Process Synthesis from Reaction Networks

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Paper: **An optimisation-based framework for the conceptual design of reaction-separation processes**

Authors: **Qingyuan Kong, Nilay Shah**
Department of Chemical Engineering, Imperial College London

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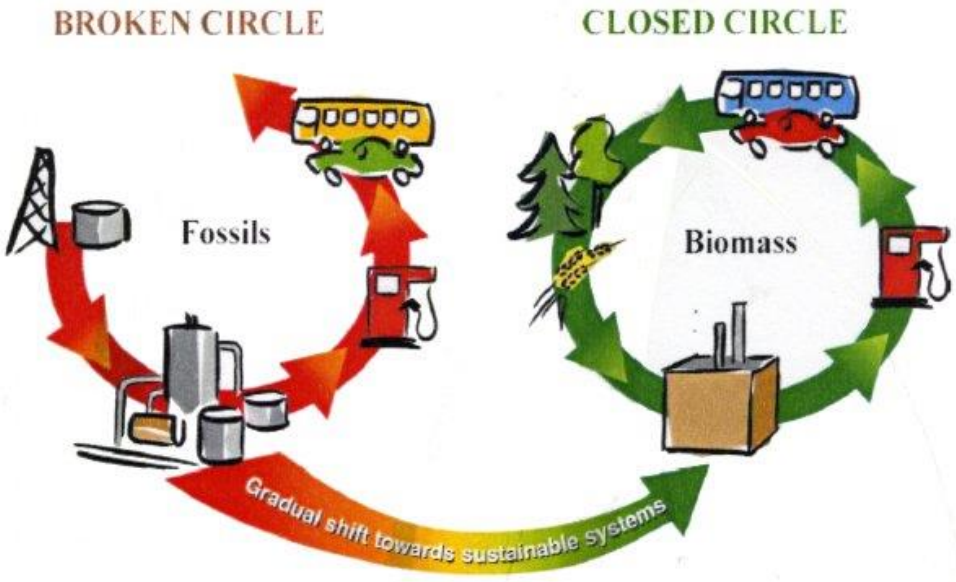


Image Courtesy: www.emaze.com

Process Synthesis from Reaction Networks

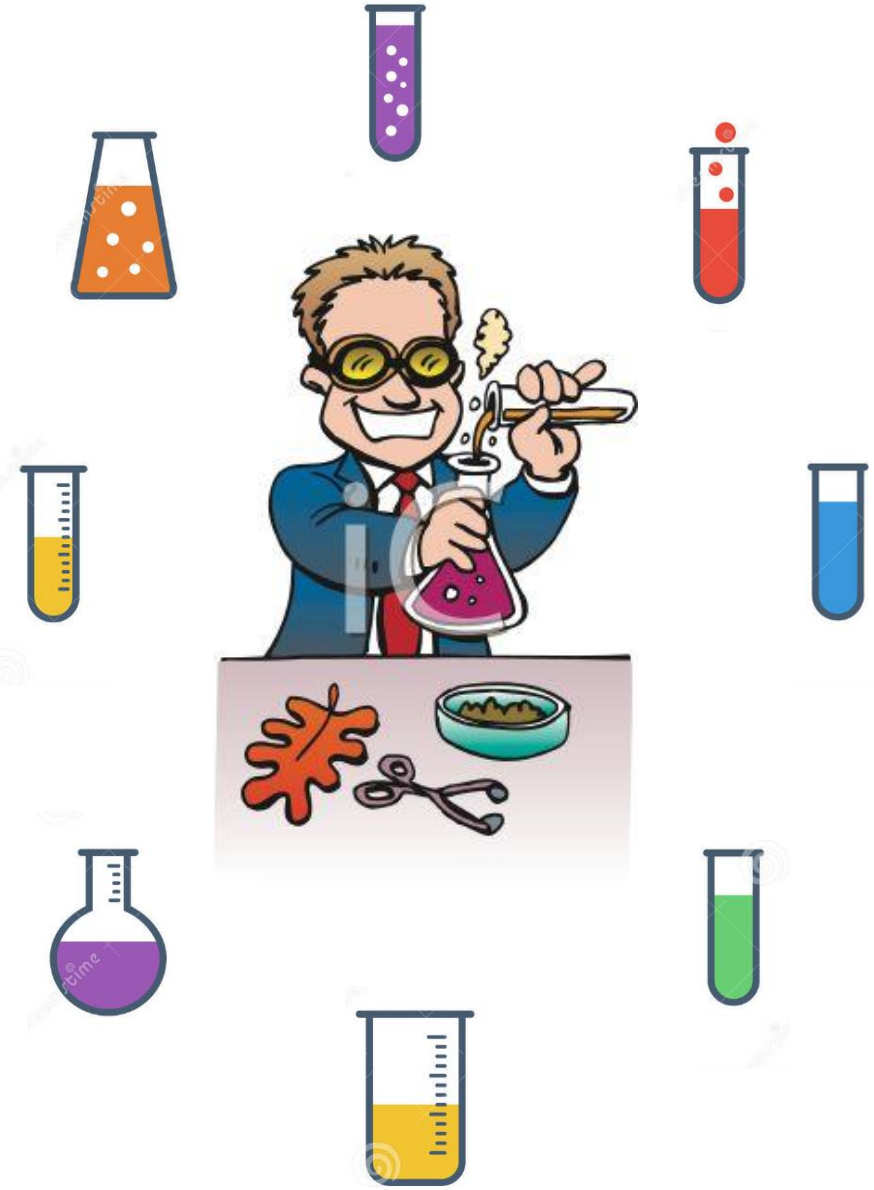
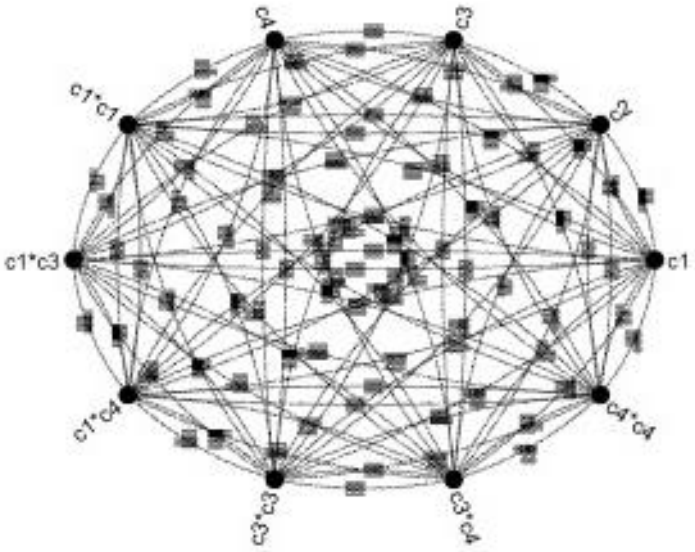


Image Courtesy: www.dreamstime.com, www.clipartguide.com

Reaction Networks



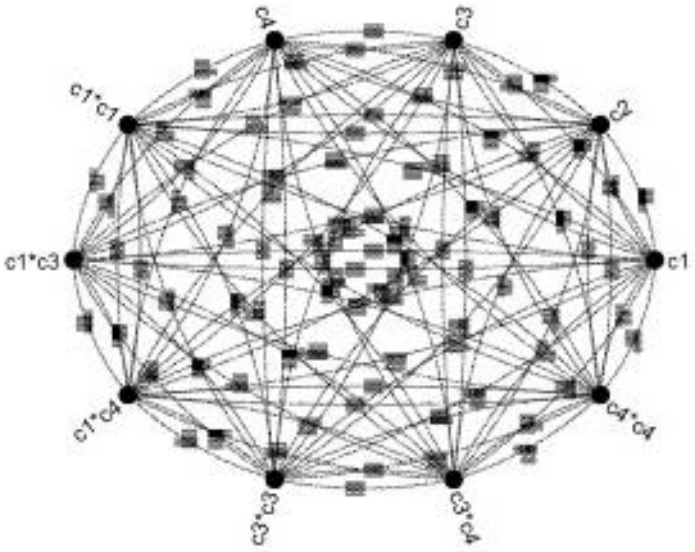
-Literature search

-Speculative reactions

-Automated tools for reaction network generation

Image Courtesy: Inference of chemical reaction networks using mixed integer linear programming

Reaction Network Data



-Yields, conversions, etc.

-Pure component property data

Image Courtesy: Inference of chemical reaction networks using mixed integer linear programming

Process Synthesis from Reaction Networks?

