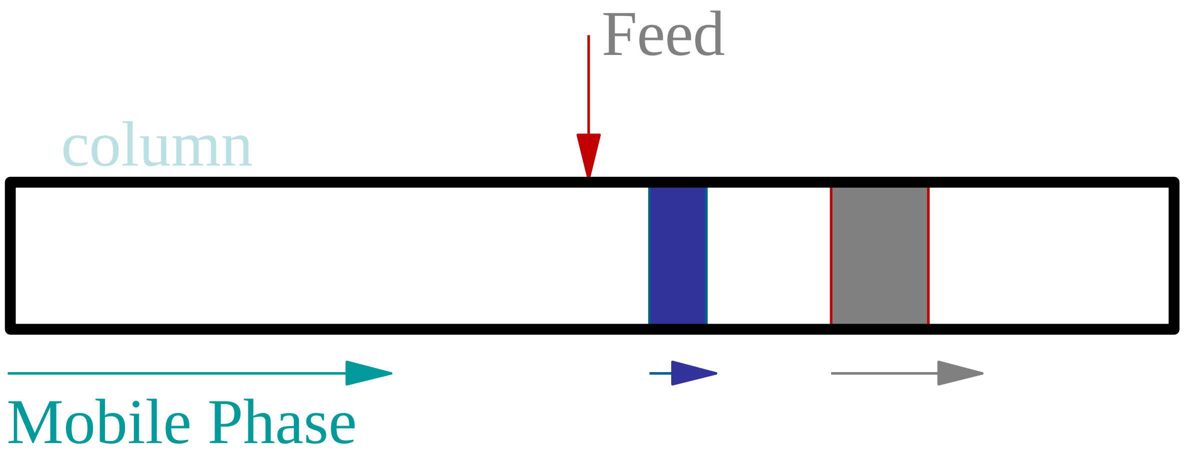
Simulated Moving Bed Liquid Chromatography (SMB)

Basic Principles

Continuous Chromatography

Basic Principle

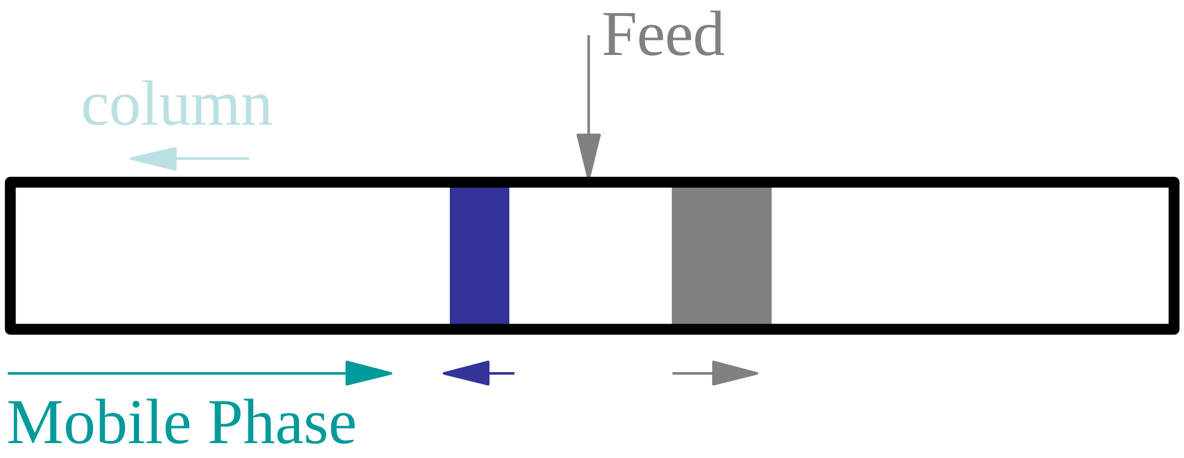


A sample is injected in the centre of a stationary column

The two components move at different speeds and are separated

Continuous Chromatography

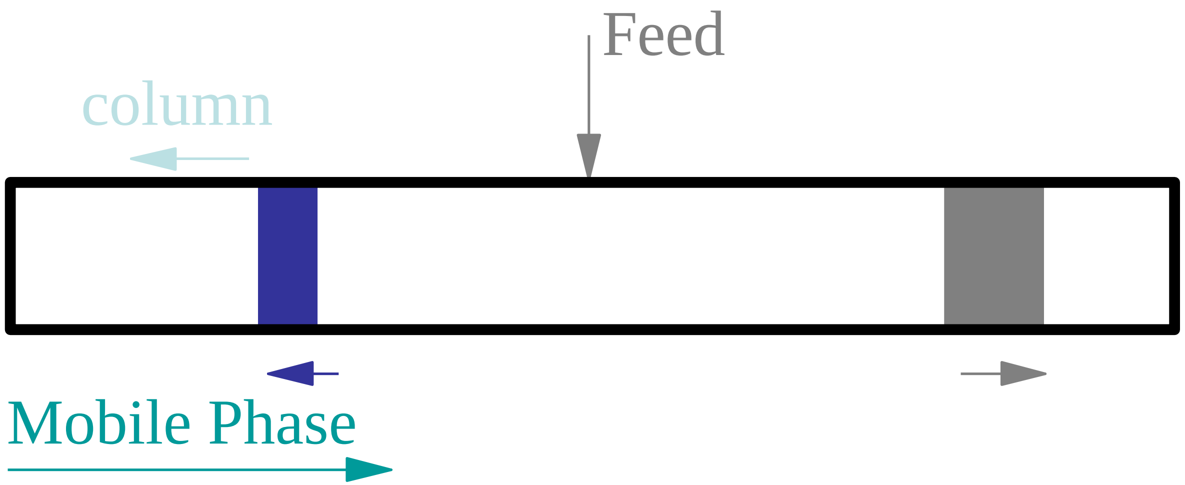
Basic Principle



If we now move the column from right to left, at a speed halfway between that of the solutes, they now move in different directions

Continuous Chromatography

Basic Principle

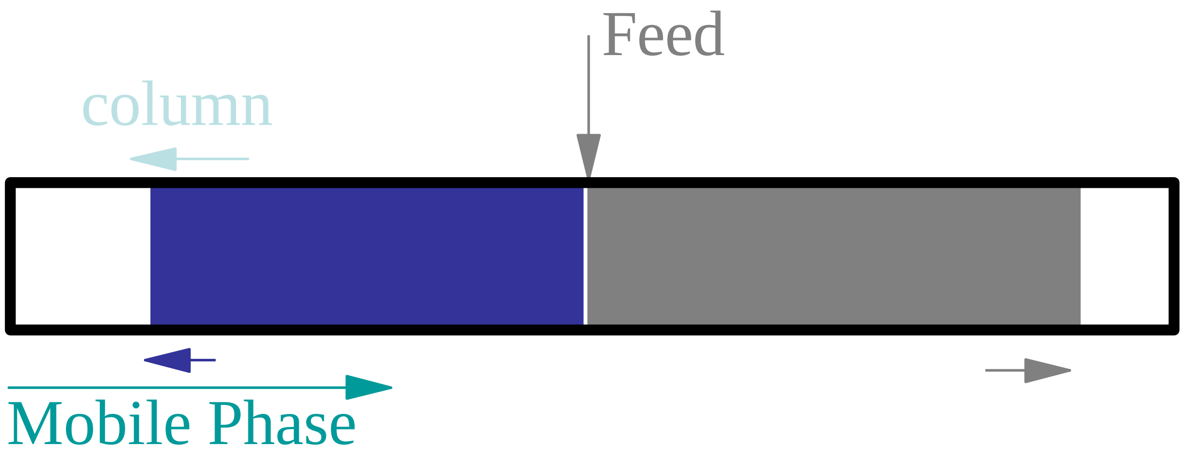


The two solutes now move in different directions relative to a stationary observer. If the column is very long, the bands will continue to separate.

