Validere

Crude oil blending problem

Anyang Peng, Oct 18 2022

Problem Statement

- Given distillation profiles of two crude oils, create a model which will give an approximate distillation profile of the mixture of the two oils with specified volumes.
- (Note: thinking of the distillation profiles as snapshots of functions is the recommended view.) The percentages to use (and get at the end) are the same as the ones in the above example, namely: [5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 95, 99]. Explain any assumptions or simplifications made.

05% : 45°C

10% : 95°C

20% : 101°C

30% : 140°C

40% : 179°C

50% : 210°C

60% : 225°C

70% : 260°C

80% : 310°C

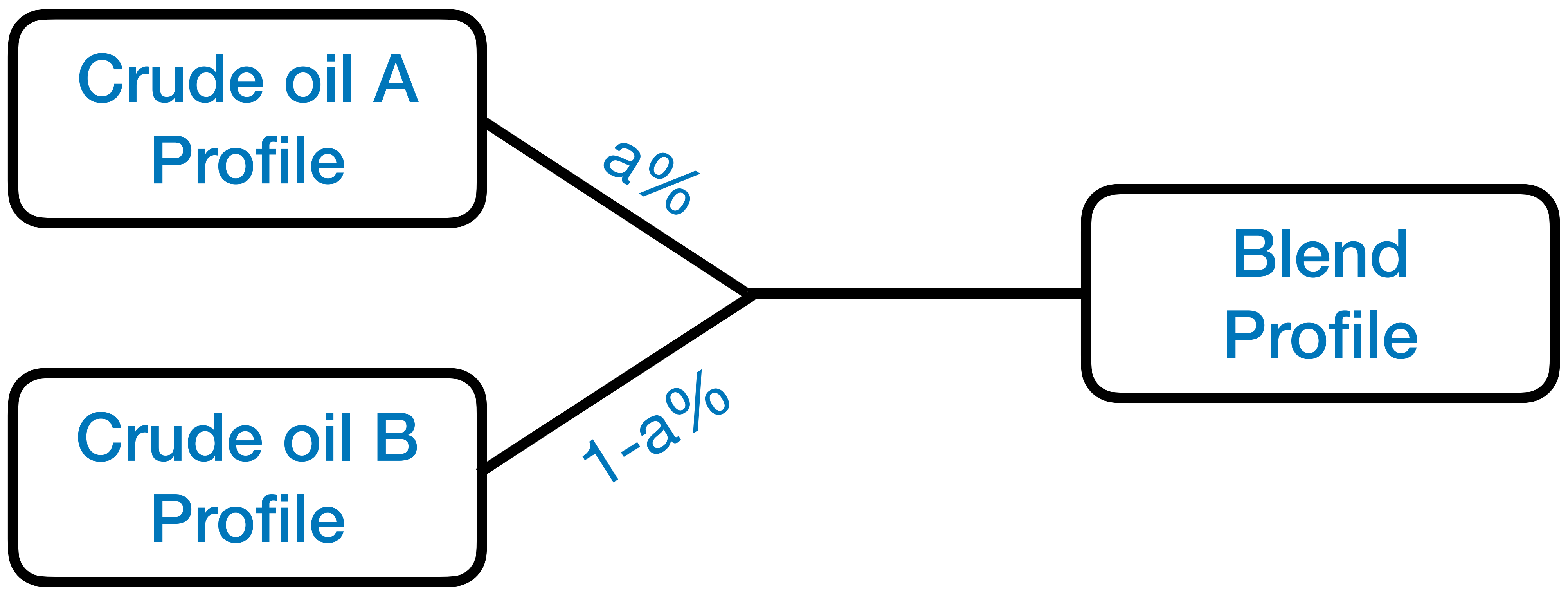
90% : 330°C

95% : 360°C

99% : 381°C

Objectives

- Create a mathematical model to predict the distillation profile of the blend given the distillation profiles of two crude oils and the mixing ratio.



Approaches

- Rule-based approach: derive the model from physics.
- Machine learning approach: learn the model from large amount of data

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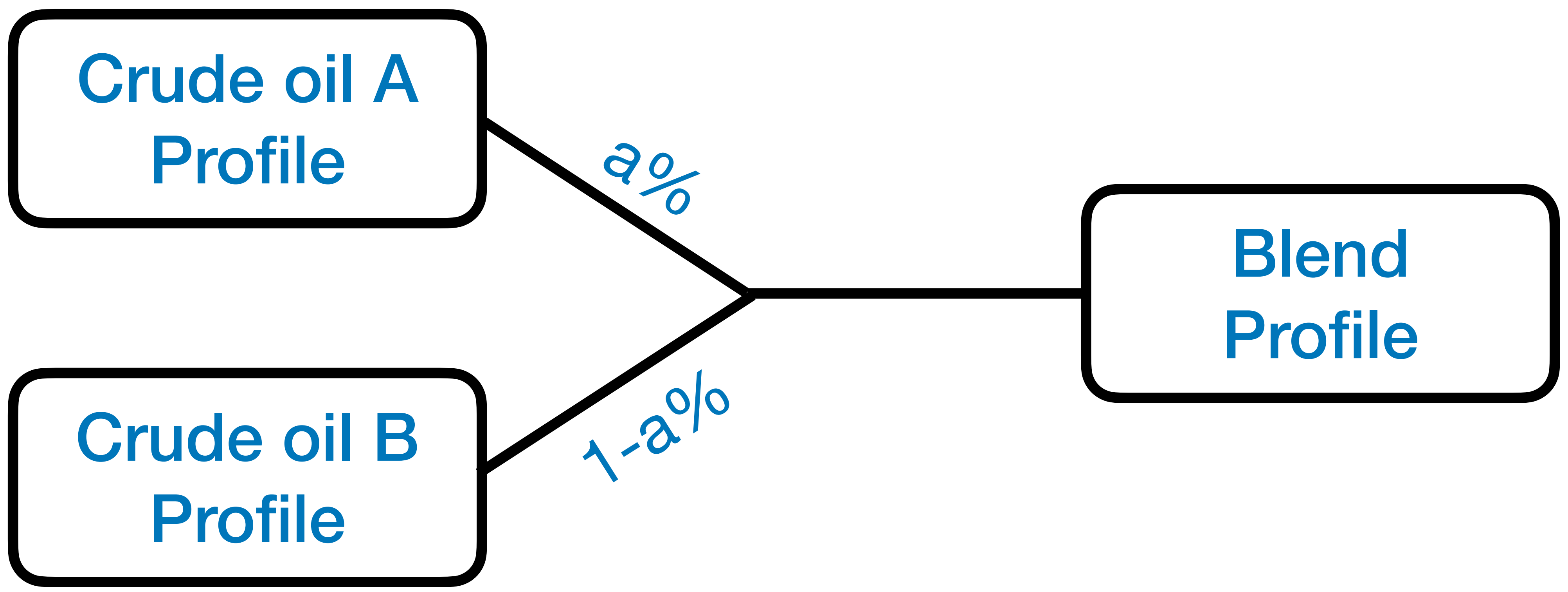

Approaches

- Rule-based approach: derive the model from physics.
- Machine learning approach: learn the model from large amount of data
- Comparison
- Uncertainty

Rule-based Approach

Background

- Distillation: the process to separate chemicals based on the difference between their boiling points.

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- What controls the boiling point?