Assumptions

-Conversion and selectivity of each reaction, as well as the boiling point and market value of each component are either known or estimated

-Distillation (sharp-split) is the method for separation

-Process operates at steady stage

-Reactor capital cost is assumed to be negligible

-A simple overall cost model based on the difficulty of separation is used

Superstructure-based Methodology

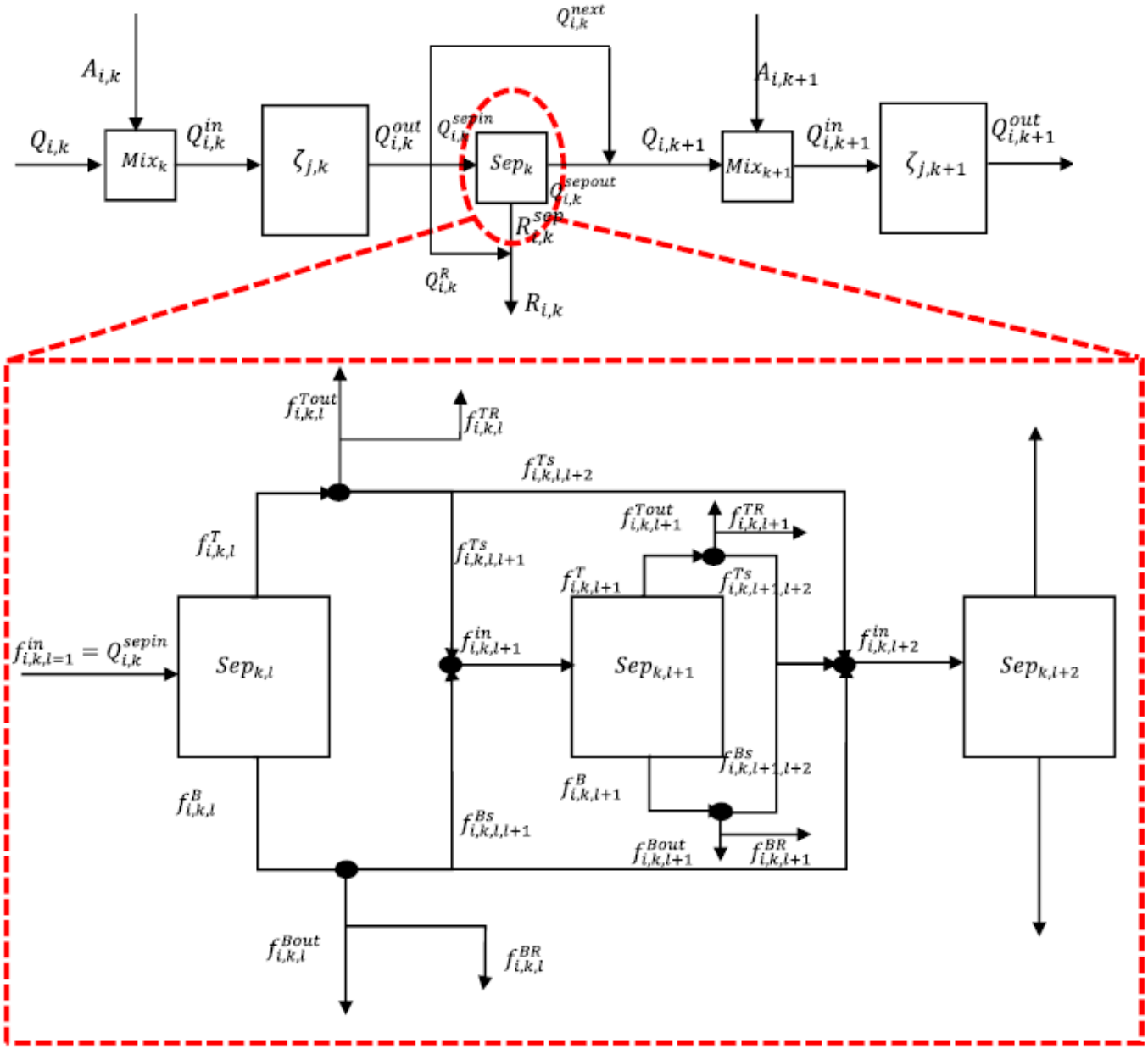
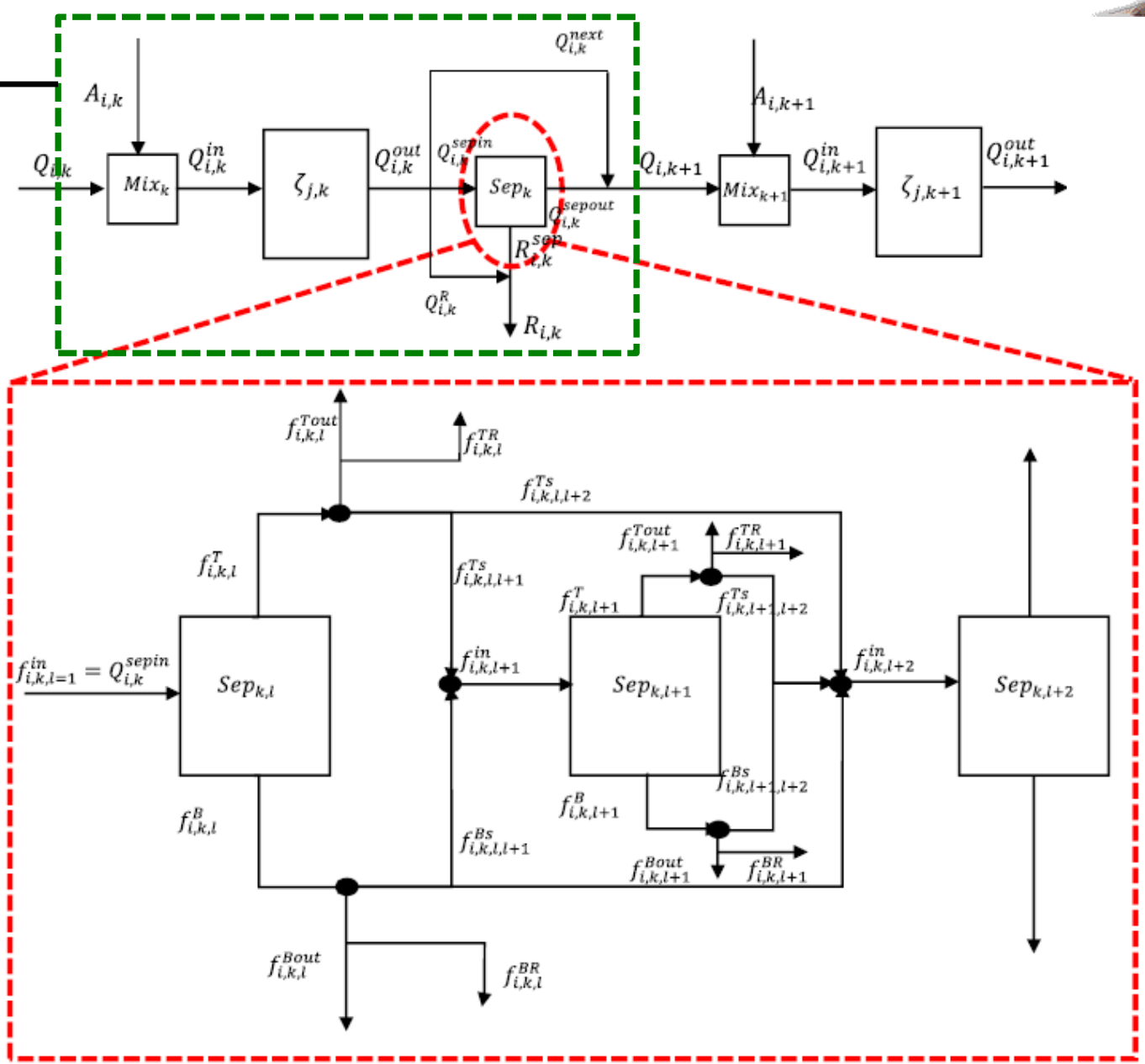


Image Courtesy: An optimisation-based framework for theconceptual design of reaction-separation processes

Superstructure-based Methodology

Master stage



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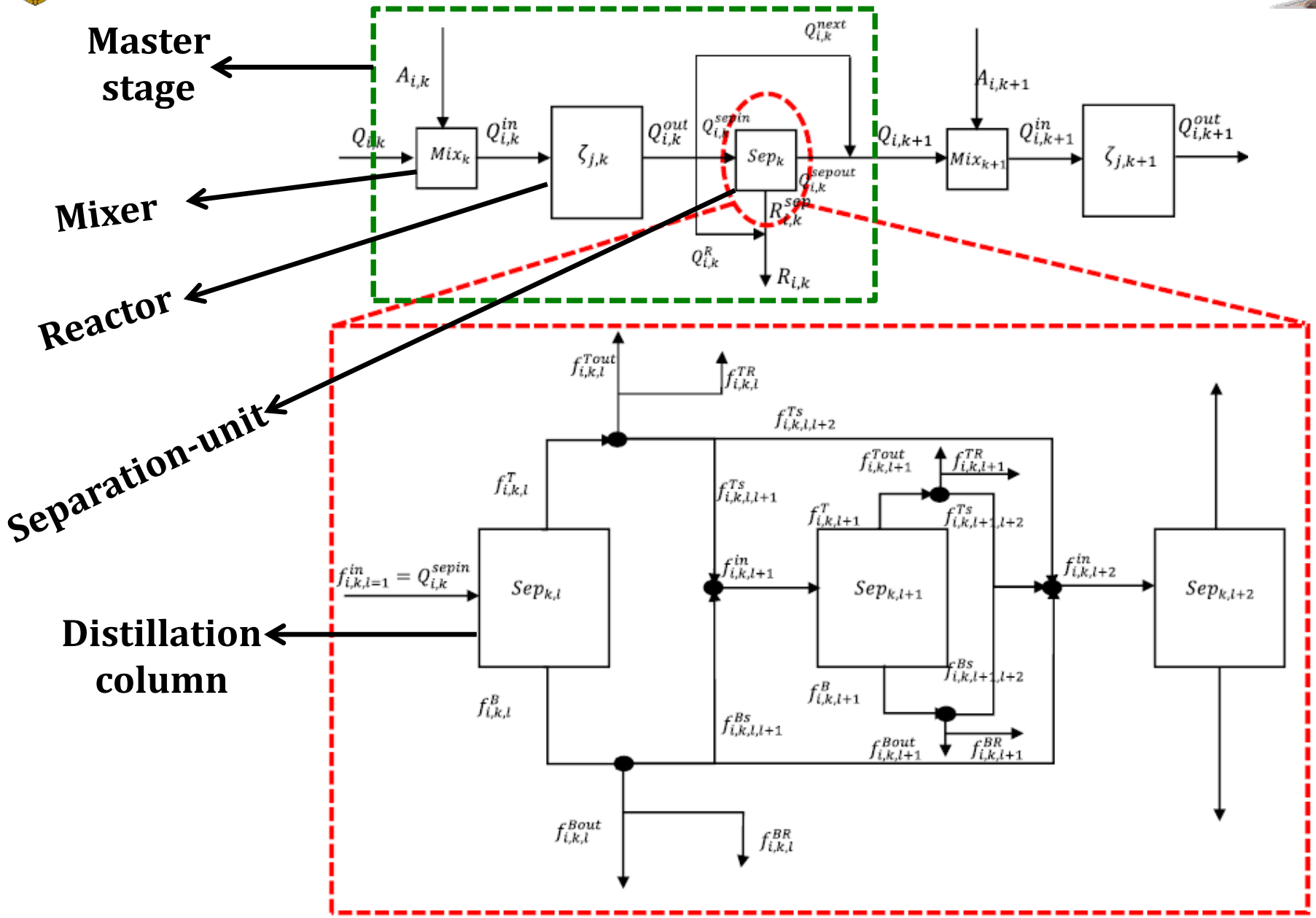