If we continue to add sample at the centre, the components will continue to separate...

Continuous Chromatography

Basic Principle

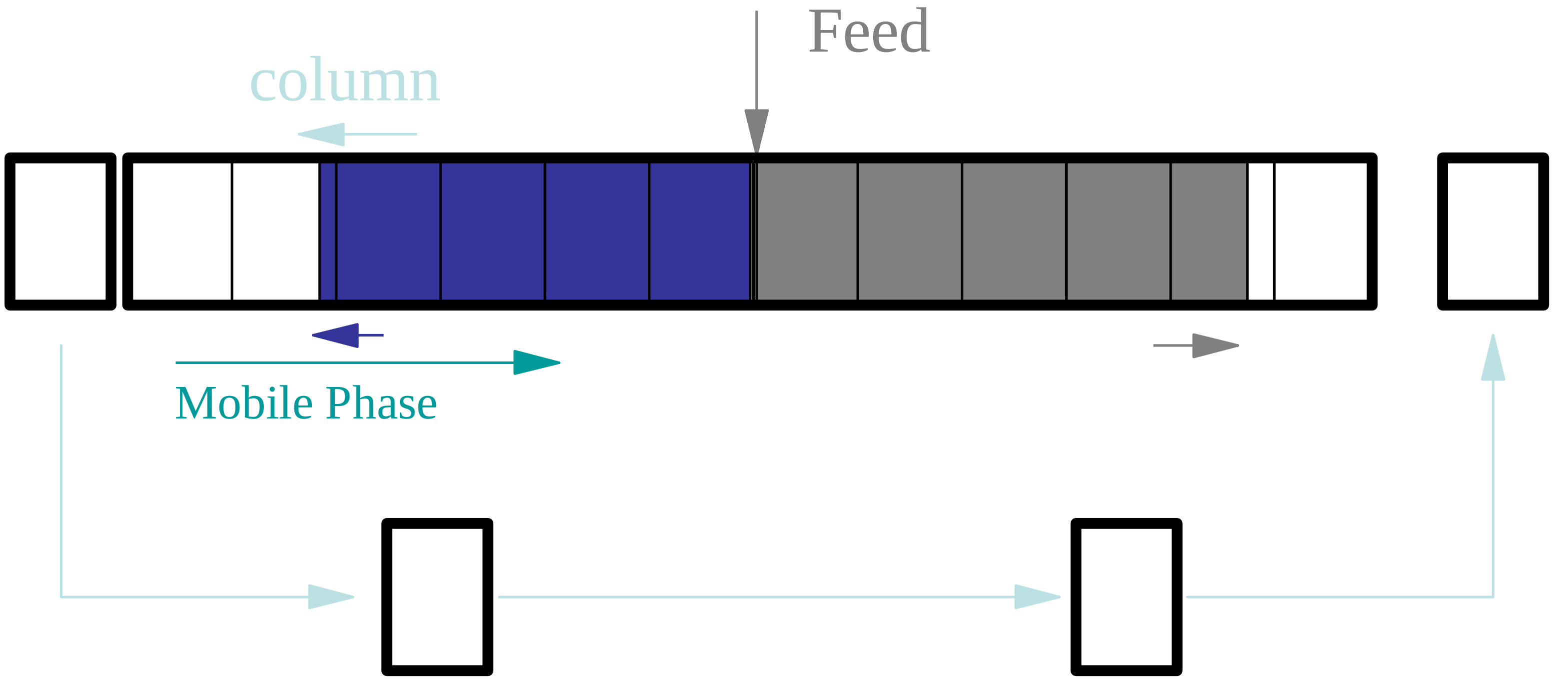


This is clearly a continuous system, but there are problems.
It needs an infinite column length and some way to introduce and remove the sample and the products.

We solve this by cutting the column into small segments and moving them

Continuous Chromatography

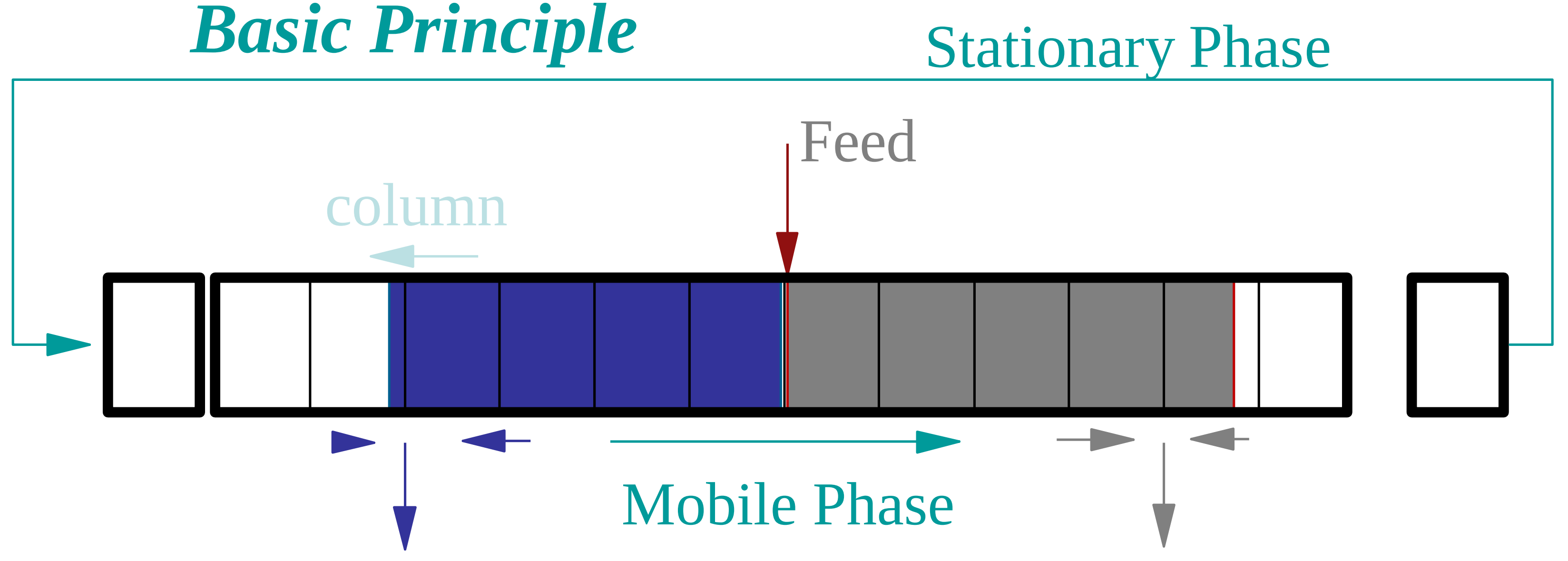
Basic Principle



The feed and solvent inlets are now placed between the segments and are moved each time a segment is moved from one end to the other