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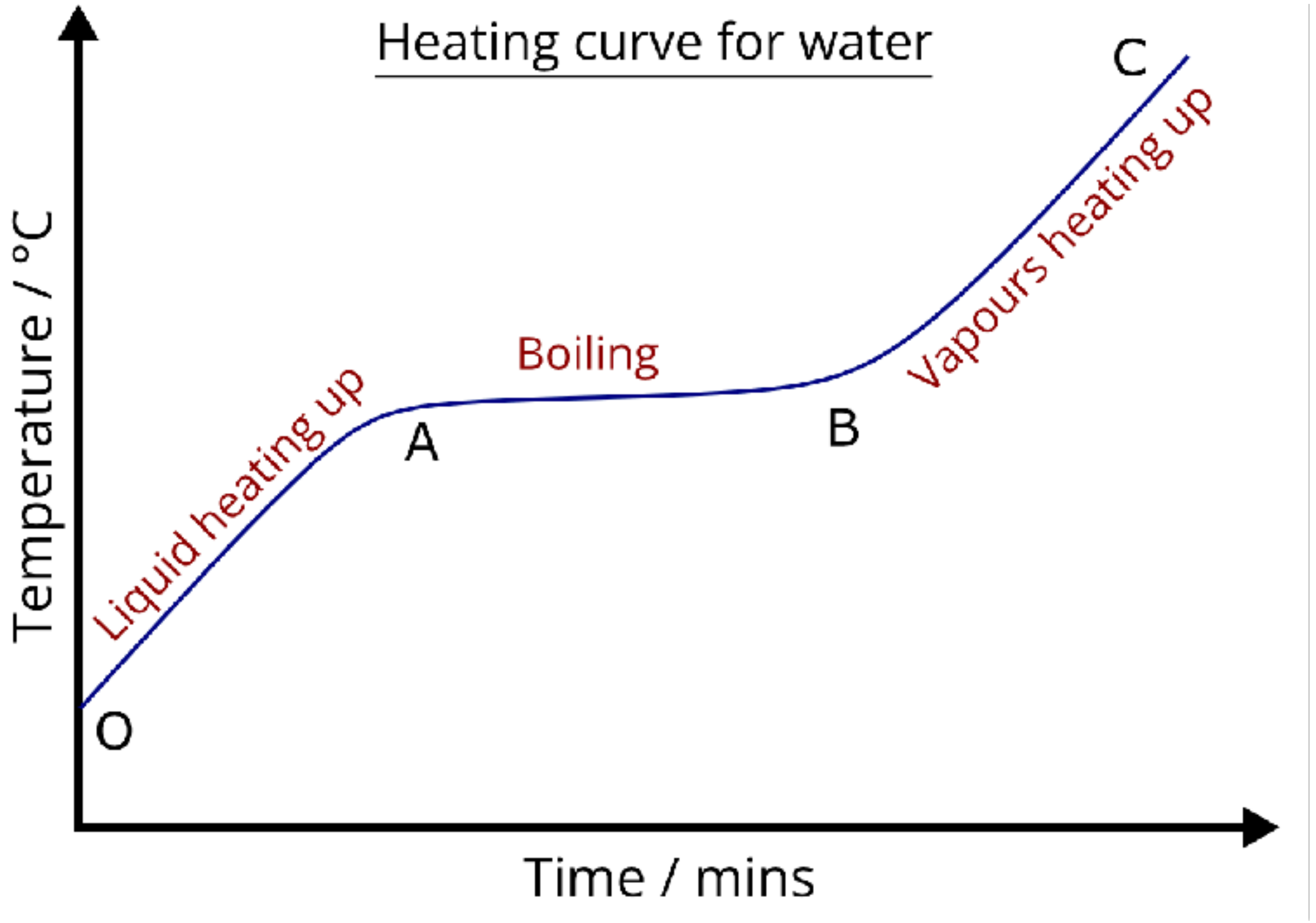
  The liquid boils when the vapor pressure is equal to the pressure of the environment



Rule-based Approach

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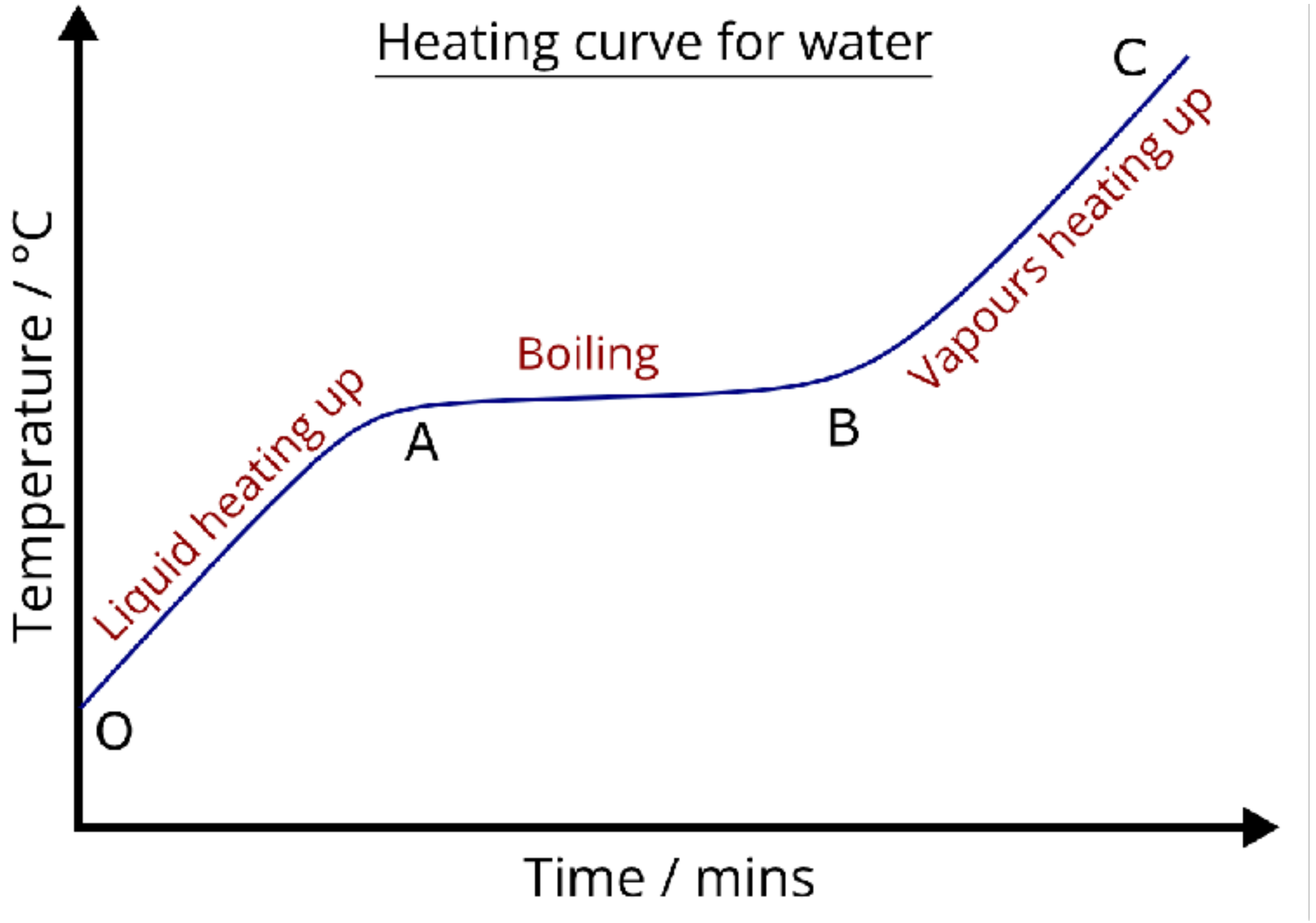