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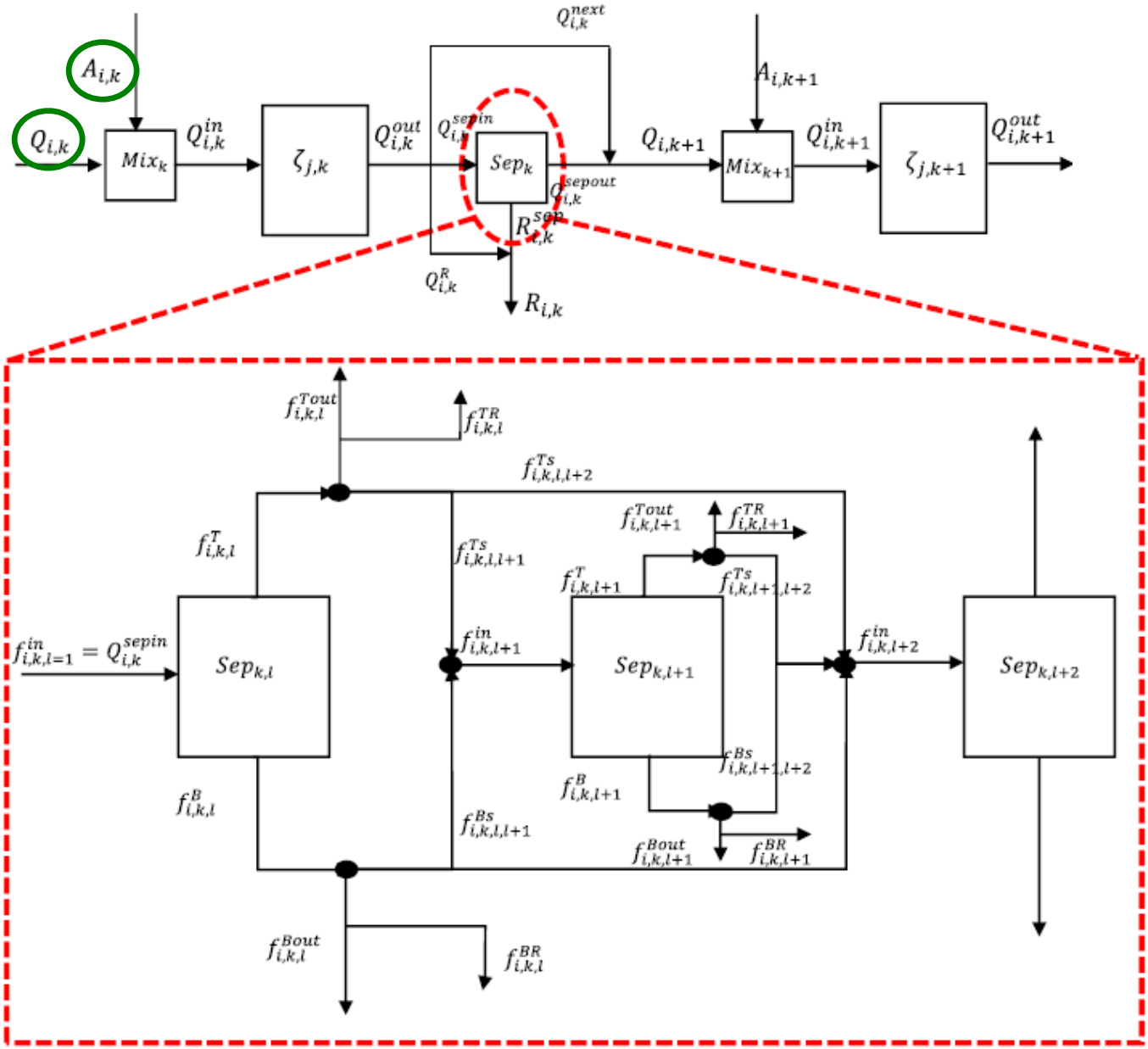

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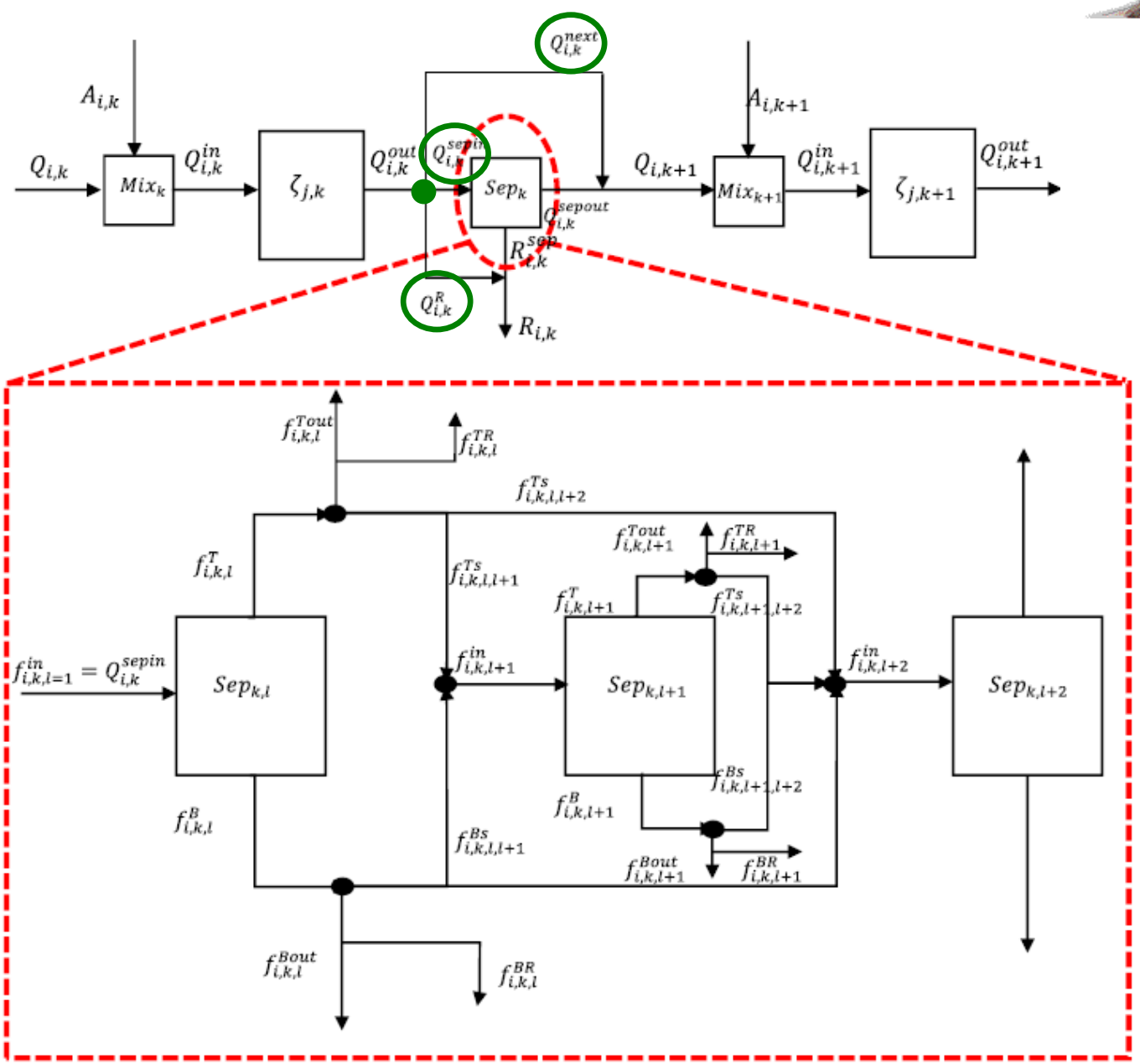