Continuous Chromatography

Basic Principle

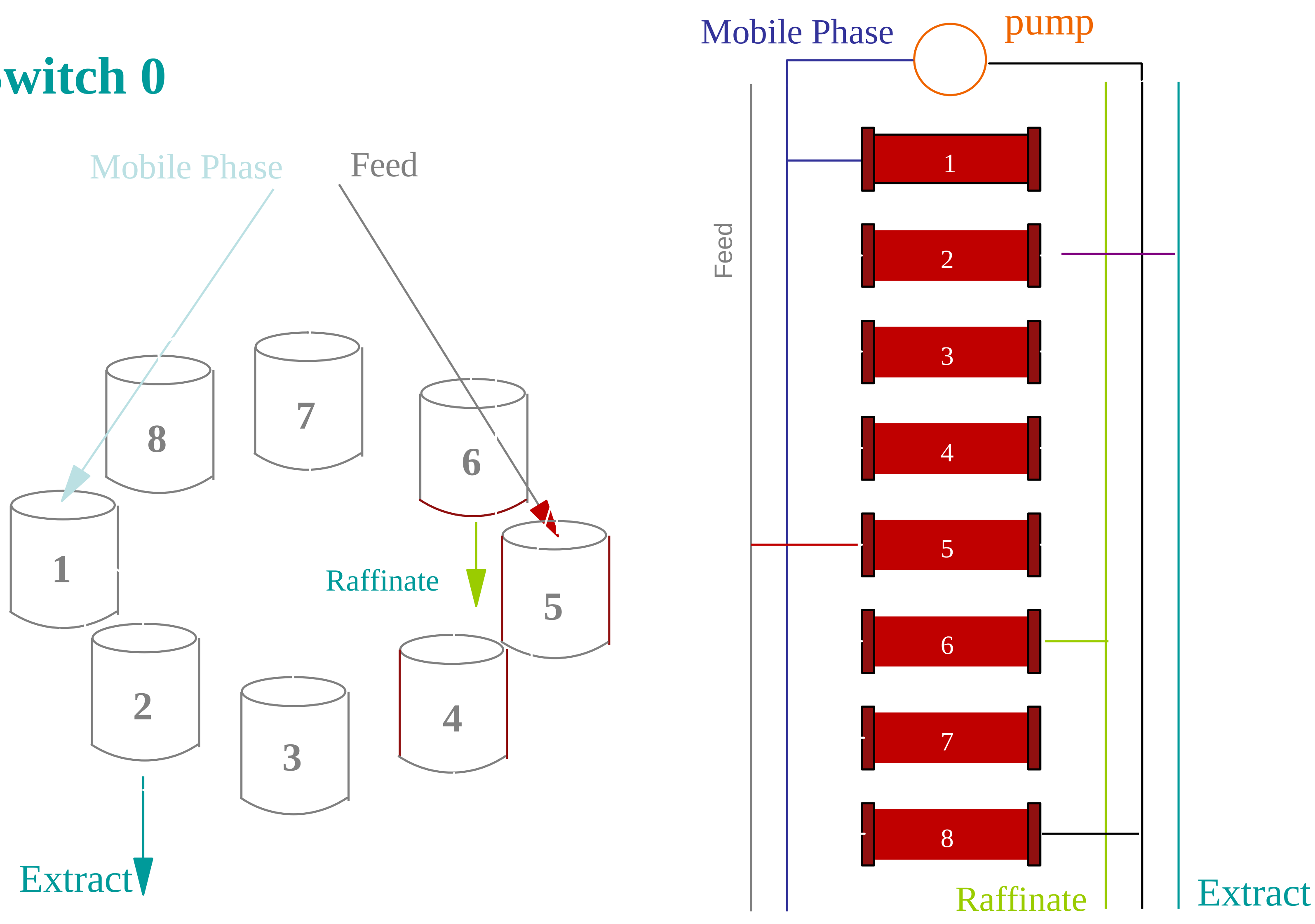


Products are removed by bleeding off a carefully calculated flow at suitable exit points. This changes the velocity of the bands in the column and forces the products to move toward the ports

This ensures that the column segments are clean before they are moved and that the solvent can be recycled directly back through the system