Rule-based Approach

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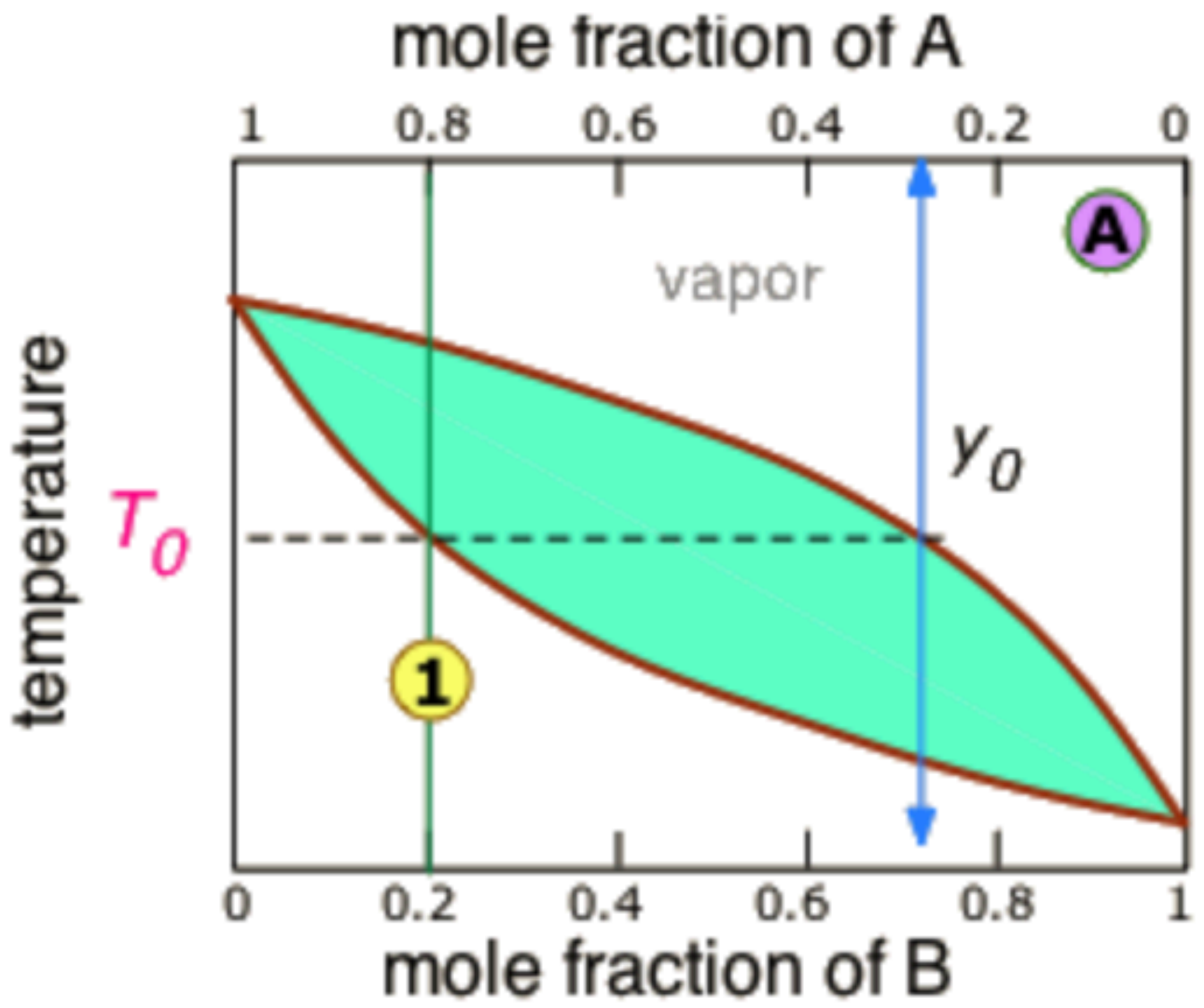
- Distillation: the process to separate chemicals based on the difference between their boiling points.

- What controls the boiling point?

  The liquid boils when the vapor pressure is equal to the pressure of the environment

- How does distillation occur in mixtures?

  For a binary mixture, the temperature at which the mixture boils depends on the composition of the mixture, and it changes throughout the boiling process.



Rule-based Approach

Background

- What about our problem?
  - Our system is not binary.
  - We don’t know the exact composition.
  - No well defined boiling points, boiling ranges overlap.

It is impossible to solve this problem analytically with the given information using the approach mentioned for the binary system.

We need to simplify the system by making assumptions

Rule-based Approach
Assumptions

- I assume the distillation settings are all the same (ramping rate, heat transfer, mixing, etc.) Fair assumption.

Rule-based Approach

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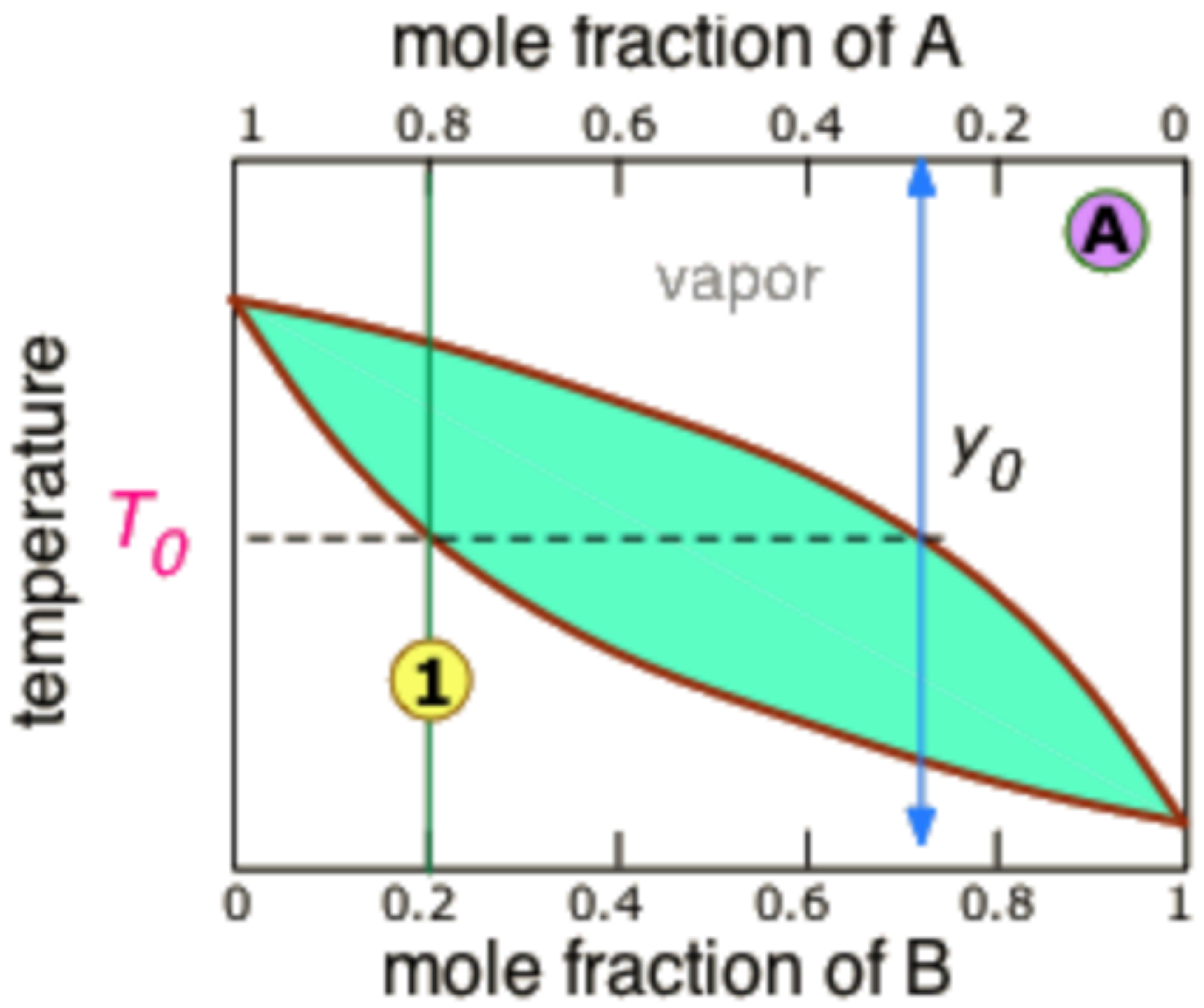
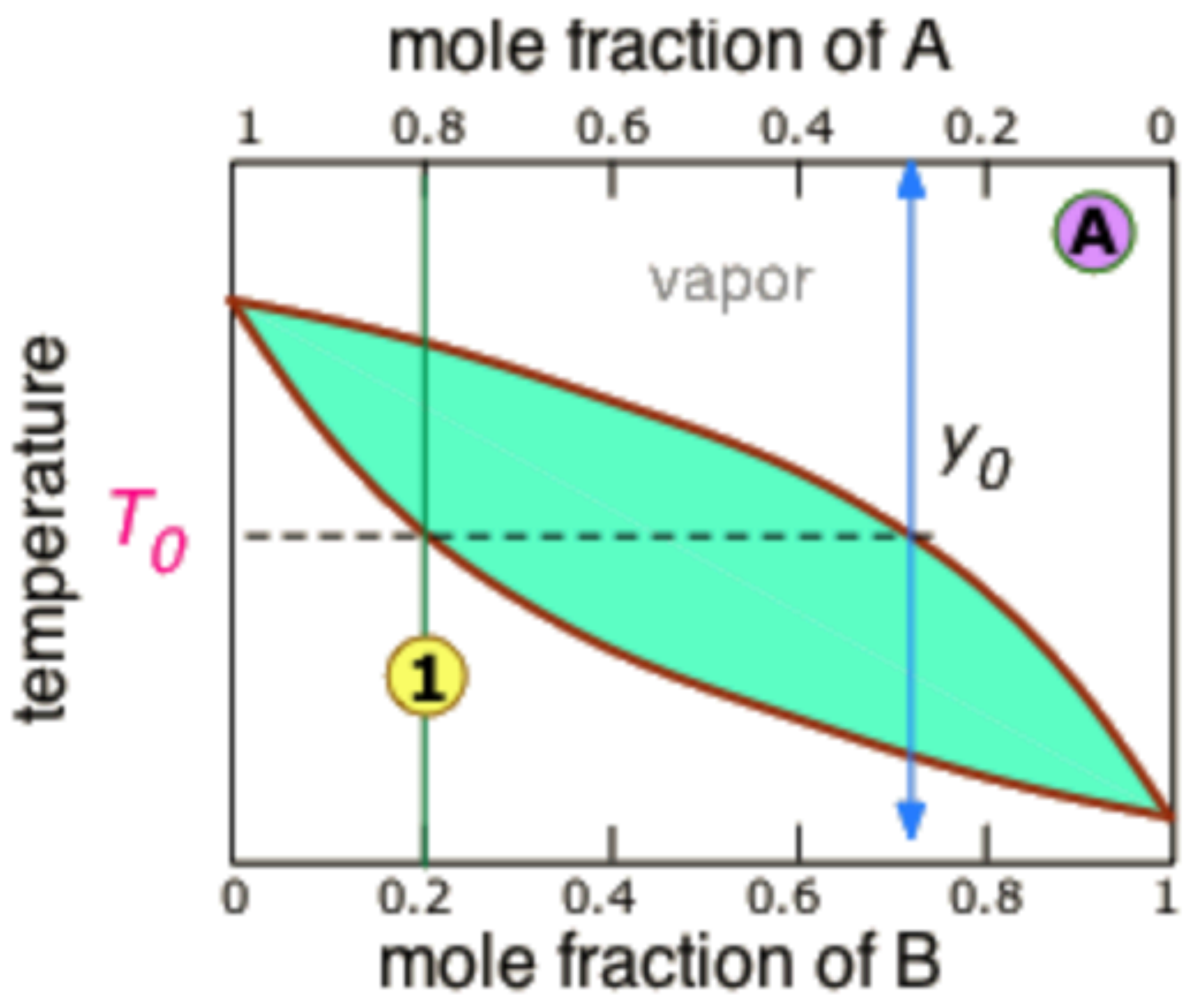
- Based on the composition list, I assume azeotropic composition is not an issue. In other words the boiling point moves along the bubble point curve in the above figure (if we consider a binary mixture) Fair assumption.



