text{ Exp} \left[ \frac{-86}{8.314 * 10^{-3} \frac{\text{tempcstr} + 459.67}{9/5}} \right];
k4cstr := 1.2 \times 10^6 \text{ Exp} \left[ \frac{-77}{8.314 \times 10^{-3} \frac{\text{tempcstr} + 459.67}{1000}} \right];
k1pfr := 1.9 * 10<sup>12</sup> Exp\left[\frac{-112}{8.314 * 10^{-3} \frac{\text{temppfr} + 459.67}{9.75}}\right];
k2pfr := 9.5 * 10^2 \text{ Exp} \left[ \frac{-52}{8.314 * 10^{-3} \frac{\text{temppfr} + 459.67}{9/5}} \right];
k3pfr := 1.0 * 10^9 \text{ Exp} \left[ \frac{-86}{8.314 * 10^{-3} \frac{\text{temppfr} + 459.67}{3.314 * 10^{-3}}} \right];
```

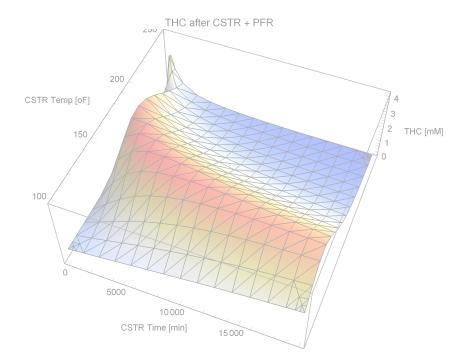
```
k4pfr := 1.2 * 10<sup>6</sup> Exp\left[\frac{-77}{8.314 * 10^{-3} \frac{\text{temppfr} + 459.67}{9.07}}\right];
p[t_, left_, right_] := HeavisideTheta[t - left] HeavisideTheta[right - t];
line1 := Line[{{taucstr, 0}, {taucstr, ca0 + cb0 + cc0 + cd0 + ce0}}];
line2 := Line[{{taucstr + taupfr, 0}, {taucstr + taupfr, ca0 + cb0 + cc0 + cd0 + ce0}}];
Manipulate[
 tempcstr;
 temppfr;
 Plot[{
    cacstrp[t, 0, taucstr],
    cbcstrp[t, 0, taucstr],
    cccstrp[t, 0, taucstr],
    cdcstrp[t, 0, taucstr],
    cecstr p[t, 0, taucstr],
    capfr p[t, taucstr, taucstr + taupfr],
   cbpfr p[t, taucstr, taucstr + taupfr],
   ccpfr p[t, taucstr, taucstr + taupfr],
   cdpfr p[t, taucstr, taucstr + taupfr],
   cepfr p[t, taucstr, taucstr + taupfr]
  }, {t, 0, taucstr + taupfr},
  Epilog → {line1, line2},
  PlotStyle → {Red, Orange, Yellow, Green, Blue},
  PlotLabel → "Series CSTR + PFR Concentrations",
  AxesLabel → {"Time [min]", "Concentration [mM]"},
  PlotLegends → {"CBDA", "CBD", "THCA", "THC", "CBN"},
  PlotRange \rightarrow {0, ca0 + cb0 + cc0 + cd0 + ce0}],
 {{tempcstr, 240, "CSTR Temp [oF]"}, 70, 500, Appearance → "Labeled"},
 {{taucstr, 30, "CSTR \tau [min]"}, 0, 5000, Appearance \rightarrow "Labeled"},
 {{temppfr, 300, "PFR Temp [oF]"}, 70, 500, Appearance → "Labeled"},
 {{taupfr, 30, "PFR \tau [min]"}, 0, 5000, Appearance \rightarrow "Labeled"},
 LocalizeVariables → False]
```



Setting PFR time and temp to recipe-specific 22 min and 212 oF, CSTR time and temp can be optimized for final THC concentration

```
ca0 = 9.1; (*mM CBDA*)
cb0 = 0; (*mM CBD*)
cc0 = 1.1; (*mM THCA*)
cd0 = 0; (*mM THC*)
ce0 = 0; (*mM CBN*)
                  ca0
ca0new := -
          1 + 60 taucstr k1cstr
cb0new := cb0 + 60 taucstr k1cstr ca0new
               1 + 60 taucstr k2cstr
                  cc0
cc0new := -
          1 + 60 taucstr k3cstr