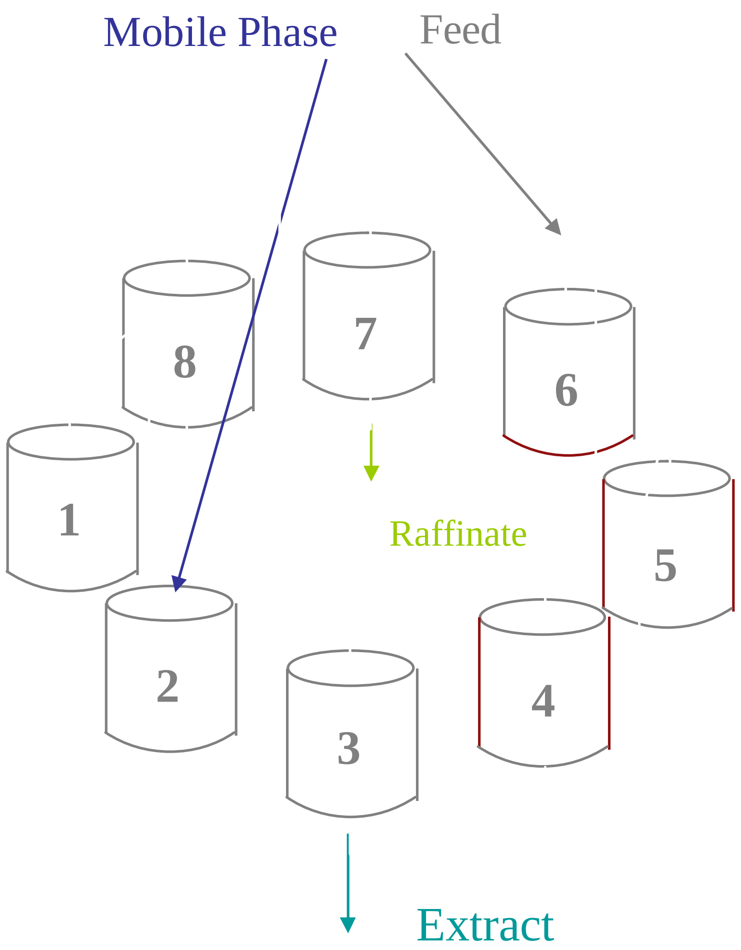
Switching

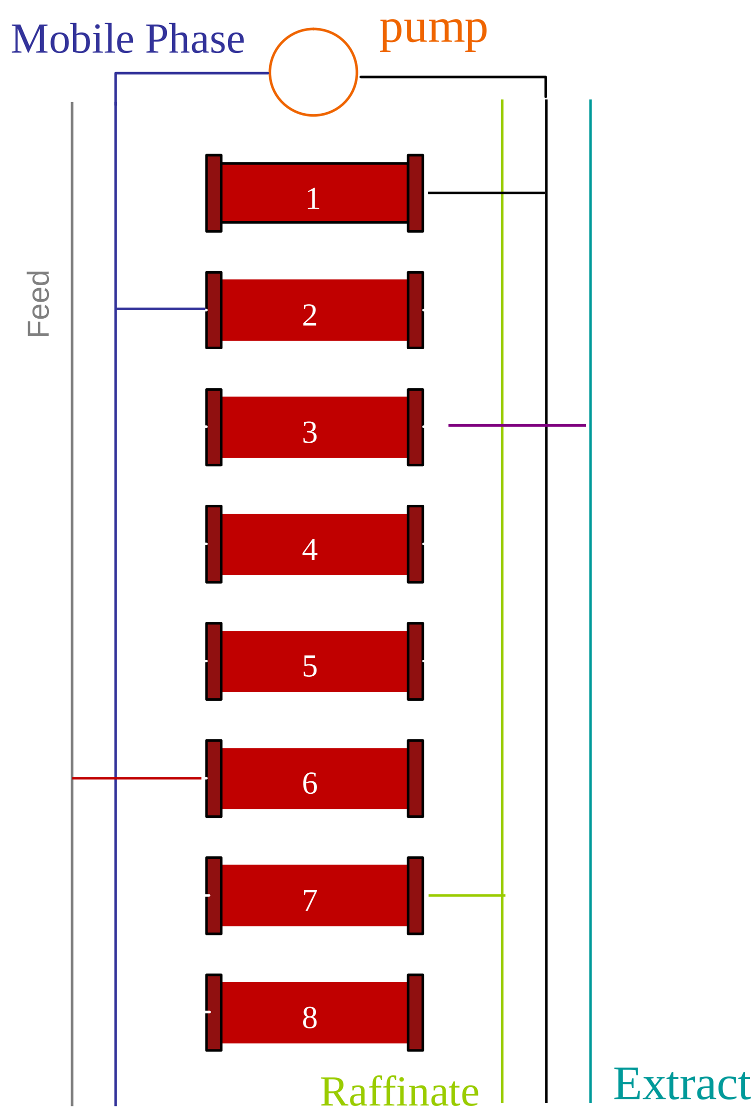
Switch 0



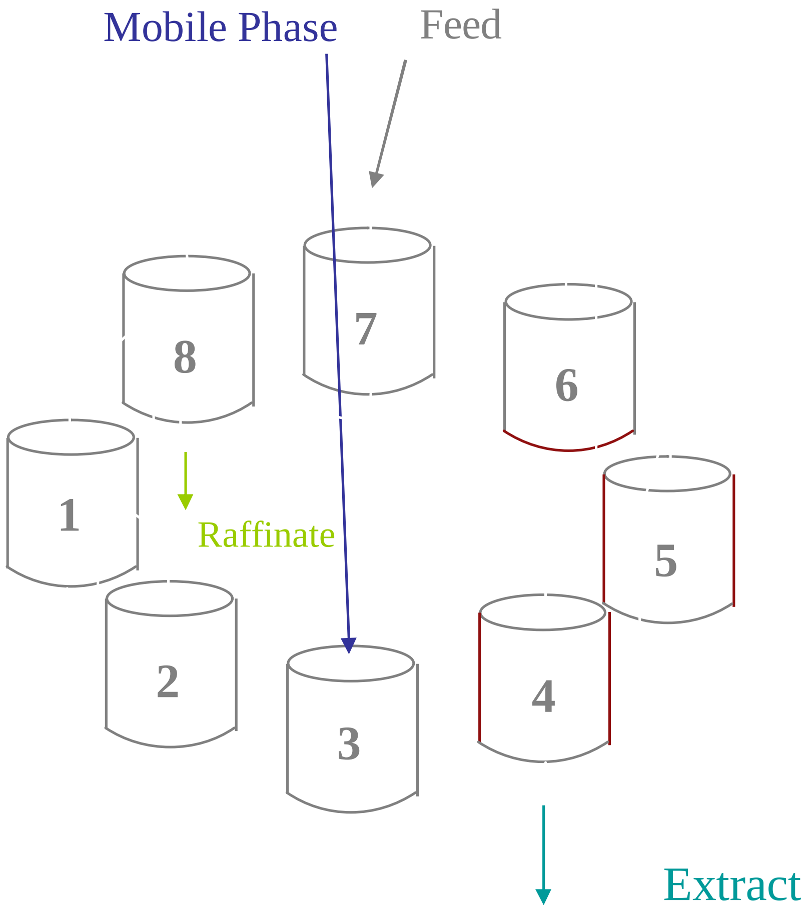
[redacted]