Rule-based Approach

Assumptions

- I simplify the curve to a straight line. As a result, the boiling temperature is approximately linearly dependent on the composition within a small range
  OK assumption.

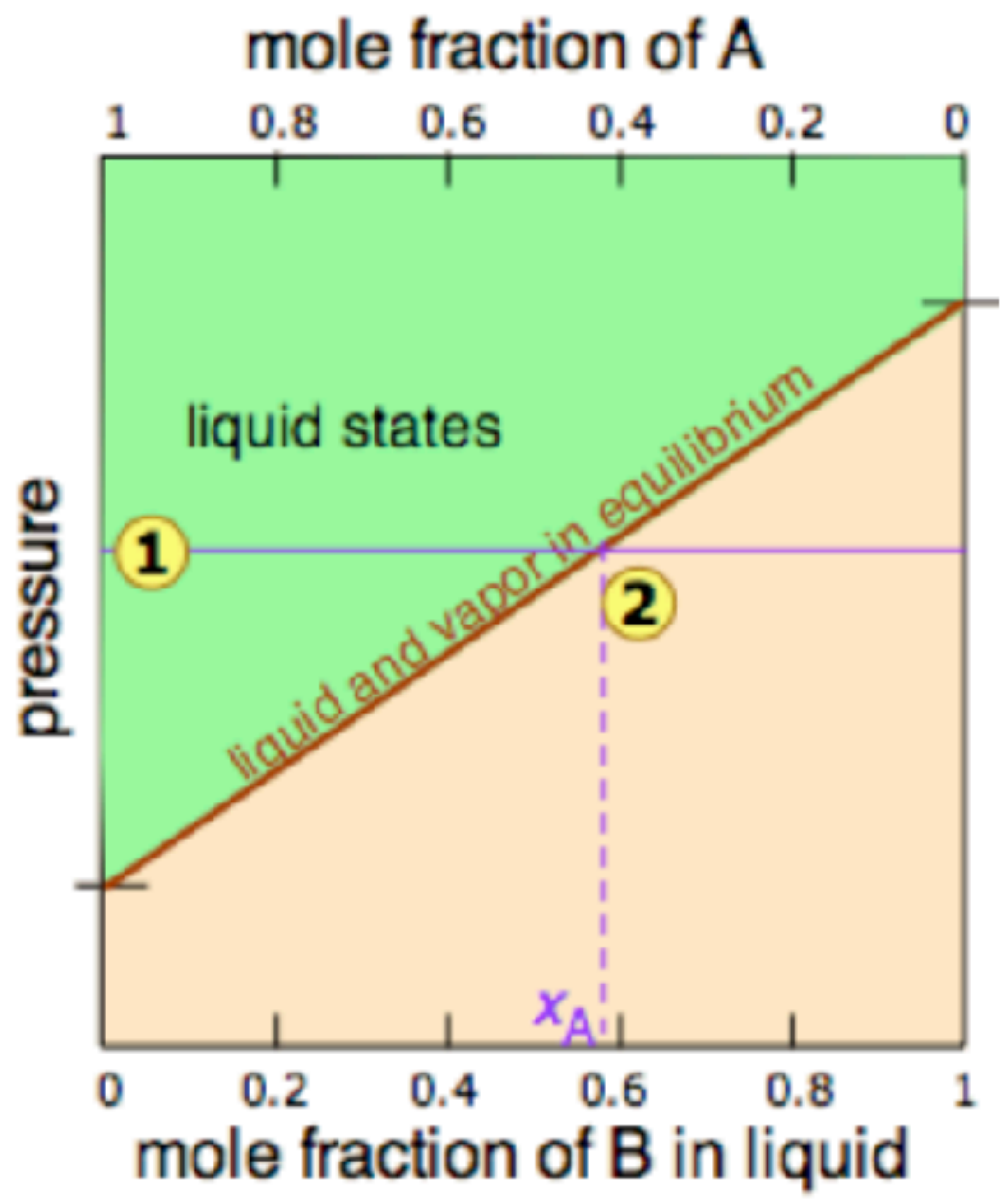


Rule-based Approach

Assumptions

- I simplify the curve to a straight line. As a result, the boiling temperature is approximately linearly dependent on the composition within a small range OK assumption.