cd0new := (cd0 + 60 taucstr k2cstr cb0new + 60 taucstr k3cstr cc0new) / (1 + 60 taucstr k4cstr);
ce0new := ca0 + cb0 + cc0 + cd0 + ce0 - ca0new - cb0new - cc0new - cd0new;
capfr := ca0new Exp[-60 taupfr k1pfr];
           k1pfr capfr + cb0new (k2pfr - k1pfr) - k1pfr ca0new Exp[-60 taupfr k2pfr];
cbpfr:= -
         k2pfr - k1pfr
                                          k2pfr - k1pfr
ccpfr := cc0new Exp[-60 taupfr k3pfr];
    vara := k1pfr k2pfr ca0new;
               k2pfr - k1pfr
            \frac{k2pfr (cb0new (k2pfr - k1pfr) - k1pfr ca0new)}{};
                             k2pfr - k1pfr
```

```
varc := k3pfr cc0new;
              vara (Exp[-60 taupfr k1pfr] - Exp[-60 taupfr k4pfr])
k4pfr - k1pfr
      \frac{1}{\text{k4pfr} - \text{k2pfr}} \text{varb} \left( \text{Exp[-60 taupfr k2pfr]} - \text{Exp[-60 taupfr k4pfr]} \right) + \frac{1}{\text{k4pfr} - \text{k3pfr}}
      varc (Exp[-60 taupfr k3pfr] - Exp[-60 taupfr k4pfr]) + cd0new Exp[-60 taupfr k4pfr];
cepfr := ca0 + cb0 + cc0 + cd0 + ce0 - capfr - cbpfr - ccpfr - cdpfr;
k1cstr := 1.9 * 10^{12} Exp \left[ \frac{-112}{8.314 * 10^{-3} \frac{tempcstr + 459.67}{100}} \right];
k2cstr := 9.5 * 10^{2} Exp \left[ \frac{-52}{8.314 * 10^{-3} \frac{tempcstr + 459.67}{9/5}} \right];
k3cstr := 1.0 * 10^9 \text{ Exp} \left[ \frac{-86}{8.314 * 10^{-3} \frac{\text{tempcstr} + 459.67}{9/5}} \right];
k4cstr := 1.2 * 10^6 \text{ Exp} \left[ \frac{-77}{8.314 * 10^{-3} \frac{\text{tempcstr} + 459.67}{3.314 * 10^{-3}}} \right];
k1pfr := 1.9 * 10^{12} Exp\left[\frac{-112}{8.314 * 10^{-3} \frac{\text{temppfr} + 459.67}{9/5}}\right];
k2pfr := 9.5 * 10^{2} Exp \left[ \frac{-52}{8.314 * 10^{-3} \frac{temppfr+459.67}{9/5}} \right];
k3pfr := 1.0 * 10^9 \exp \left[ \frac{-86}{8.314 * 10^{-3} \frac{\text{temppfr} + 459.67}{10^{-3}}} \right];
k4pfr := 1.2 * 10^6 \text{ Exp} \left[ \frac{-77}{8.314 * 10^{-3} \frac{\text{temppfr} + 459.67}{3.314 * 10^{-3}}} \right];
temppfr = 212;
taupfr = 22;
Plot3D[{cdpfr(*,4.05*)},
  {taucstr, 0, 20000}, {tempcstr, 100, 250},
  PlotRange → Automatic,
  AxesLabel → {"CSTR Time [min]", "CSTR Temp [oF]", "THC [mM]"},
  PlotLabel → "THC after CSTR + PFR",
  ColorFunction → ColorData["TemperatureMap"],
  Mesh \rightarrow All
```



Out[404]=

Optimization

ca0 = 9.1; (*mM CBDA*)

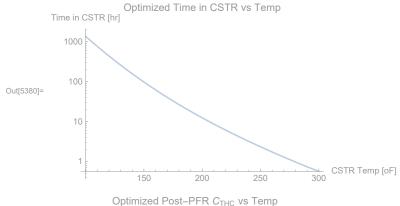
CSTR time [min] and temp [oF] could not be optimized for CBD because concentration diverged with infinite temp for 0 time.