Switch 1

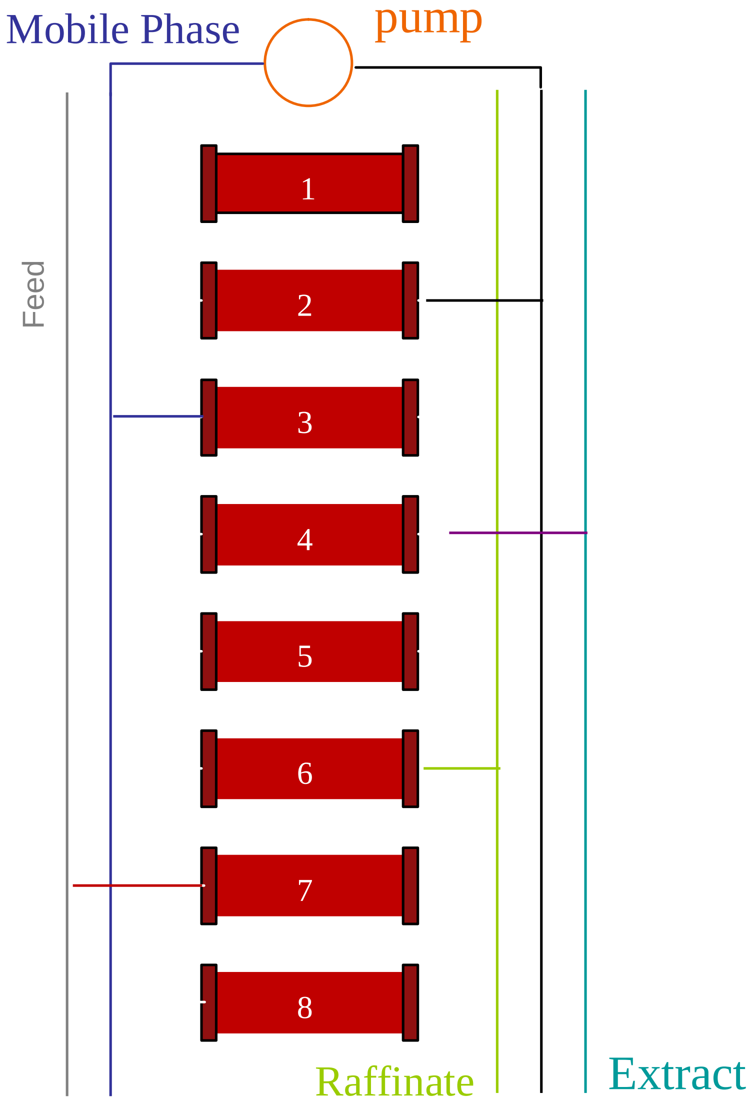




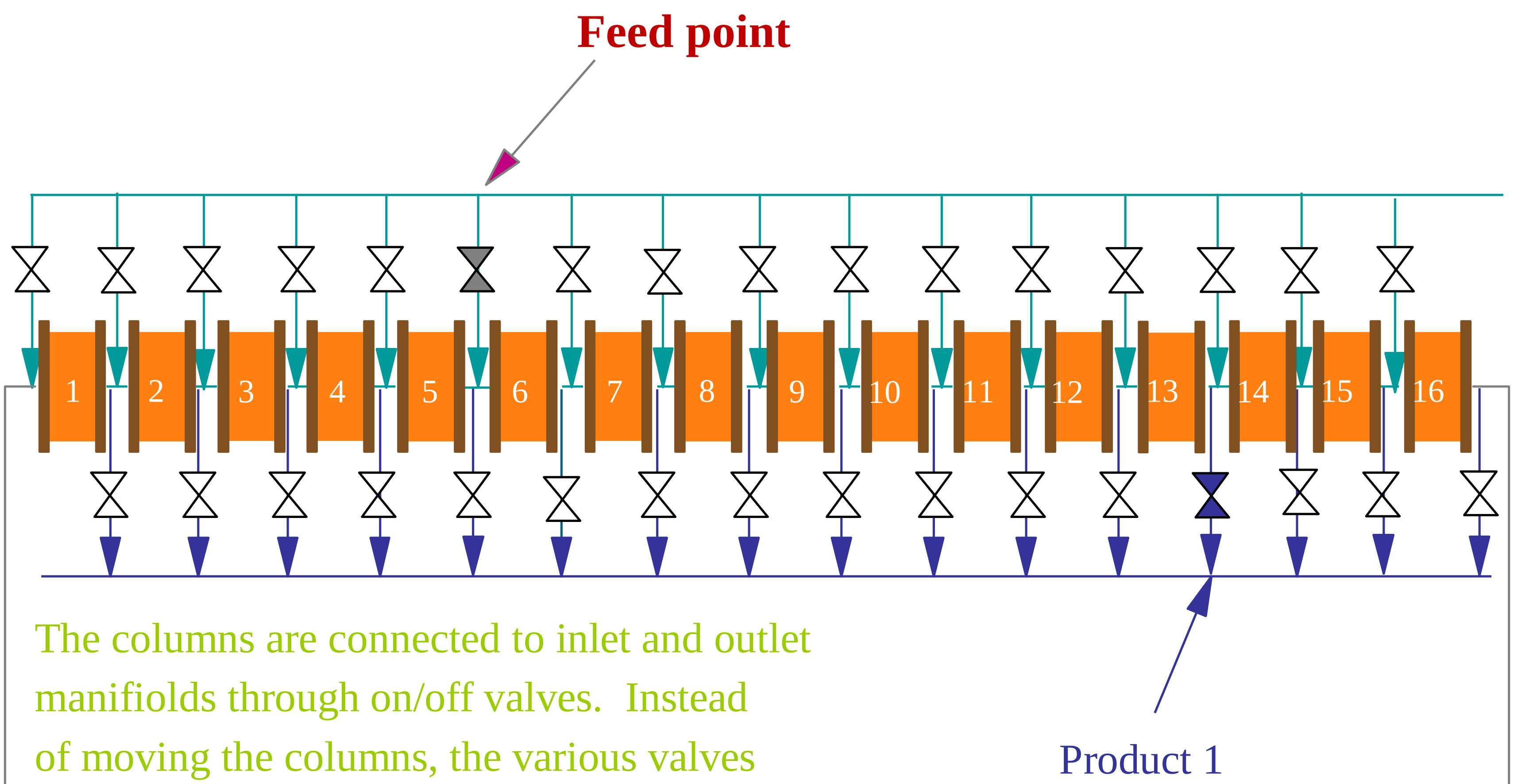
Switch 2



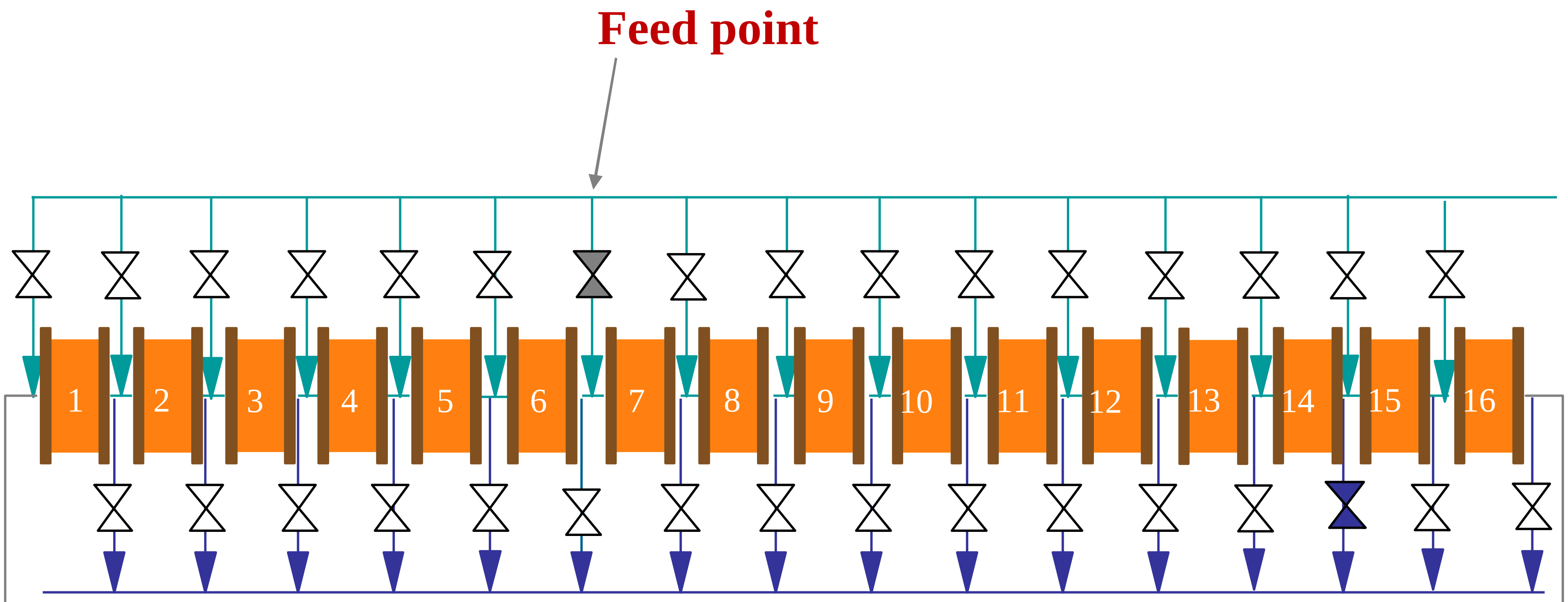
Mobile Phase
Feed
8
7
6
1
Raffinate
5
2
3
4
Extract



Mobile Phase
pump
Feed
1
2
3
4
5
6
7
8
Raffinate
Extract



The columns are connected to inlet and outlet manifiolds through on/off valves. Instead of moving the columns, the various valves are opened and closed to SIMULATE the movement.