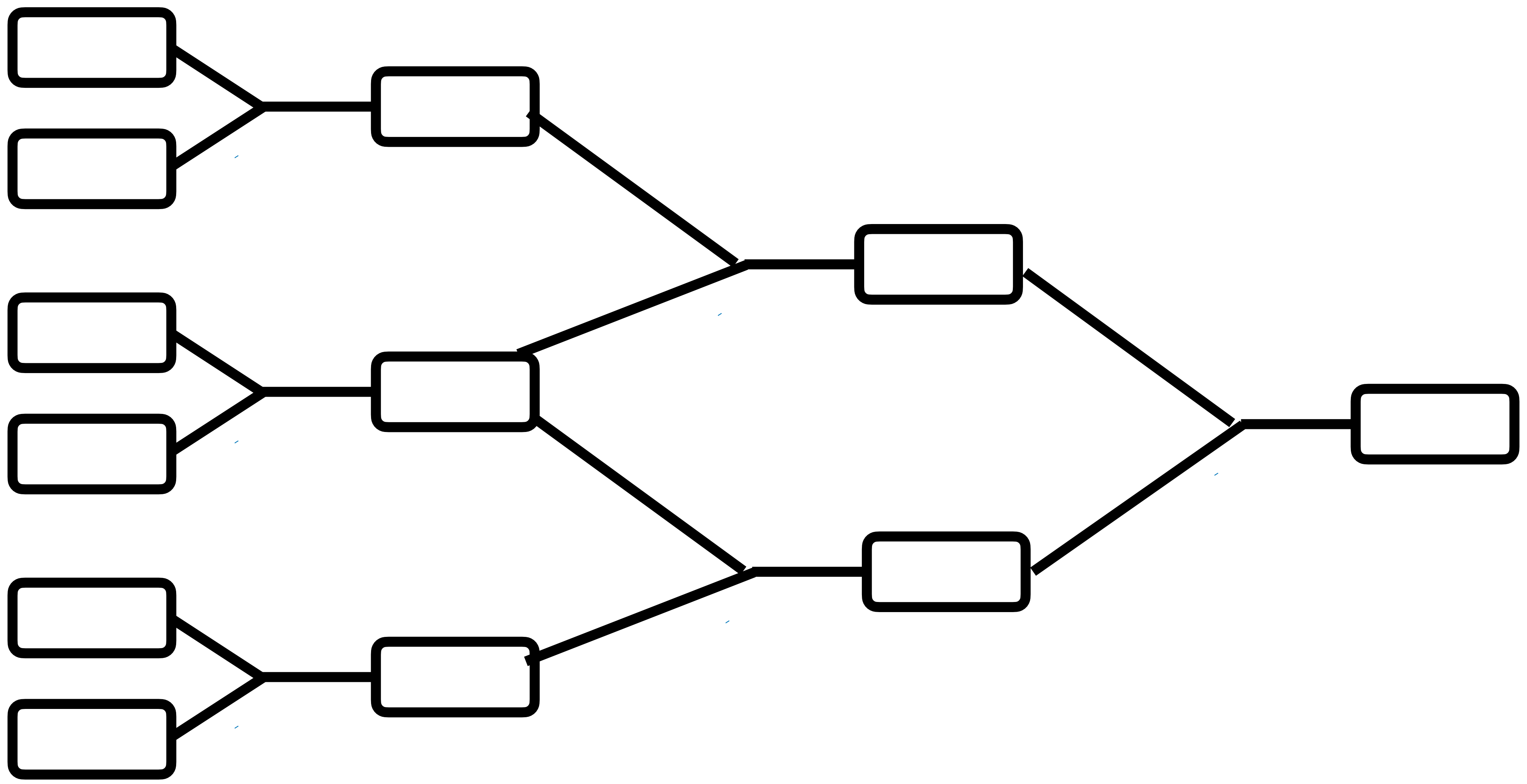
- This also implies the dew point curve is close to the boiling point curve, and the distillation does not change the molar fraction of each components in the liquid phase. (This is not a valid assumption, but necessary to simplify the problem.)

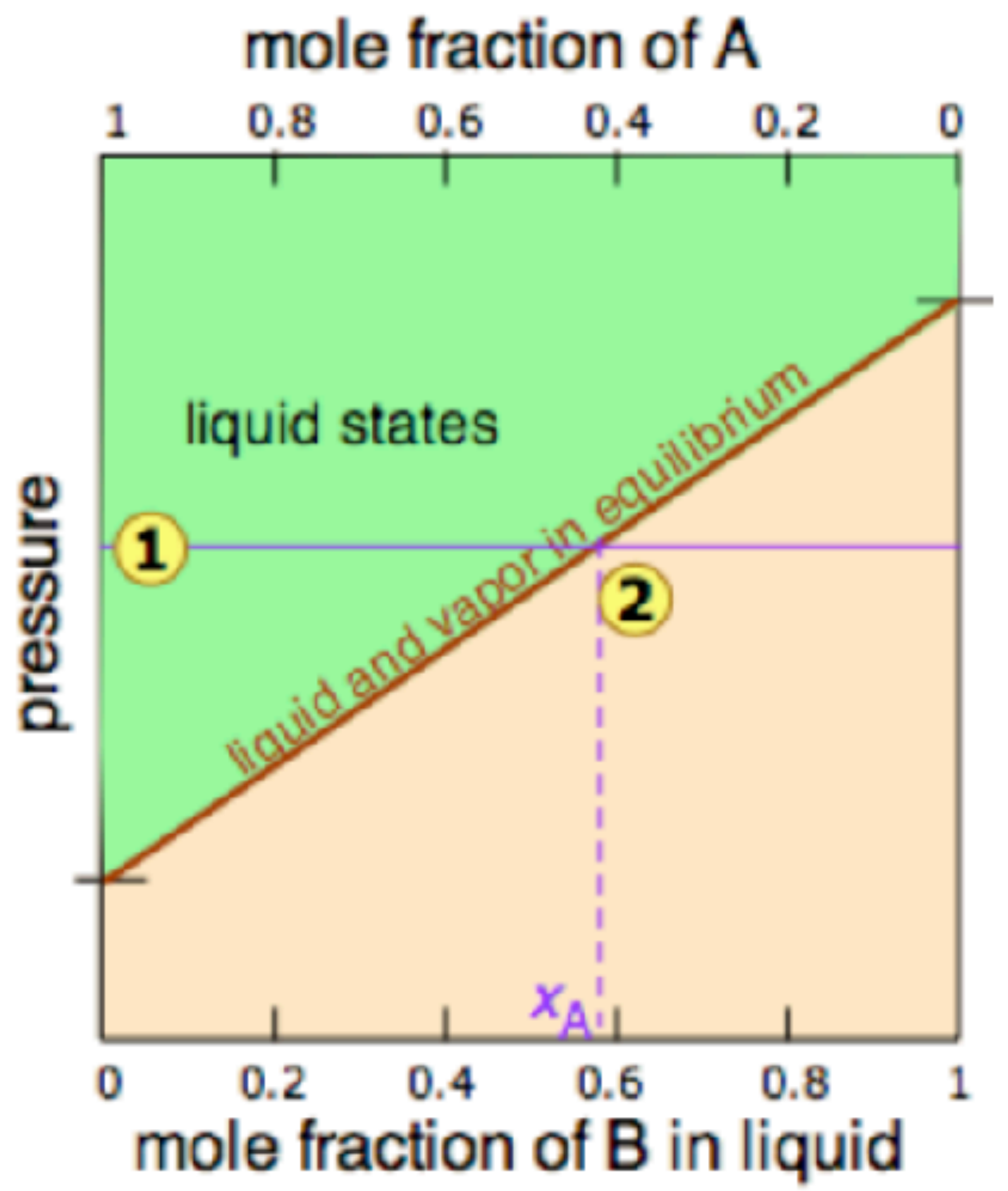


Rule-based Approach

Assumptions

- At each time snapshot, microscopically, I simplify the multi-component mixture to many binary mixture systems (this neglects the interaction between those systems which inevitably leads to error). This is a bold assumption, but necessary to simplify the problem.





Rule-based Approach

Demo

Given the above information, we can get a very rough estimation on the distillation profile of the blend using a linear combination of the starting crude oil.

- Sanity Check
  - 50% A + 50% A = A
  - 99% A + 1% B should be similar to A.
  - 1% A + 99% B shouldd be similar to B.
  - if A has no residue, B has 20% residue, mix in a 1:1 ratio, we should have 10% residue.