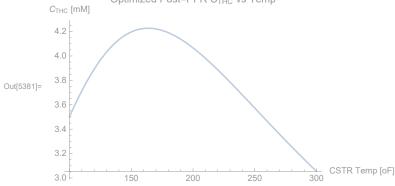
THC concentration is maximized at 0.264232 mM (post-16x dilution in the PFR) for time [min] and temp [oF] below

```
k3cstrop := 1.0 * 10^9 \text{ Exp} \left[ \frac{-86}{8.314 * 10^{-3} \frac{\text{tempcstrop} + 459.67}{9/5}} \right];
k4cstrop := 1.2 * 10^6 \text{ Exp} \left[ \frac{-//}{8.314 * 10^{-3} \frac{\text{tempcstrop} + 459.67}{3.314 * 10^{-3}}} \right];
k1pfr := 1.9 * 10^{12} Exp\left[\frac{-112}{8.314 * 10^{-3} \frac{temppfr+459.67}{1.000}}\right];
k2pfr := 9.5 * 10^{2} Exp \left[ \frac{-52}{8.314 * 10^{-3} \frac{temppfr + 459.67}{9/5}} \right];
k3pfr := 1.0 * 10^9 \text{ Exp} \left[ \frac{-86}{8.314 * 10^{-3} \frac{\text{temppfr} + 459.67}{9/5}} \right];
k4pfr := 1.2 * 10^6 \text{ Exp} \left[ \frac{-77}{8.314 * 10^{-3} \frac{\text{temppfr} + 459.67}{10^{-3}}} \right];
ca0new := \frac{\text{ca0}}{1 + 60 \text{ taucstrop k1cstrop}};
cb0new := \frac{\text{cb0} + 60 \text{ taucstrop k1cstrop ca0new}}{1 + 60 \text{ taucstrop k2cstrop}};
ccOnew := \frac{\text{ccO}}{1 + 60 \text{ taucstrop k3cstrop}};
cd0new := (cd0 + 60 taucstrop k2cstrop cb0new + 60 taucstrop k3cstrop cc0new) /
       (1 + 60 taucstrop k4cstrop);
ce0new := ca0 + cb0 + cc0 + cd0 + ce0 - ca0new - cb0new - cc0new - cd0new;
ca0newmax := \frac{\text{ca0}}{1 + 60 \text{ taucstrmax k1cstrop}};
cb0newmax := cb0 + 60 taucstrmax k1cstrop ca0newmax
                                1 + 60 taucstrmax k2cstrop
ccOnewmax := \frac{\text{ccO}}{1 + 60 \text{ taucstrmax k3cstrop}};
cd0newmax := (cd0 + 60 taucstrmax k2cstrop cb0newmax + 60 taucstrmax k3cstrop cc0newmax) /
       (1 + 60 taucstrmax k4cstrop);
ce0newmax := ca0 + cb0 + cc0 + cd0 + ce0 - ca0newmax - cb0newmax - cc0newmax - cd0newmax;
temppfr = 212;
taupfr = 22;
capfr := ca0new Exp[-60 taupfr k1pfr];
cbpfr := \frac{\text{k1pfr}}{\text{k2pfr} - \text{k1pfr}} \operatorname{capfr} + \frac{\text{cbOnew}\left(\text{k2pfr} - \text{k1pfr}\right) - \text{k1pfr} \operatorname{caOnew}}{\text{k2pfr} - \text{k1pfr}} \operatorname{Exp}\left[-60 \operatorname{taupfr} \operatorname{k2pfr}\right];
ccpfr := cc0new Exp[-60 taupfr k3pfr];
       vara := \frac{k1pfr \ k2pfr \ ca0new}{k2pfr - k1pfr};
```

```
varb := \frac{k2pfr (cb0new (k2pfr - k1pfr) - k1pfr ca0new)}{k2pfr - k1pfr};
     varc := k3pfr cc0new;