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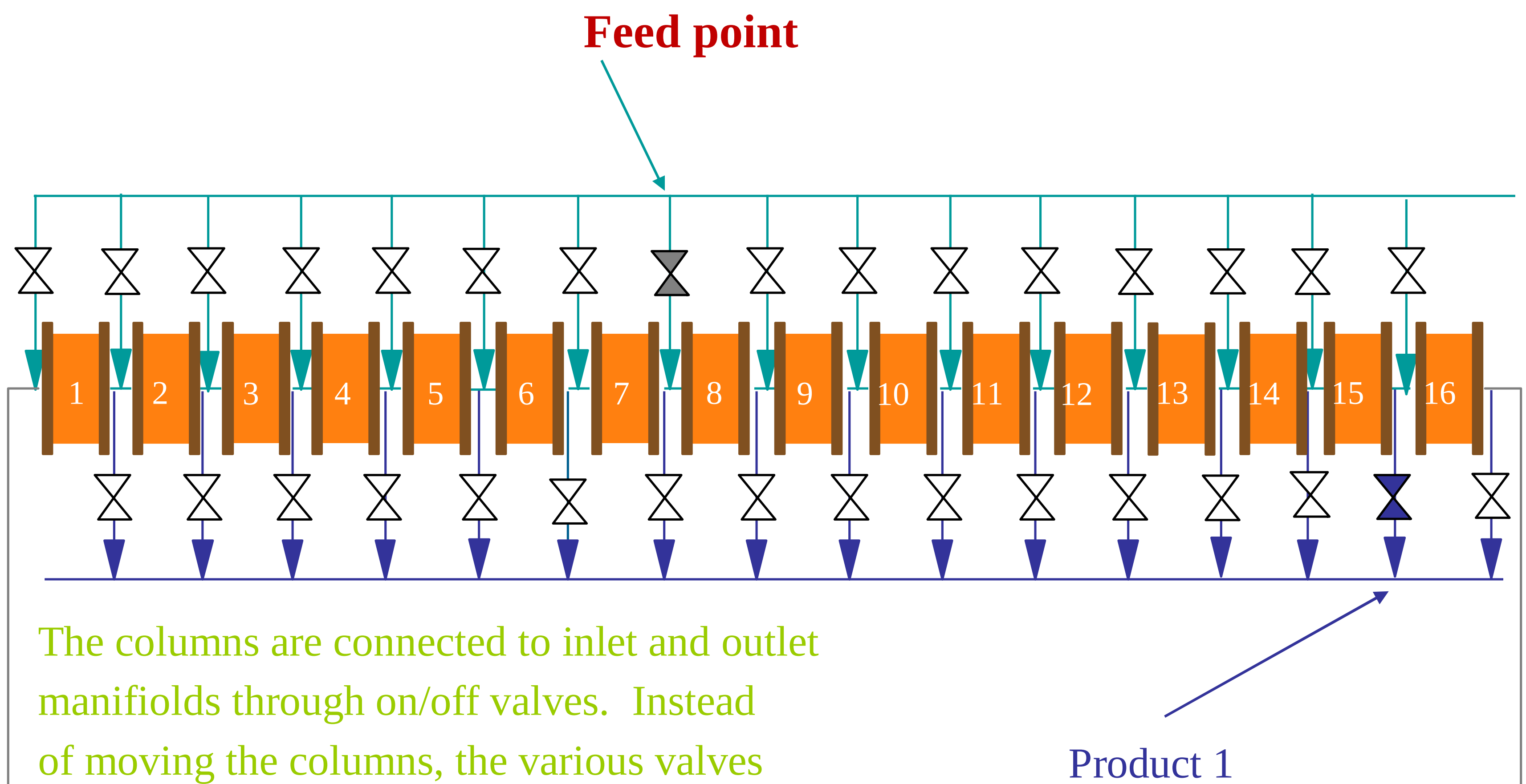
Product 1



