Cannabis Brownie Kinetics

$$\text{CBDA} \xrightarrow{k1} \text{CBD} \xrightarrow{k2} \text{THC}$$
$$\text{THCA} \xrightarrow{k3} \text{THC} \xrightarrow{k4} \text{CBN}$$

or

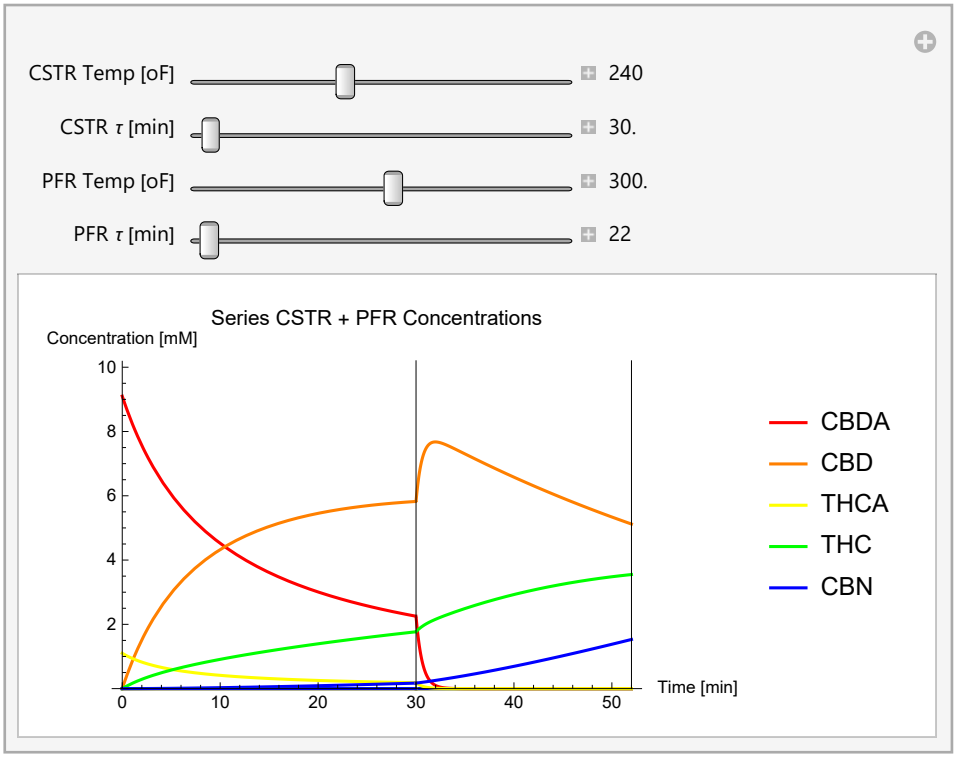
$$\text{A} \xrightarrow{k1} \text{B} \xrightarrow{k2} \text{D}$$
$$\text{C} \xrightarrow{k3} \text{D} \xrightarrow{k4} \text{E}$$

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

Out[5335]=

Rate Constant	A $[s^{-1}]$	E_a [kJ/mol]
k1	1.9×10^{12}	112
k2	950.	52
k3	$1. \times 10^{9}$	86
k4	1.2×10^{6}	77