cdpfr := \frac{1}{k4pfr - k1pfr} vara \left( Exp[-60 taupfr k1pfr] - Exp[-60 taupfr k4pfr] \right) +
     \frac{1}{\text{k4pfr} - \text{k2pfr}} \text{ varb } \left( \text{Exp[-60 taupfr k2pfr]} - \text{Exp[-60 taupfr k4pfr]} \right) + \frac{1}{\text{k4pfr} - \text{k3pfr}} \text{ varc}
      (Exp[-60 taupfr k3pfr] - Exp[-60 taupfr k4pfr]) + cd0new Exp[-60 taupfr k4pfr];
cepfr := ca0 + cb0 + cc0 + cd0 + ce0 - capfr - cbpfr - ccpfr - cdpfr;
capfrmax := ca0newmax Exp[-60 taupfr k1pfr];
cbpfrmax :=
   \frac{\text{k1pfr}}{\text{k2pfr}-\text{k1pfr}} \operatorname{capfrmax} + \frac{\text{cb0newmax} \left(\text{k2pfr}-\text{k1pfr}\right) - \text{k1pfr} \operatorname{ca0newmax}}{\text{k2pfr}-\text{k1pfr}} \operatorname{Exp[-60 \, taupfr \, k2pfr]};
ccpfrmax := cc0newmax Exp[-60 taupfr k3pfr];
     varamax := \frac{k1pfr \ k2pfr \ ca0newmax}{k2pfr - k1pfr};
     varbmax := \frac{k2pfr \left(cb0newmax \left(k2pfr - k1pfr\right) - k1pfr ca0newmax\right)}{k2pfr - k1pfr};
      varcmax := k3pfr cc0newmax;
cdpfrmax := \frac{1}{k4pfr - k1pfr} varamax (Exp[-60 taupfr k1pfr] - Exp[-60 taupfr k4pfr]) +
     \frac{1}{k4pfr - k2pfr} varbmax (Exp[-60 taupfr k2pfr] - Exp[-60 taupfr k4pfr]) +
     \frac{1}{\text{k4pfr} - \text{k3pfr}} \, \text{varcmax} \, \left( \text{Exp[-60 taupfr k3pfr]} \, - \, \text{Exp[-60 taupfr k4pfr]} \right) \, + \,
     cd0newmax Exp[-60 taupfr k4pfr];
cepfrmax := ca0 + cb0 + cc0 + cd0 + ce0 - capfrmax - cbpfrmax - ccpfrmax - cdpfrmax;
(*4.2277190685 mM before dilution*)
NArgMax[{cdpfr, taucstrop ≥ 0, tempcstrop ≥ 0}, {taucstrop, tempcstrop}]
taucstrmax := NArgMax[{cdpfr, taucstrop ≥ 0}, taucstrop];
LogPlot \left[\frac{\mathsf{taucstrmax}}{\mathsf{60}}\right]
  {tempcstrop, 100, 300},
 PlotLabel → "Optimized Time in CSTR vs Temp",
 AxesLabel → {"CSTR Temp [oF]", "Time in CSTR [hr]"},
 MaxRecursion → 0
Plot[cdpfrmax,
  {tempcstrop, 100, 300},
 PlotRange → All,
 PlotLabel → "Optimized Post-PFR C<sub>THC</sub> vs Temp",
 AxesLabel → {"CSTR Temp [oF]", "C<sub>THC</sub> [mM]"},
 MaxRecursion → 0]
```







Final Concentrations (Diluted 16x)

```
Grid[{
  {"Compound", "CBDA", "CBD", "THCA", "THC", "CBN"},
  {"Label", "CA", "CB", "CC", "CD", "CE"},
  {"Initial Conc [mM]", 9.1, 0, 1.1, 0, 0},
  {"Final Conc [mM]", 0.989 / 16, 2.619 / 16, 0.0159 / 16, 4.227 / 16, 2.349 / 16}