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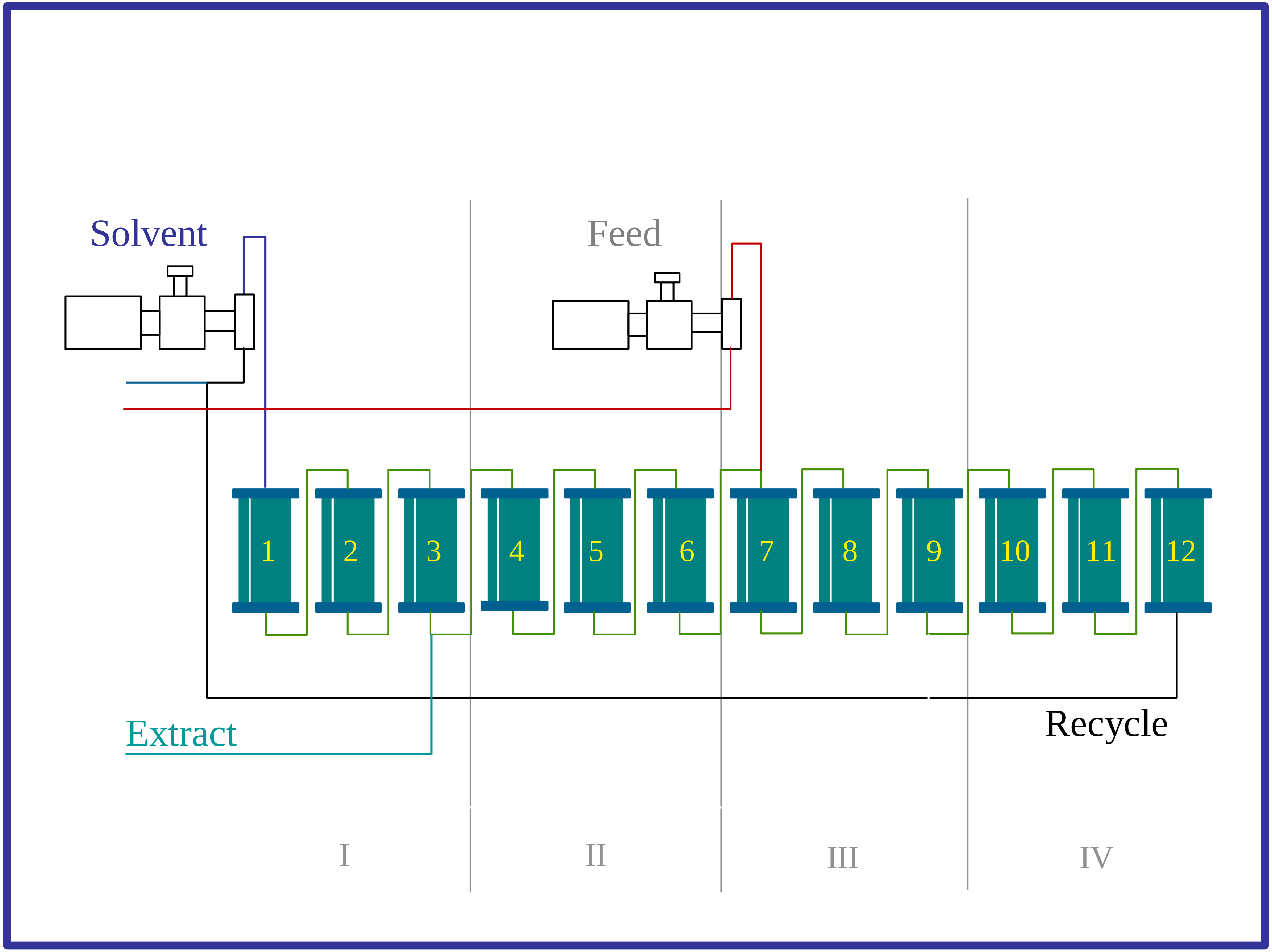
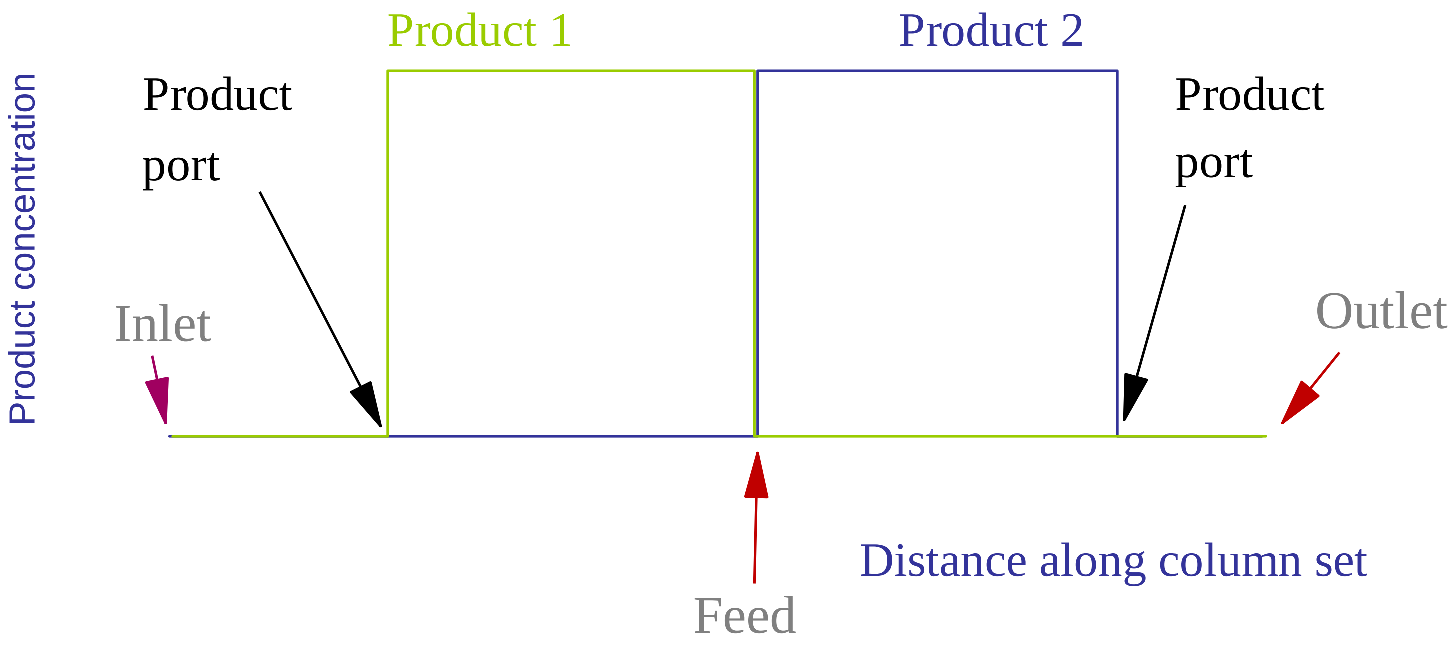

Solvent
Feed
1
2
3
4
5
6
7
8
9
10
11
12
Extract
Recycle
I
II
III
IV

Determination of Operating Conditions

If we know how fast the bands move,
we can calculate the speeds required
for the solvents and the column.

The speed of the band relative
to the mobile phase may be
calculated from the capacity factor.

The choice of operating conditions in continuous chromatography
is a difficult one without some theoretical decription of the process
To make it easy, we assume that the columns are infinitely efficient



For linear adsorption isotherms:

Equations which relate the band velocities to known parameters exist. There is an exact solution for the conditions required

For non-linear and interacting isotherms:

Band velocities are dependent upon the band concentrations (which are not known) and there is no longer an exact solution.

Operating Conditions

For non-linear and interacting isotherms:

The concentration of the band is a function of the band velocity in the column which is in turn dependent upon:

solute capacity factor

feed flow rate

mobile phase flow rate

"speed" of the column

Unfortunately, the capacity factor of a solute depends on:

the concentration

the concentration of other solutes at the same point in the column.

Operating Conditions

The model is used to calculate:

- In-column concentrations of the solutes from the:
  - Feed composition
  - Flow rates and column speed
  - Analytical capacity factors
- Capacity factors for the calculated concentrations
  - Concentration values
  - Adsorption isotherm
- New concentration values from:
  - New capacity factors
  - Feed composition
  - Flow rates and column speed

After several iterations, the values converge.

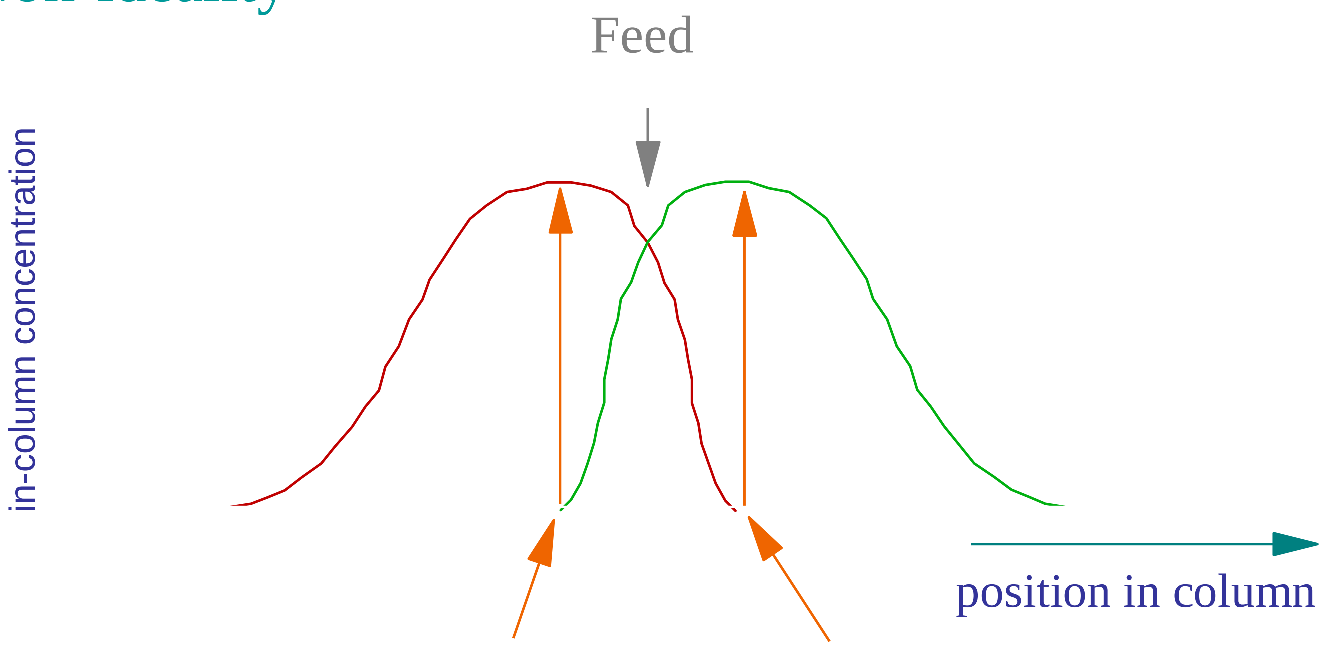
Once we know the values of capacity factors in the system, we can use previously derived equations for sugar separations to calculate the ideal operating conditions.