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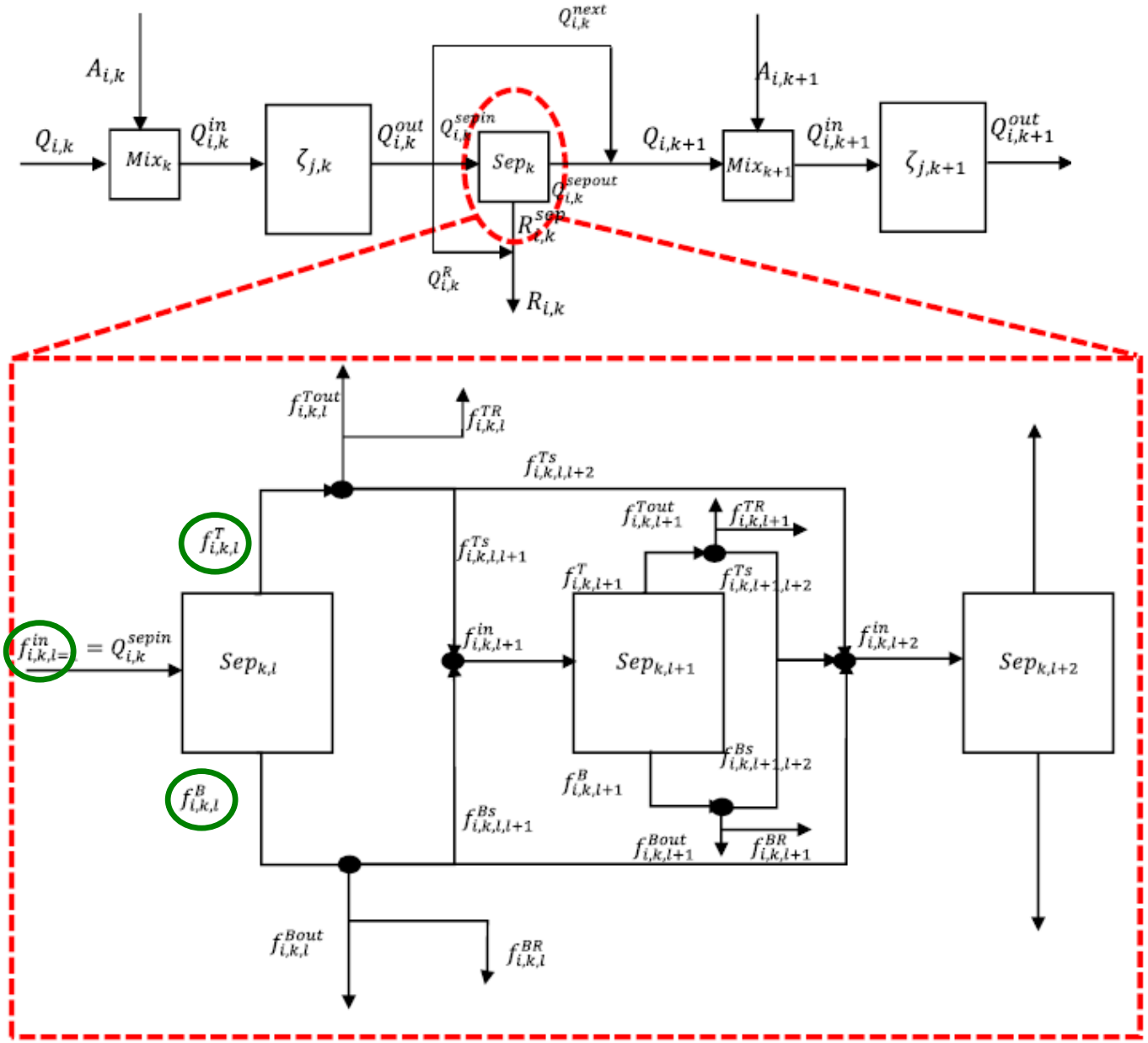

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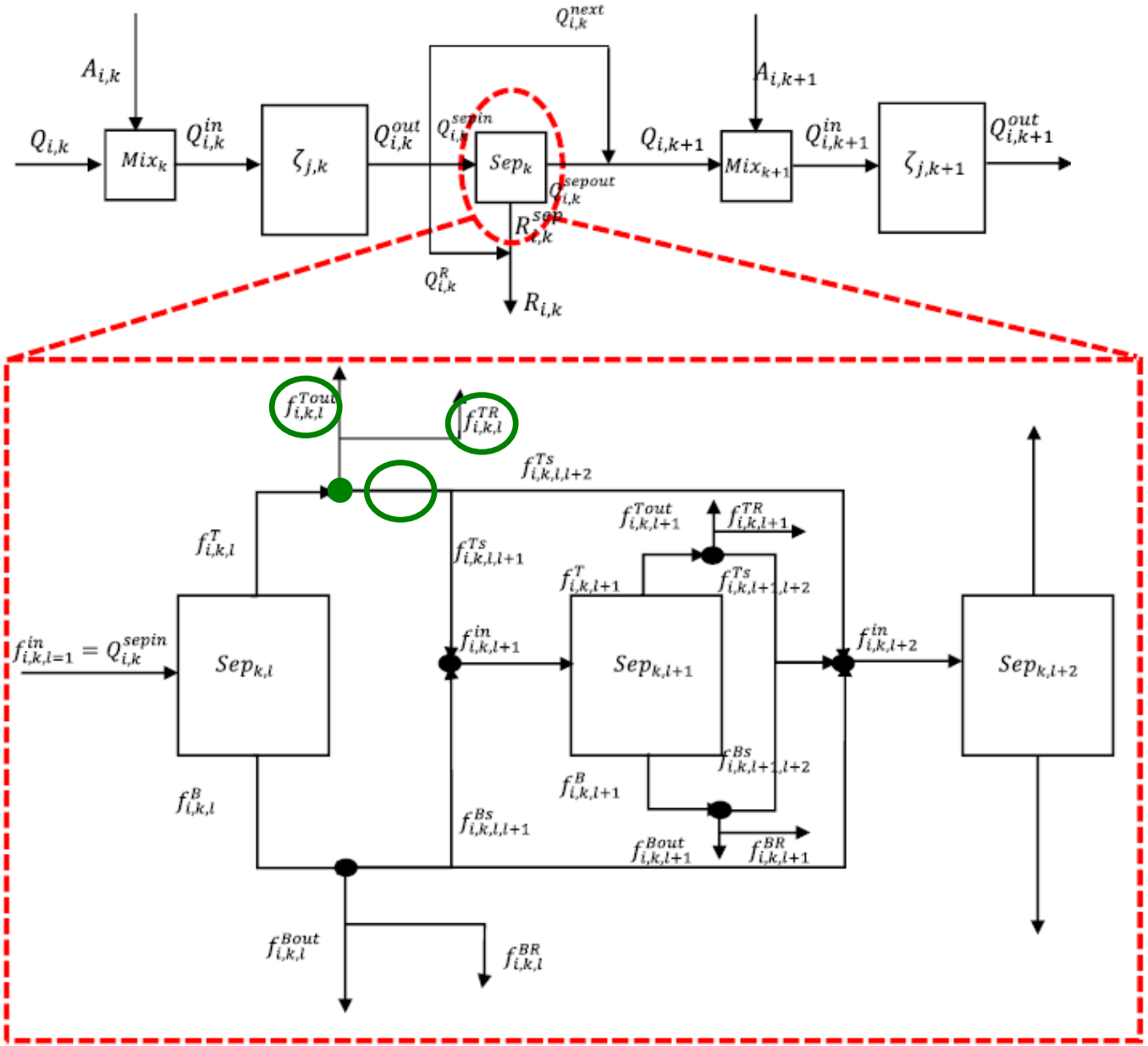

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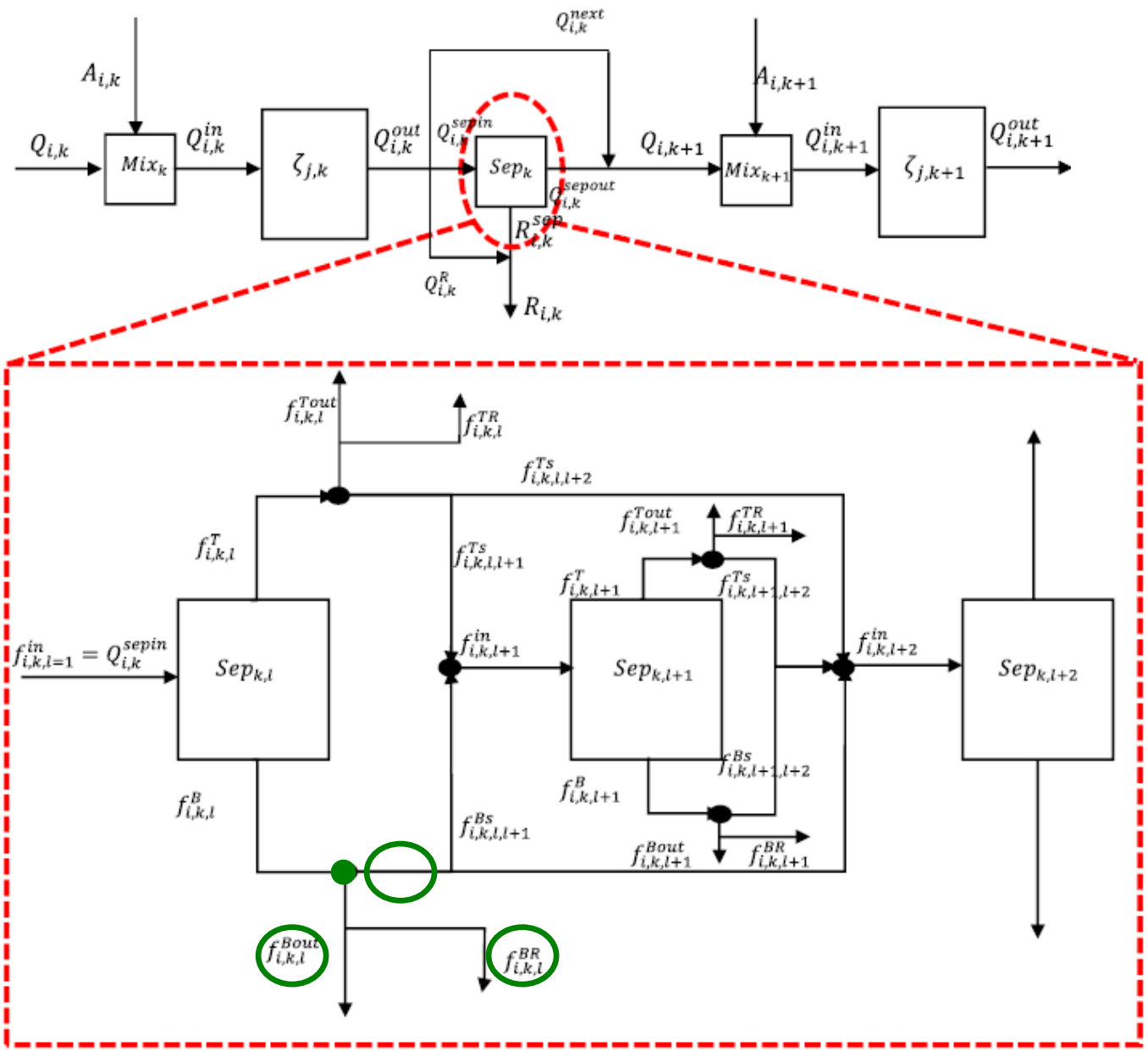