 , Frame → All]
```

Compound	CBDA	CBD	THCA	THC	CBN
Label	CA	СВ	CC	CD	CE
Initial Conc [mM]	9.1	0	1.1	0	0
Final Conc [mM]	0.0618125	0.163688	0.00099375	0.264188	0.146813

Reactor Calculations

THC = 4.227719069 mM at 163.72 oF for $3182 \text{ min} \approx 53 \text{ hr} \approx 2.2 \text{ days}$ CBD concentration max at ∞ temp for 0 time

13x9x1 in³ pan has a surface area to volume ratio of 2.376 A pipe matching this would have diameter 3.025 in For 1 in thick brownies to be produced every 1 s, volumetric flow rate would be

```
\pi * (3.025/2)^2 1 = 7.187 \text{ in}^3/\text{s} = 424 \text{ L/hr}
```

Including the 16x dilution from CSTR to PFR, 26.5 L oil/hr required 424 L/hr brownie mix * 22 min = 155.467 L = 9487 in³ PFR length = $V/(\pi (D/2)^2)$ = 1320 in = 110 ft long PFR

1 oz cannabis / 13*9*1 in³ batch = 1.74 g / brownie

26.5 L/hr for 53 hrs \rightarrow 1404 L CSTR

Reactor calculations hidden above

Batch SA/V ratio = 2.376 Match PFR → 3" diam 1" thick brownie per second (1.75 g ea) \rightarrow 424 L/hr 22 min → 155 L PFR (110' long)

16x dilution \rightarrow 27 L/hr 2.2 days → 1400 L CSTR THC = 4.2 mM at 163.72 oF

Wholesale \$1400 / lb 14 lb / hr Costs \$20,000 / hr Sold for \$20 ea \rightarrow \$72,000 / hr revenue

Expenditure

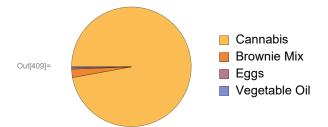
Prices

1 oz cannabis / 0.5 cup vegetable oil = 14 lbs cannabis + 26.5 L vegetable oil / hr Wholesale \$1400 / lb \$20,000 / hr for cannabis \$0.06 / fl oz vegetable oil \$54 / hr for oil brownie mix + 2 eggs + 0.25 cup water = 16.3 brownies \$0.10 / egg = \$0.02 / brownie\$2 / brownie mix box = \$0.13 / brownie \$468 / hr for mix \$72 / hr for eggs

~\$20,000 / hr total

\$20 / brownie = \$72,000 / hr

In[409]:= PieChart[{20000, 468, 72, 54}, ChartLegends \rightarrow {"Cannabis", "Brownie Mix", "Eggs", "Vegetable Oil"}]



Cannabis Curve

```
ln[407] = r := (1 + 0.9 \cos[8 \theta]) (1 + 0.1 \cos[24 \theta]) (0.9 + 0.1 \cos[200 \theta]) (1 + \sin[\theta]);
       Animate[
        PolarPlot[r, \{\theta, 0, 2\pi\},
         Axes → False,
         ColorFunction \rightarrow Function[{x, y, t, r}, Hue[r + color]],
         ColorFunctionScaling → False,
         MaxRecursion → 5,
         PlotRange \rightarrow All],
        {color, 0, 4},
        AnimationRunning → False]
```