In fact, the values used are modified to take into account the non-ideality of the system so that the predictions approach reality

Once the values are calculated, they are confirmed by simulation

Operating Conditions

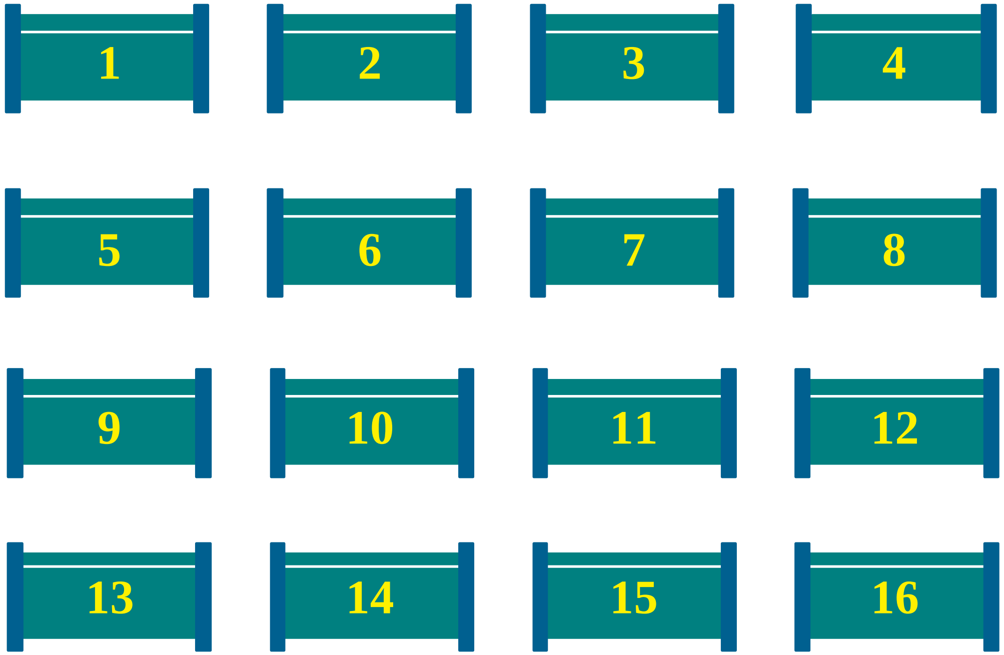
Non-ideality



Although the concentration of the solute is low
the capacity factor does not take its analytical value
The actual value depends on the isotherms
and the concentration of the other species.

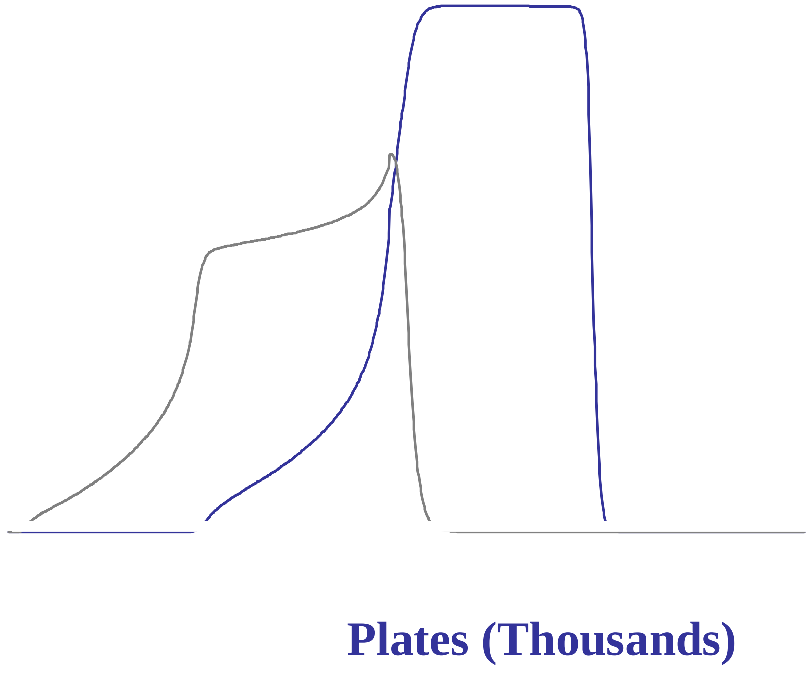
Computer Simulations

The computer simulation is carried out for each section of the SMB system separately, saving the output of one section for use as the input for the next. At the same time, the column movement is simulated by movement of all points upstream by the column length after the switch time has elapsed.



Computer Simulations

The output is a "frozen" snapshot of the concentrations within the column set at a given point of time.



The program calculates the output concentrations from a given feed and operating parameters.

Operating Conditions

Besides calculating the operating conditions for a specific application, the model is used to find the effects of various chromatographic parameters on the separation conditions required.

In addition, the model can be used to determine the characteristics of equipment required for a particular application area. In this case, from "typical" chromatographic parameters and production needs, it is possible to determine the size and capabilities of the instrumentation which must be constructed for the application.

Economics

Chromatographic Parameters:

Selectivity = 1.2

Solubility 100 mg/ml

Composition 50:50

Langmuir isotherms

Saturation capacity 100 mg/g

Costs

Solvent : 30 FF/l

Recovered solvent: 5 FF/l

Labour: 310 FF/hr

Crude costs: from 1 000 to 100 000 FF/kg

95% solvent recovery

Economics

Operating Conditions:

Pressure: 30 bar

Column Diameter: 20 cm

Required Purity: 99%

Batch

Column Length (batch): 25 cm

Separate conditions for the 1st & 2nd components

SMB

Economics

Batch Chromatography

Product purity = 99%

k' (1st component) = 1

Column Efficiency = 4000

Crude Cost (FF/kg)		1000	20000	100000
Recovery	Product 1 Product 2	80 80	85 90	90 90
Cost (FF/kg)	Product 1 Product 2	9100 15263	13370 18744	23360 27633
Production (kg/yr)	Product 1 Product 2	1529 904	1379 821	1108 821

Economics

Continuous Chromatography

Product purity = 99%; All material recovered.

k' (1st component) = 1

Input Concentration (g/l)	10	12.5	12.5
Efficiency	1840	2270	2270
Single Column Length (cm)	5	10	15
Product cost (FF/kg)	6056	5756	5638
Production rate (kg/year)	1353	1496	1638

Conclusions

Rapid calculation of operating conditions for SMB separations

Refinement of conditions by use of computer simulations

Determination of the sensitivity to variations in conditions

Determination of the effects of changes to parameters

Estimation of separation economics for SMB separations