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Reactor Modeling

-Operating conditions (temperature, pressure, catalyst)

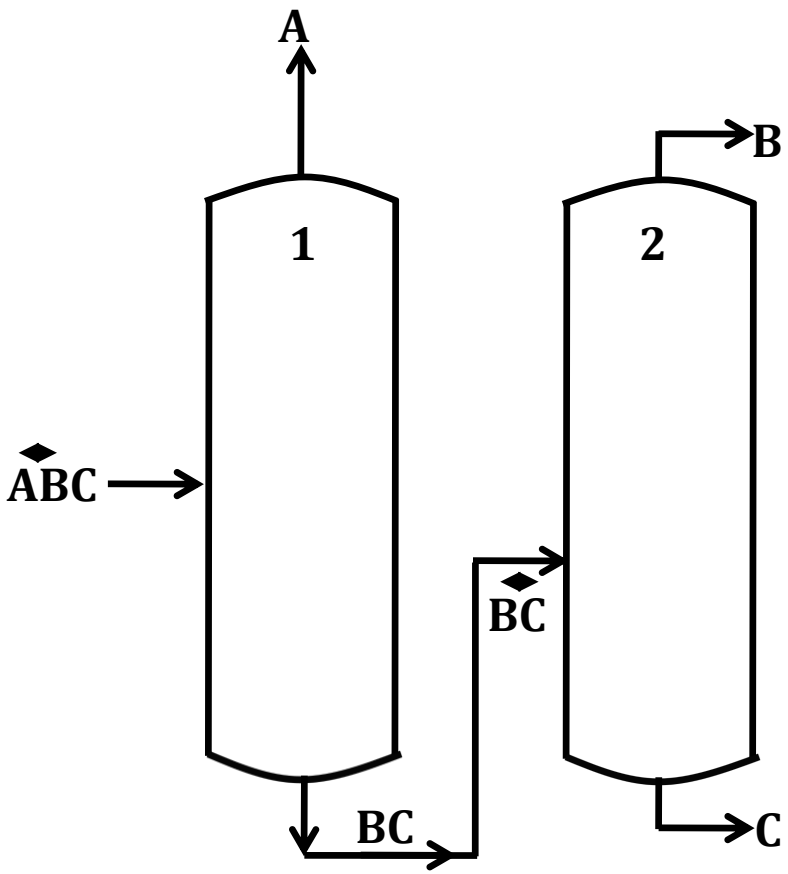
-One reaction can occur (not one of the parallel reactions; binary)
-Mass balance based on conversion data w.r.t. a reference component (binary)

-Parallel reactions must occur simultaneously (binaries)
-Mass balance based on conversion data and selectivity between reactions (binaries)

-One stream can leave the splitter

Distillation Column Basics

Example: Distillation of a mixture of 3 components A, B & C



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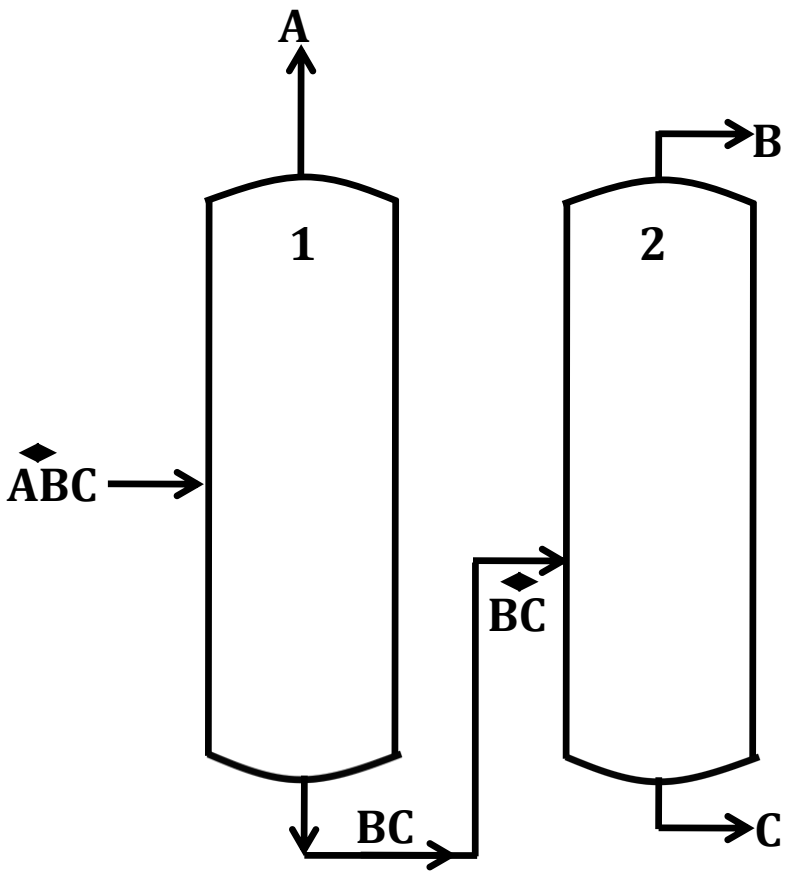

A: Light key **B: Light key**
B: Heavy key **C: Heavy key**

Distillation Column Basics

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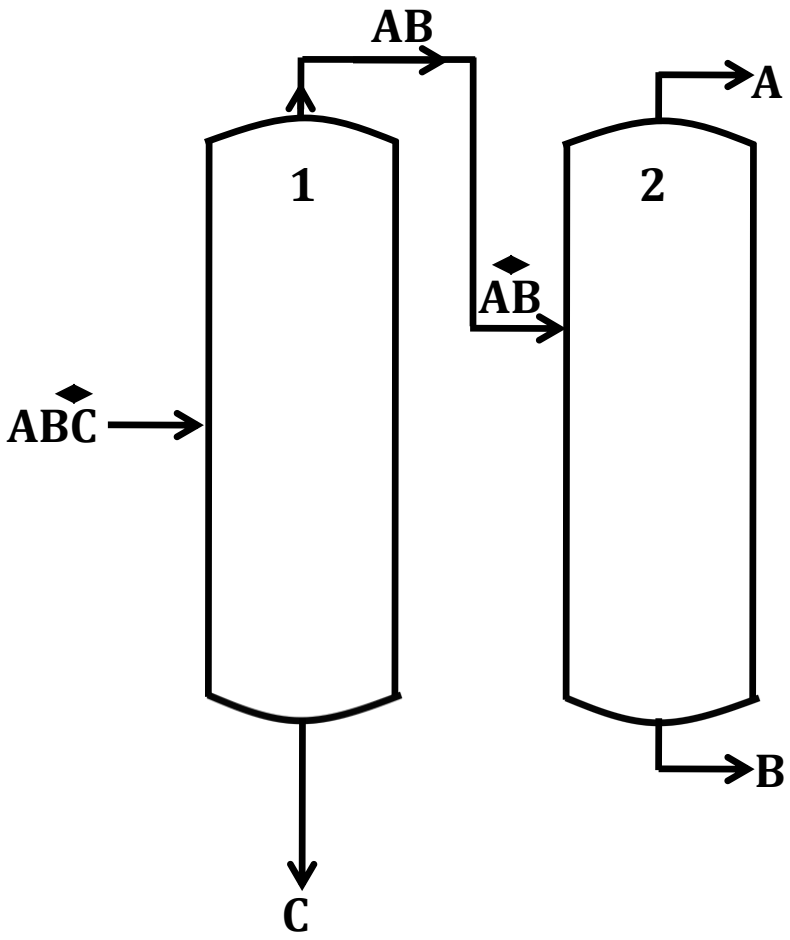
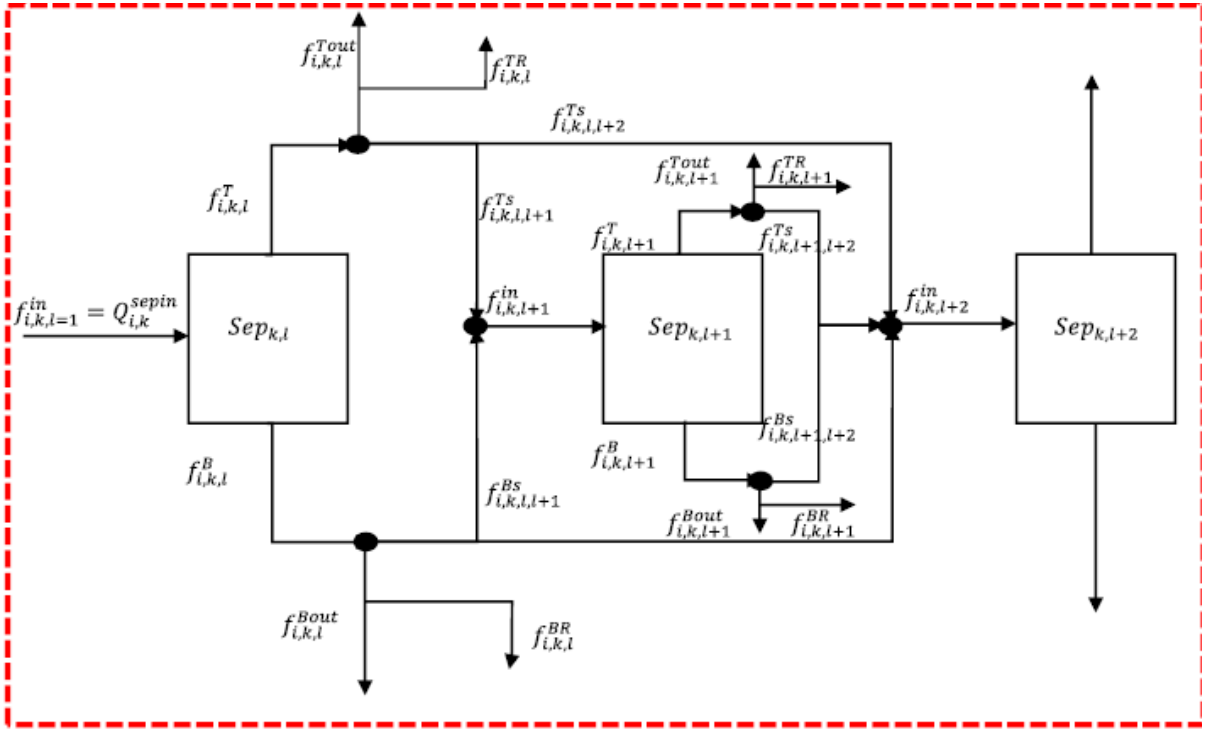