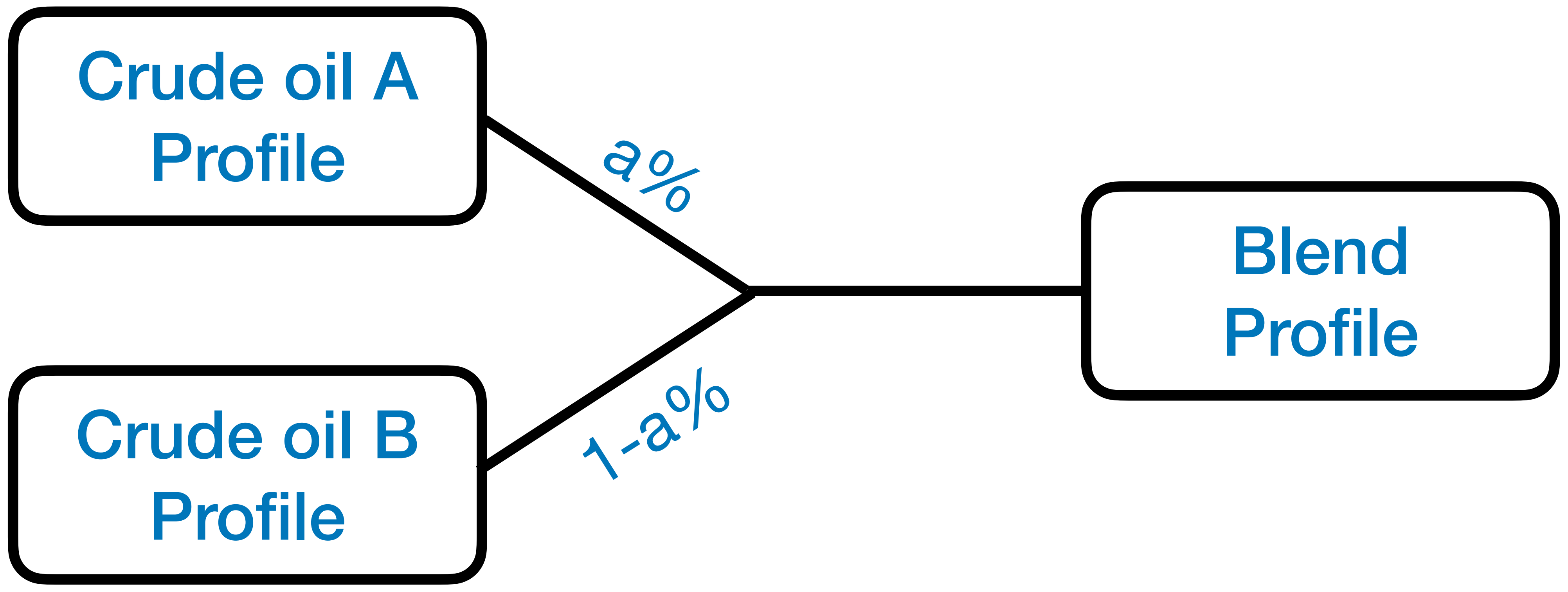
```python
if __name__ == '__main__':
    #A is BG past Avg(Feb 04, 2008), B is AWB past Avg(Jun 29, 2010)
    compA = Distill([28.0, 52.7, 78.7, 117.9, 160.2, 207.9, 264.8, 324.9, 393.3, 478.7, 571.4, 619.2, 685.2])
    compB = Distill([34.2, 46.8, 82.5, 235.4, 350.8, 426.4, 498.3, 582.4, 658.7, 708.9, float('inf'), float('inf'), float('inf')])

    m = Model(compA, compB)
    print(m.blend(0.8))
    assert m.blend(0) == compB.temp
    assert m.blend(1) == compA.temp
```

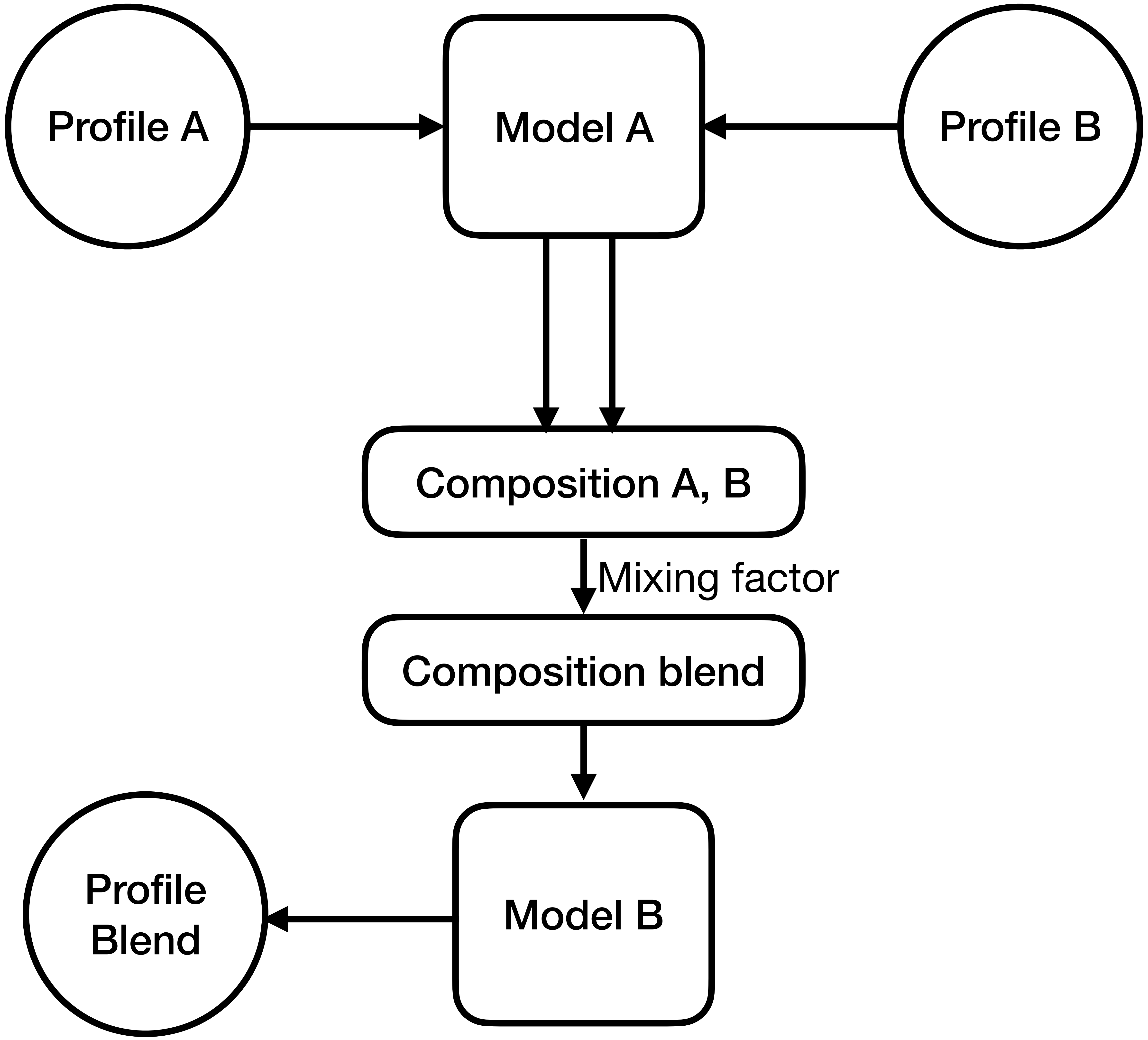
```
[(base) Anyangs-MacBook-Pro-2:Desktop anyangpeng$ python basemode.py
[29.24, 51.52, 79.46, 141.4, 198.32, 251.6, 311.5, 376.4, 446.38, 524.74, 619.2, 685.2, inf]
```

Machine Learning Approach

Problem statement

- Input: 2* List [float] + float
- Output: List [float]





Machine Learning Approach

Data

- ~5000 reports from the Crude Monitor database

https://crudemonitor.ca/library/archives/batch/BDY/BDY090831.pdf

Crude: **Boundary Lake** **Location:** **Kamloops**
Batch: **BDY-831** **SampleDate:** **August 31, 2009**

Yield on Crude (Vol %)

	Observed	Past Avg	Std Dev
C4 and lighter (mass%)	1.8	1.8	0.3
Naphtha (C5 - 190°C)	-	22.8	2.3
Kerosine (190°C - 277°C)	-	17.7	0.7
Distillate (277°C - 343°C)	-	13.1	1.6
Gas Oil (343°C - 565°C)	-	31.5	1.8
Residue (565°C +)	-	13.1	1.9

Distillation Information (°C)

% Off	Observed	Past Avg	Std Dev
IBP	-	32.4	5.5
1%	-	34.7	4.6
5%	-	87.7	10.9
10%	-	112.6	7.1
15%	-	137.3	6.0
20%	-	162.6	6.0
25%	-	188.0	7.2
30%	-	215.1	7.1
35%	-	240.0	7.1
40%	-	264.3	7.5
45%	-	290.0	8.1
50%	-	314.0	8.3
55%	-	339.8	9.8
60%	-	368.0	10.2
65%	-	397.7	10.6
70%	-	427.8	10.4
75%	-	460.3	11.7
80%	-	497.3	13.5
85%	-	543.2	18.5
90%	-	604.5	25.8
95%	-	668.1	32.0
98%	-	691.7	17.3
99%	-	696.7	2.2
100%	-	-	-
FBP	-	701.4	6.7
Residue (%)	-	5.35	1.93