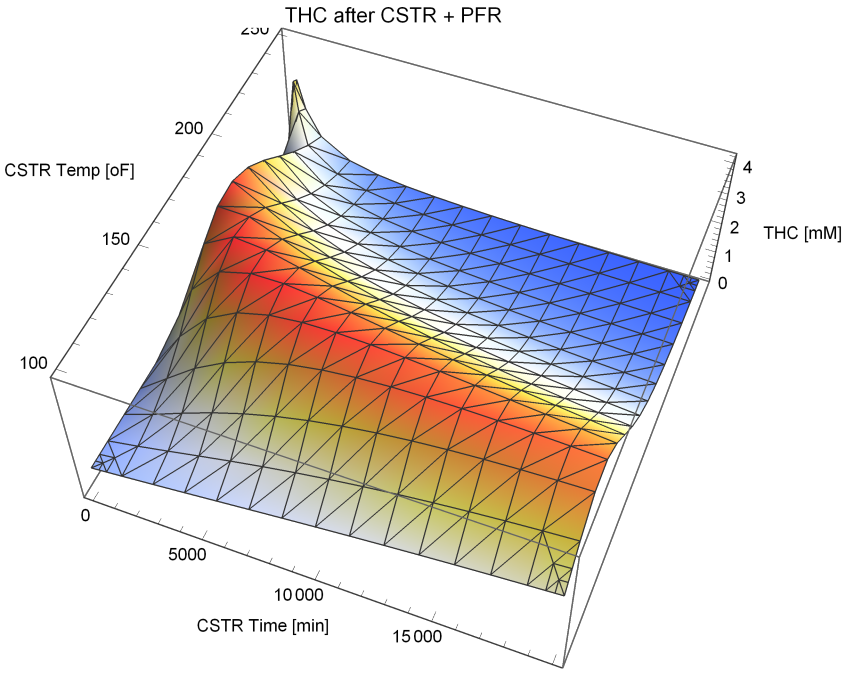
Out[5414]=



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

for final THC concentration

Out[404]=



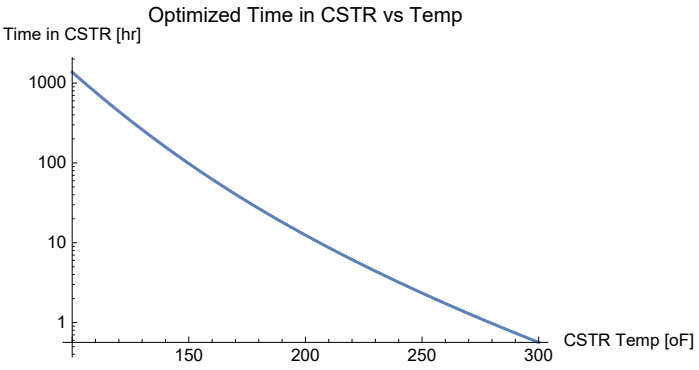
Optimization

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

Out[5378]= {3182.09, 163.718}

Out[5380]=



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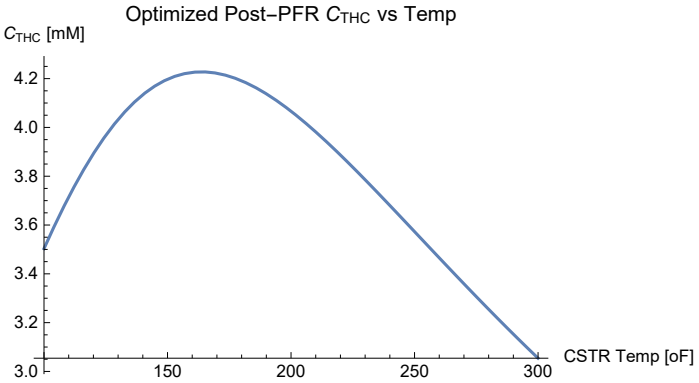


Final Concentrations (Diluted 16x)

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]	0.0618125	0.163688	0.00099375	0.264188	0.146813

Reactor Calculations

Reactor calculations hidden above

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

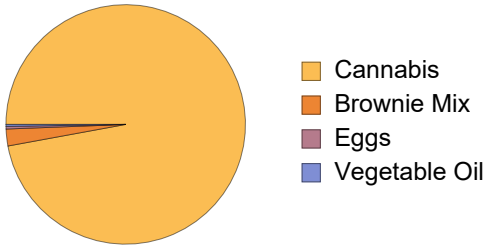
16x dilution → 27 L/hr
2.2 days → 1400 L CSTR

THC = 4.2 mM at 163.72 oF

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

Expenditure

Out[409]=



Cannabis Curve

Out[408]=