B: Light key **A: Light key**

C: Heavy key **B: Heavy key**

Distillation Columns Modeling



-Each column: 1 light key, 1 heavy key

-Any component: light/heavy key in only one column

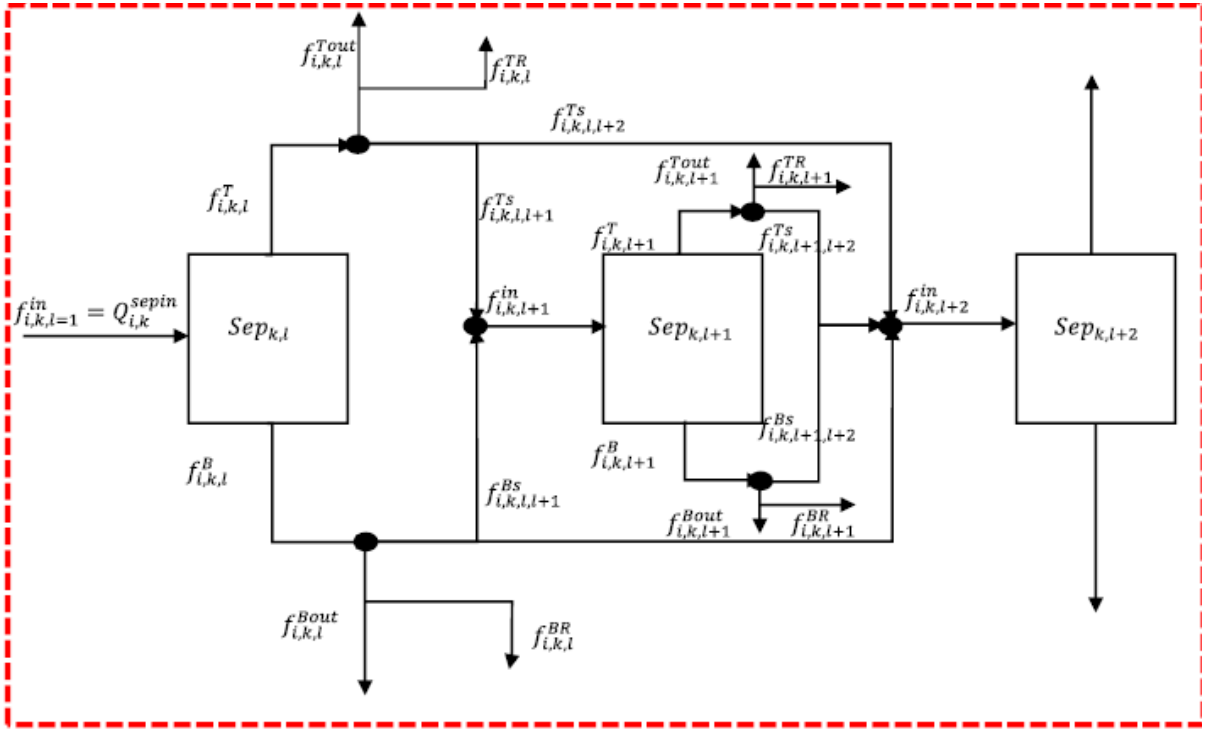
-Detect the present inlet components

-Light/heavy key from among present inlet components

-Components lighter than light key -> top product

Image Courtesy: An optimisation-based framework for theconceptual design of reaction-separation processes

Distillation Columns Modeling



-Components heavier than heavy key -> bottom product

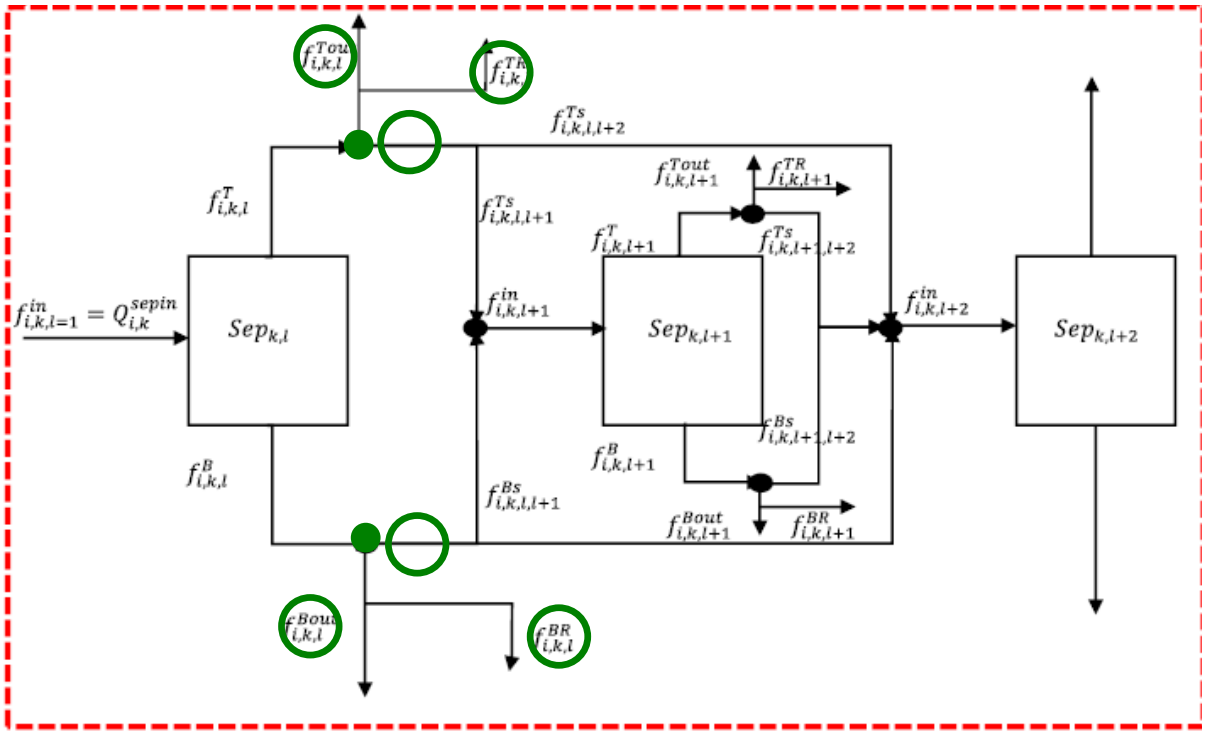
-Heavy key: component with the next highest BP than that of the light key

-A prior column absent => all subsequent columns are absent

-Mass balance

Image Courtesy: An optimisation-based framework for theconceptual design of reaction-separation processes