Machine Learning Approach

Data

Web Scrape with Selenium

```
1   AWB100629
2   AWB100527
3   AWB100428
4   AWB100323
5   AWB100216
6   AWB100122
7   AWB091222
8   AWB091122
9   AWB091023
10  AWB090920
11  AWB090827
12  AWB090723
13  AWB090628
14  AWB090616
15  AWB090528
16  AWB090516
17  AWB090429
18  AWB090415
19  AWB090329
20  AWB090315
```

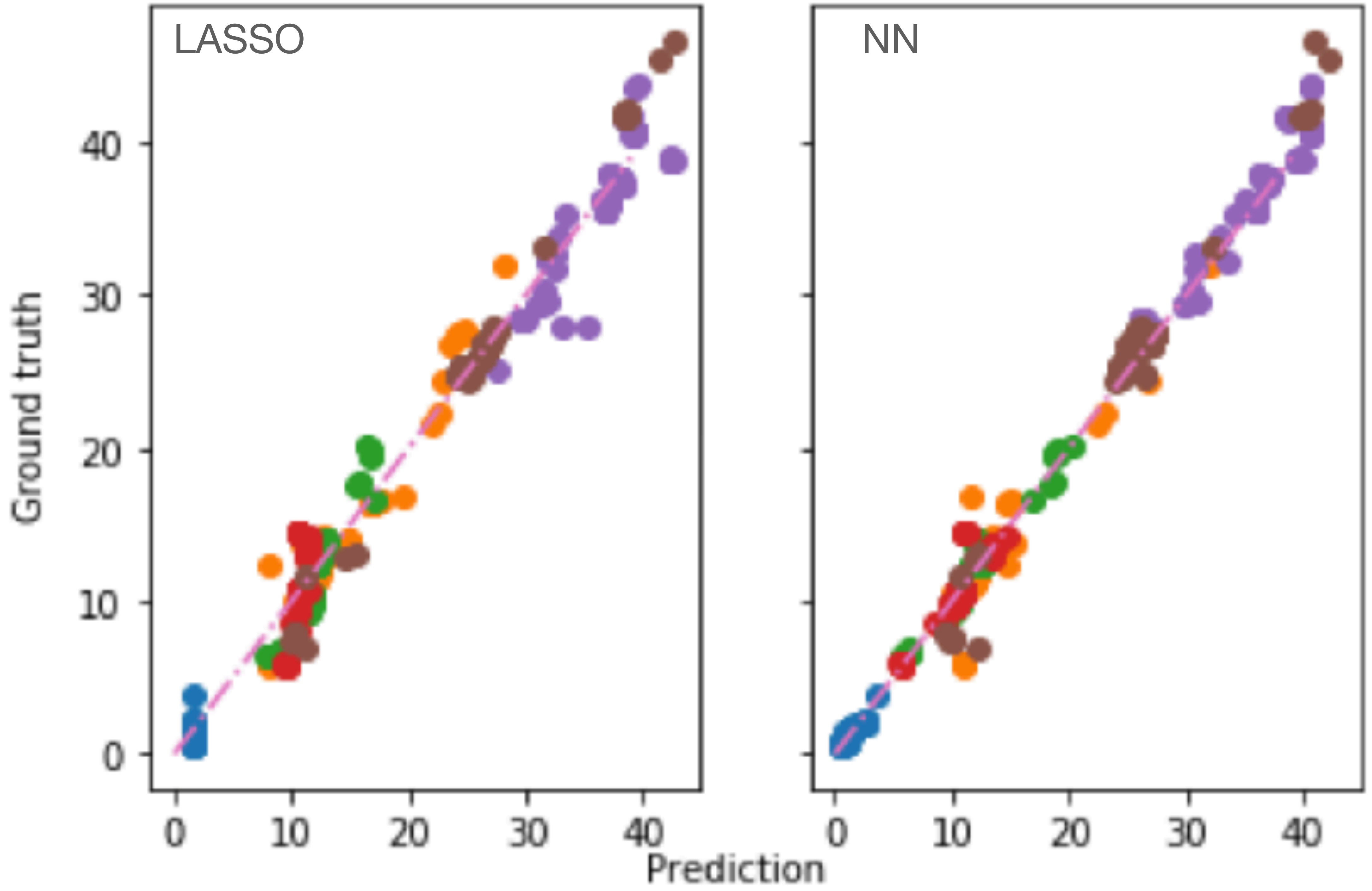
https://crudemonitor.ca/library/archives/batch/BDY/BDY090831.pdf

```
[              Observed.1  Past Avg.1  Std Dev.1
 % Off
 IBP                 2000       34.20       2.30
 1%                  2000       34.70       2.30
 5%                  2000       46.80       9.70
 10%                 2000       82.50      15.10
 15%                 2000      139.50      40.70
 20%                 2000      235.40      42.50
 25%                 2000      306.00      24.30
 30%                 2000      350.80      20.80
 35%                 2000      390.00      19.40
 40%                 2000      426.40      17.60
 45%                 2000      461.20      19.00
 50%                 2000      498.30      20.30
 55%                 2000      538.60      22.80
 70%                 2000      658.70      22.90
 75%                 2000      685.70      14.70
 80%                 2000      708.90      10.90
 85%                 2000      719.00    2000.00
 90%                 2000     2000.00    2000.00
 95%                 2000     2000.00    2000.00
 98%                 2000     2000.00    2000.00
 99%                 2000     2000.00    2000.00
 100%                2000     2000.00    2000.00
 FBP                 2000      716.80       1.40
 Residue (%)         2000       21.23       3.56,
                               Obs   His   Std
 Composition
 C4 and lighter (mass%)        0.9   0.7   0.2
 Naphtha (C5 - 190°C)            -  16.3   2.5
 Kerosine (190°C - 277°C)        -   6.9   0.4
 Distillate (277°C - 343°C)      -   6.0   0.3
 Gas Oil (343°C - 565°C)         -  28.4   0.5
 Residue (565°C +)               -  41.7   2.7]
```

Machine Learning Approach

Model A

- Use distillation profile to predict composition.
- Map the dataset from (500,22) to (500,6).



The real compositions from reprot are

- A: [3.9, 31.8, 16.6, 10.7, 24.9, 12.0]
- B: [0.7, 16.3, 6.9, 6.0, 28.4, 41.7]