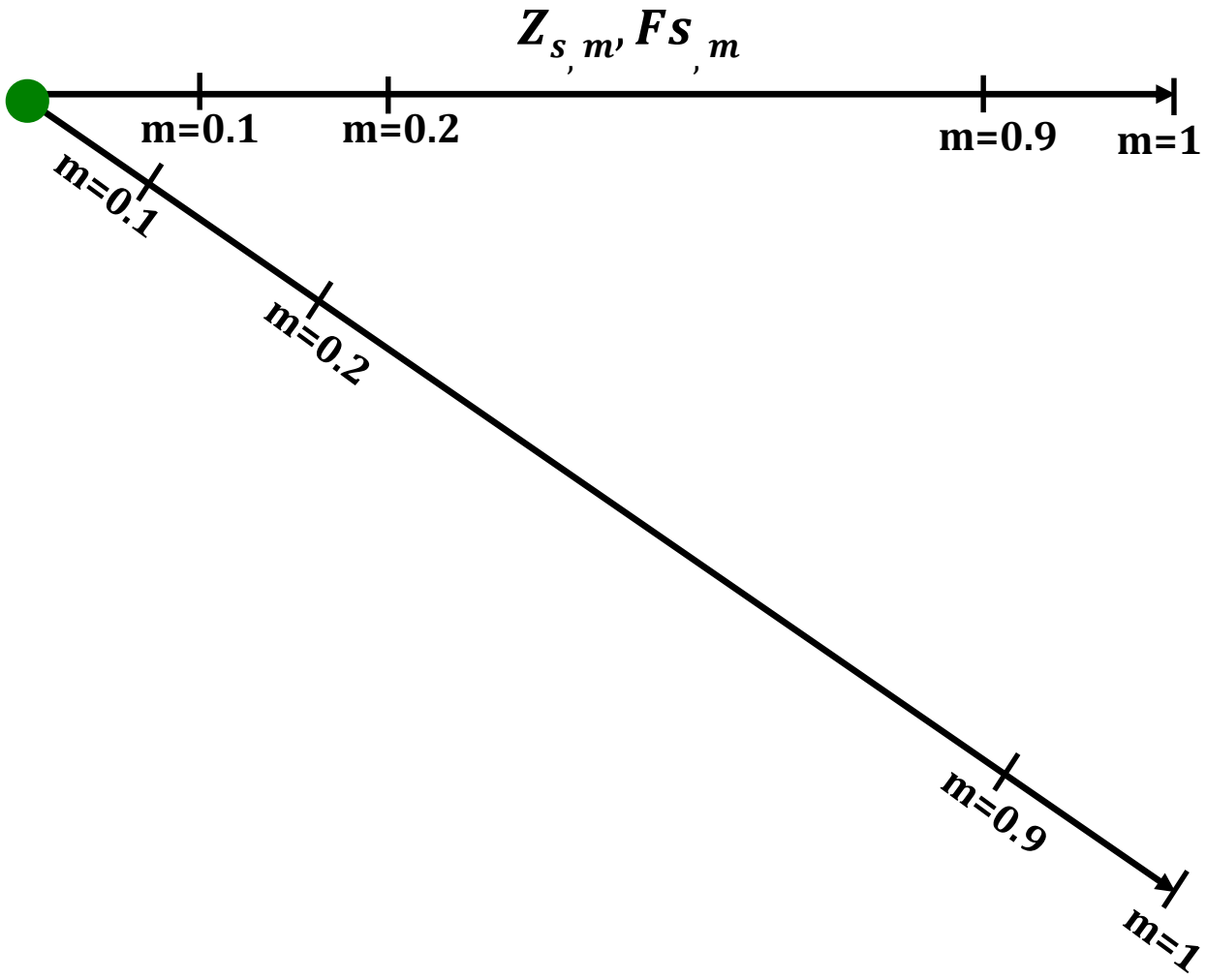
Splitter Modeling



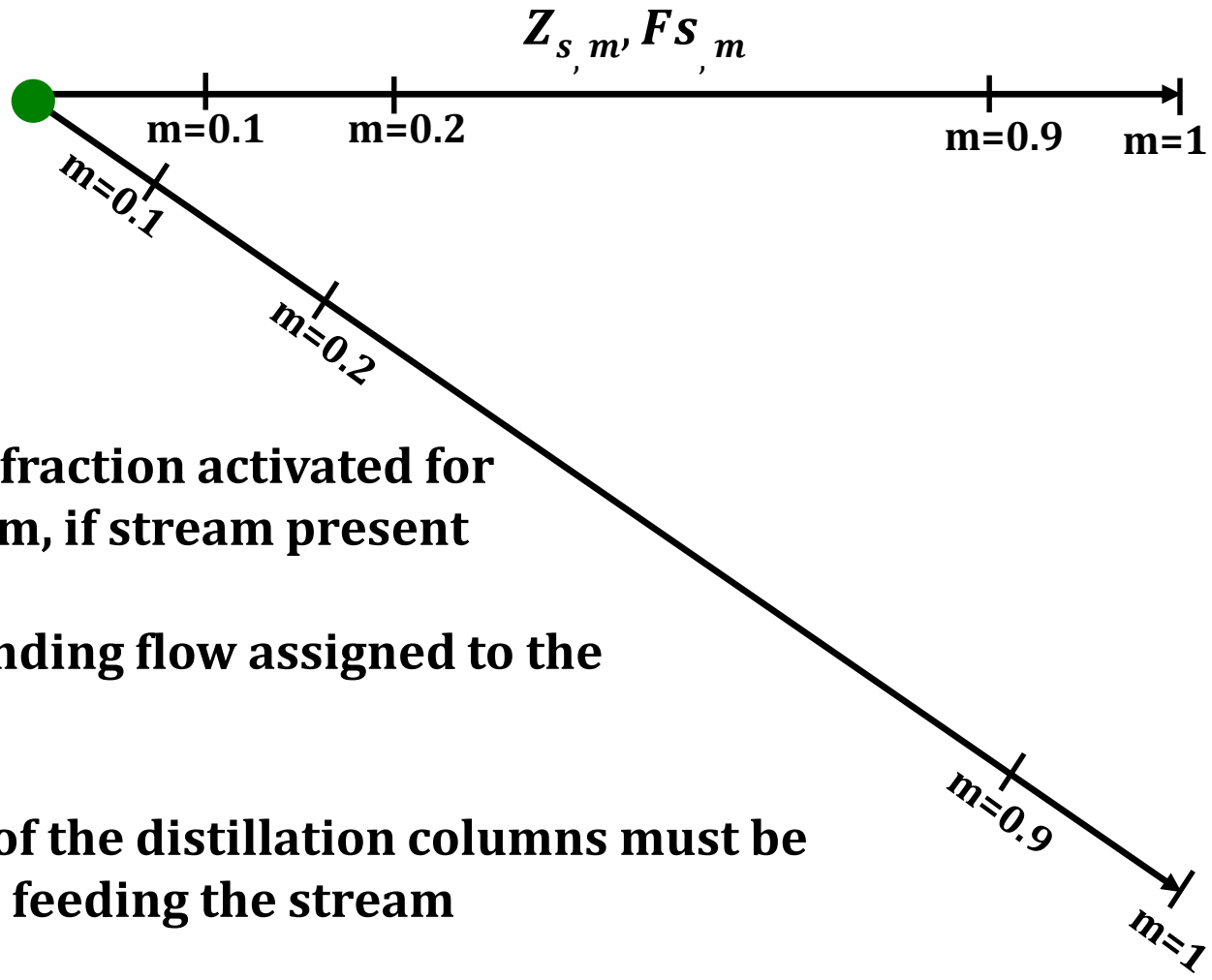
-Splitters associated with distillate/bottoms: non linear constraints

Image Courtesy: An optimisation-based framework for theconceptual design of reaction-separation processes

Splitter Modeling



Splitter Modeling



-One split-fraction activated for each stream, if stream present

-Corresponding flow assigned to the Stream

-Only one of the distillation columns must be chosen for feeding the stream

-Sum of the chosen split-fractions=1

Economic Considerations

-Revenue from products

-Raw material costs

-Annualized separation cost (column) = $\frac{\beta(\text{Total feed flowrate to the column})}{\text{BP difference b/w the light and heavy key}}$

-Profit

-MILP formulation

Case Study

-D:limonene as starting material

-Worldwide production of d-limonene ≥ 70,000 t in 2013

-Assumption: plant processing 15,000 t limonene per annum

Case Study: Reaction Network

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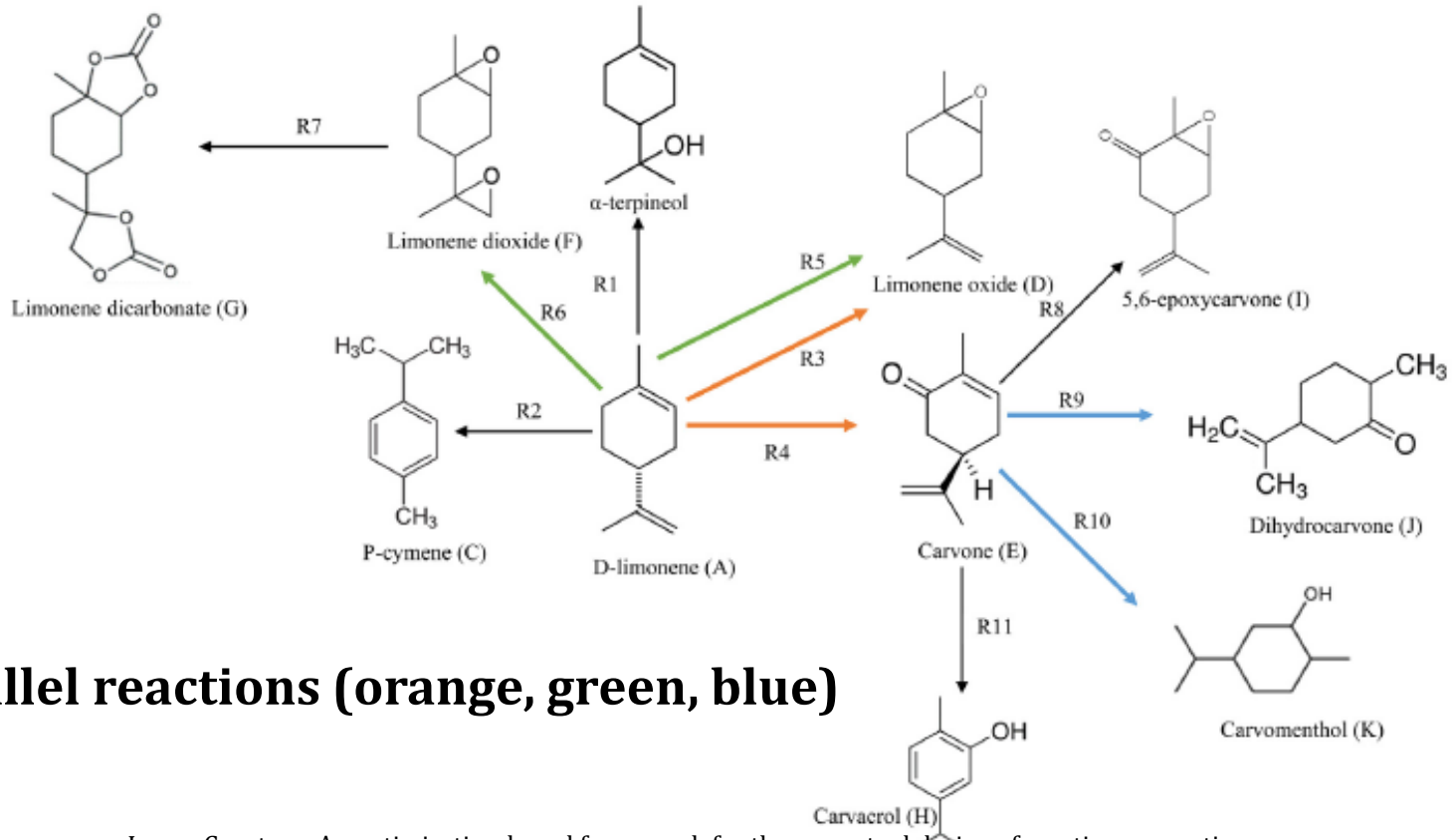