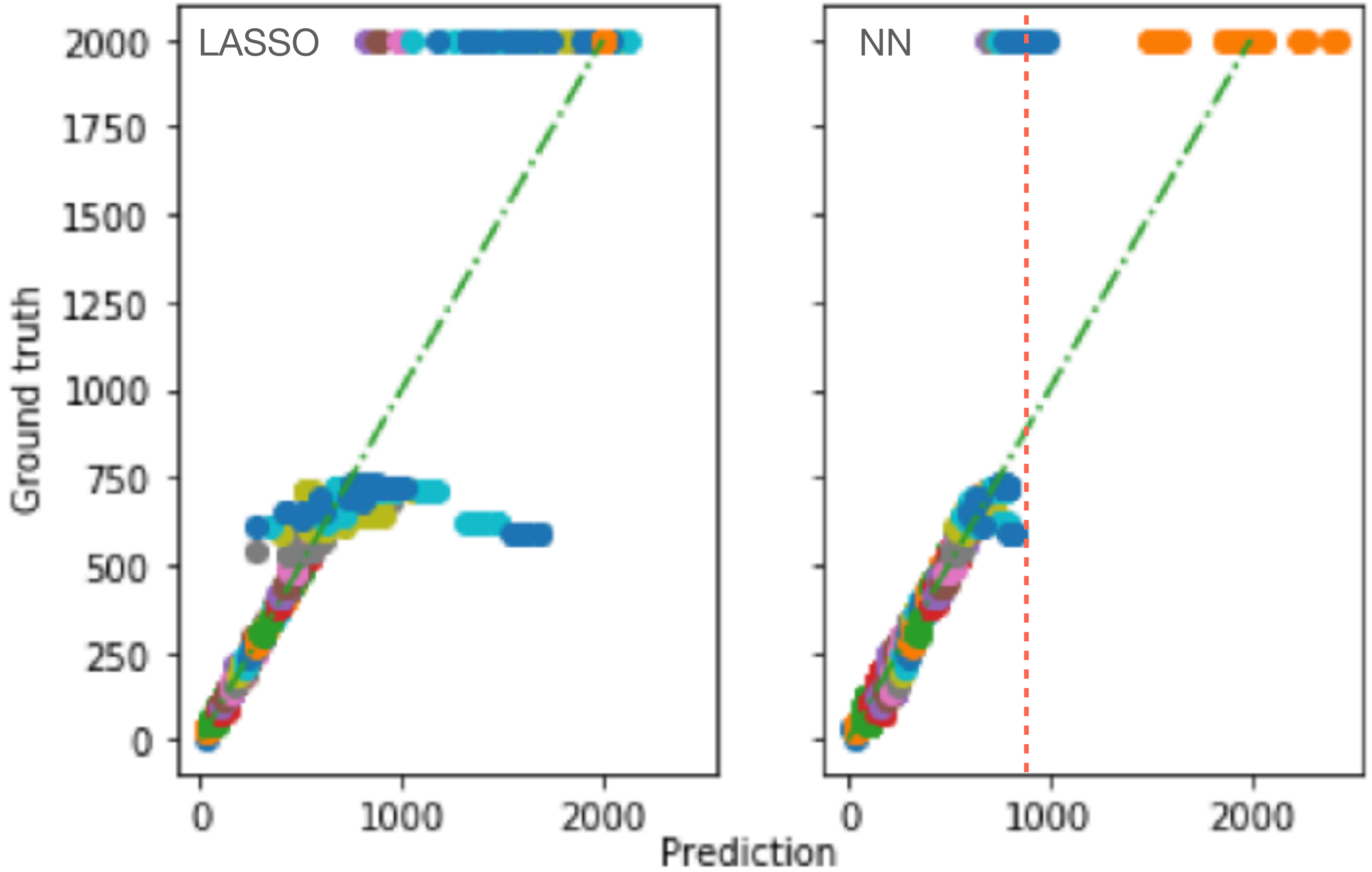
Model Prediction

- A: [3.7, 31.0, 16.5, 11.0, 24.5, 11.6]
- B: [0.5, 15.1, 6.7, 6.2, 29.4, 40.4]

Machine Learning Approach

Model B

- Use composition to predict distillation profile.
- Map the dataset from (500,6) to (500,22).




```
[               Observed.1  Past Avg.1  Std Dev.1
 % Off
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 Gas Oil (343°C - 565°C)       -   28.4   0.5
 Residue (565°C +)             -   41.7   2.7]
```
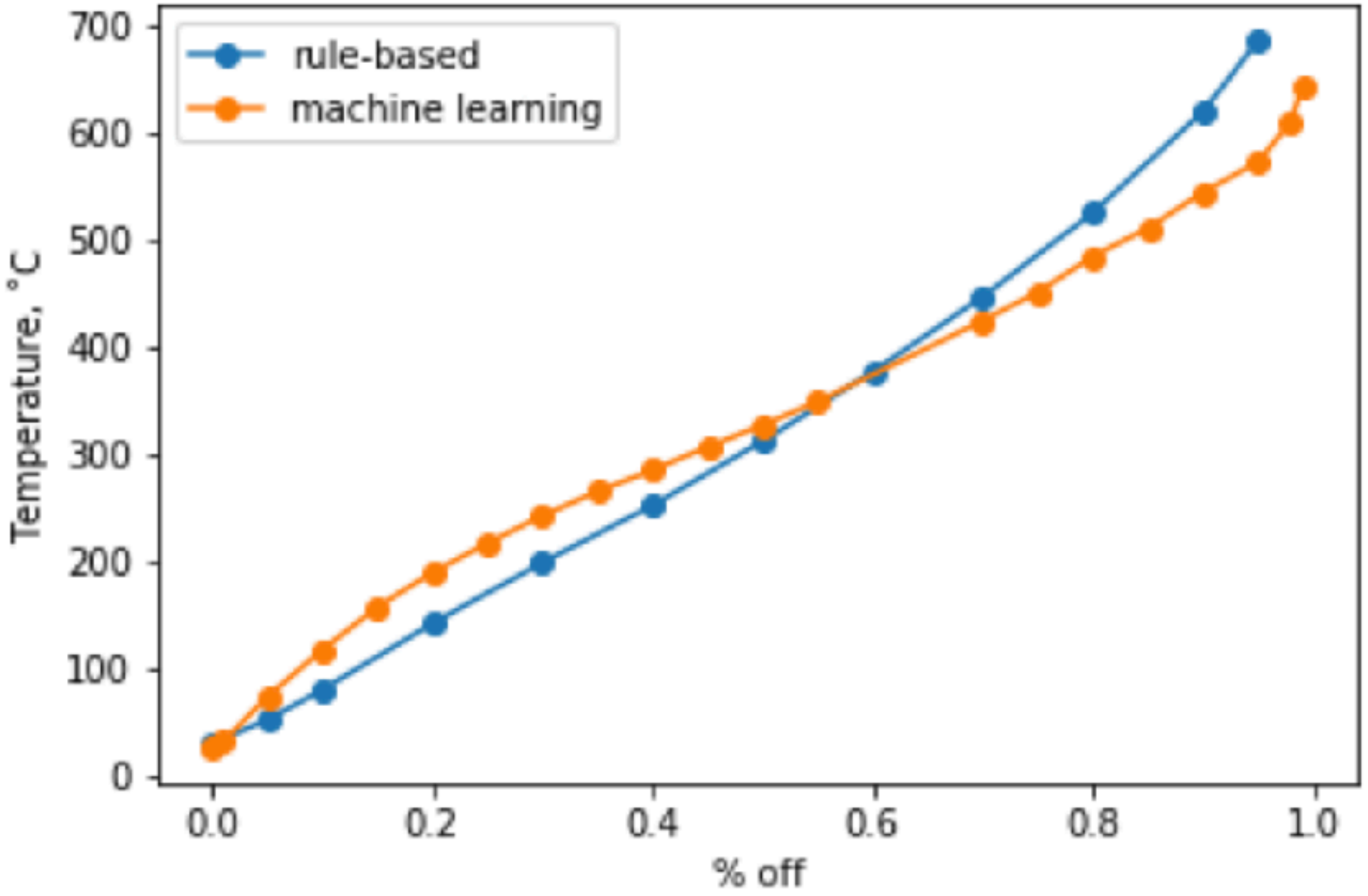

Results

Comparison

- The rule-based model only provide a rough estimation of the distillation profile.

- The machine learning model seems to have much better performance.



Uncertainties

Dollar values

- Mostly two sources of uncertainties, from the data and from the model. The uncertainty on the data is provided in the distillation profile by standard deviations.

- We can try to estimate the uncertainties from the model by looking at the differences between predictions and ground truth values.

```
[2.6661078674044294,
 3.7853287583453232,
 20.804998521404688,
 30.627578859785025,
 33.540537474328026,
 30.219574970287837,
 29.818411406191093,
 30.46654935382515,
 30.646288539084285,
 29.953156852905387,
 28.231576679813745,
 25.90739039826376,
 23.870054884760066,
 19.383965422277242,
 nan,
 nan,
 nan,
 nan,
 nan,
 nan,
 nan,
 nan]
```

Uncertainties
Dollar values

How can we add dollar value to the error? Few facts before we make the estimation (in US$):

- A barrel of crude oil is 42 gal, which can be made into ~20 gal gasoline (C4-C12), ~12 gal diesel fuel (C9-C25). Most of this product comes out below 350˚C
- Refinery cost $3 per barrel.
- Crude oil cost ~$85 per barrel.
- Gasoline is ~$4 per gal, diesel is ~$6 per gal

Looking at the estimated error of the model (+- ~30˚), let's consider the case where we only collected products below 320˚C (350-30=320), we could potentially lose about 10% of the product which is equal to (20 * 4 + 12 * 8) * 10% = $18 per barrel. The error at a higher temperature may not be as important because most profitable products have come out already.