-Parallel reactions (orange, green, blue)

Image Courtesy: An optimisation-based framework for theconceptual design of reaction-separation processes

Case Study: Reaction Network Data

Reaction	Conversion	Selectivity (mol%)	Conditions	Source
R1	93	–	25 °C, 1atm	Literature
R2	100	–	170 °C, 1atm	Literature
R3	100	59.5	75 °C, 1atm	Literature
R4	100	40.5	75 °C, 1atm	Assumed
R5	98	74.5	40 °C, 1atm	Literature
R6	98	25.5	40 °C, 1atm	Assumed
R7	100	–	140 °C, 30bar	Literature
R8	32	–	50 °C, 1atm	Literature
R9	90	62.6	100 °C	Literature
R10	90	37.4	100 °C	Assumed
R11	80	–	–	Literature

-Boiling points: from databases

-Market price of certain molecules: group contribution method

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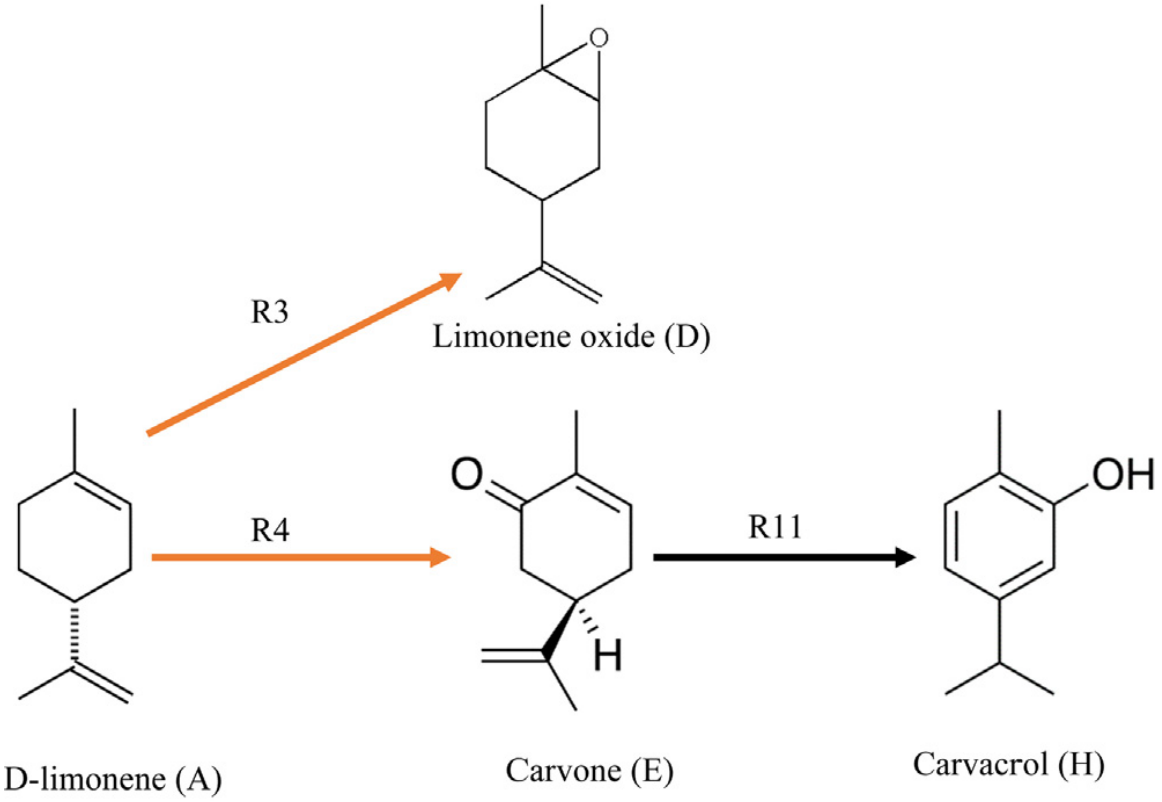
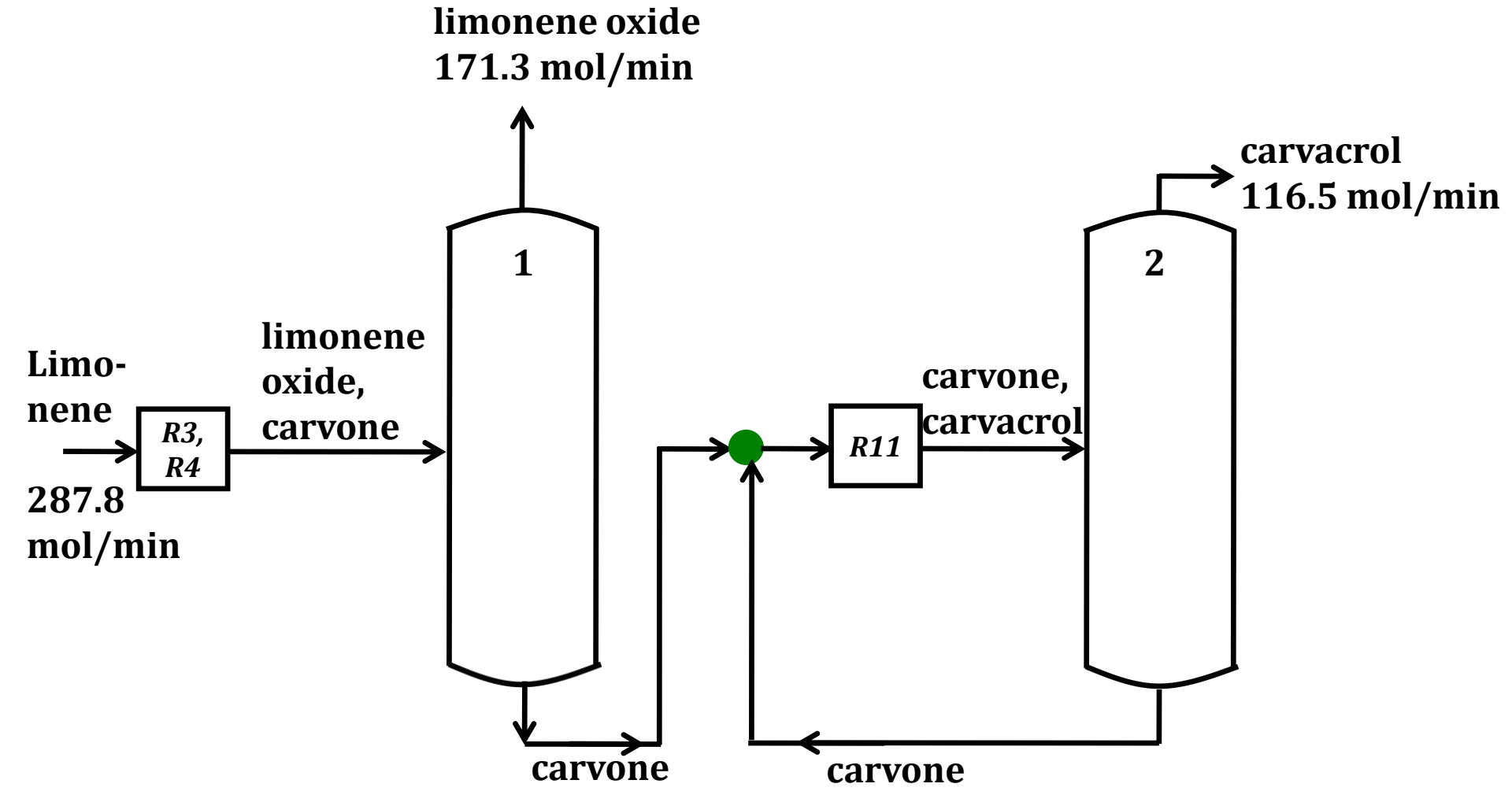
Optimal Reaction Network



Optimal Process Flowsheet



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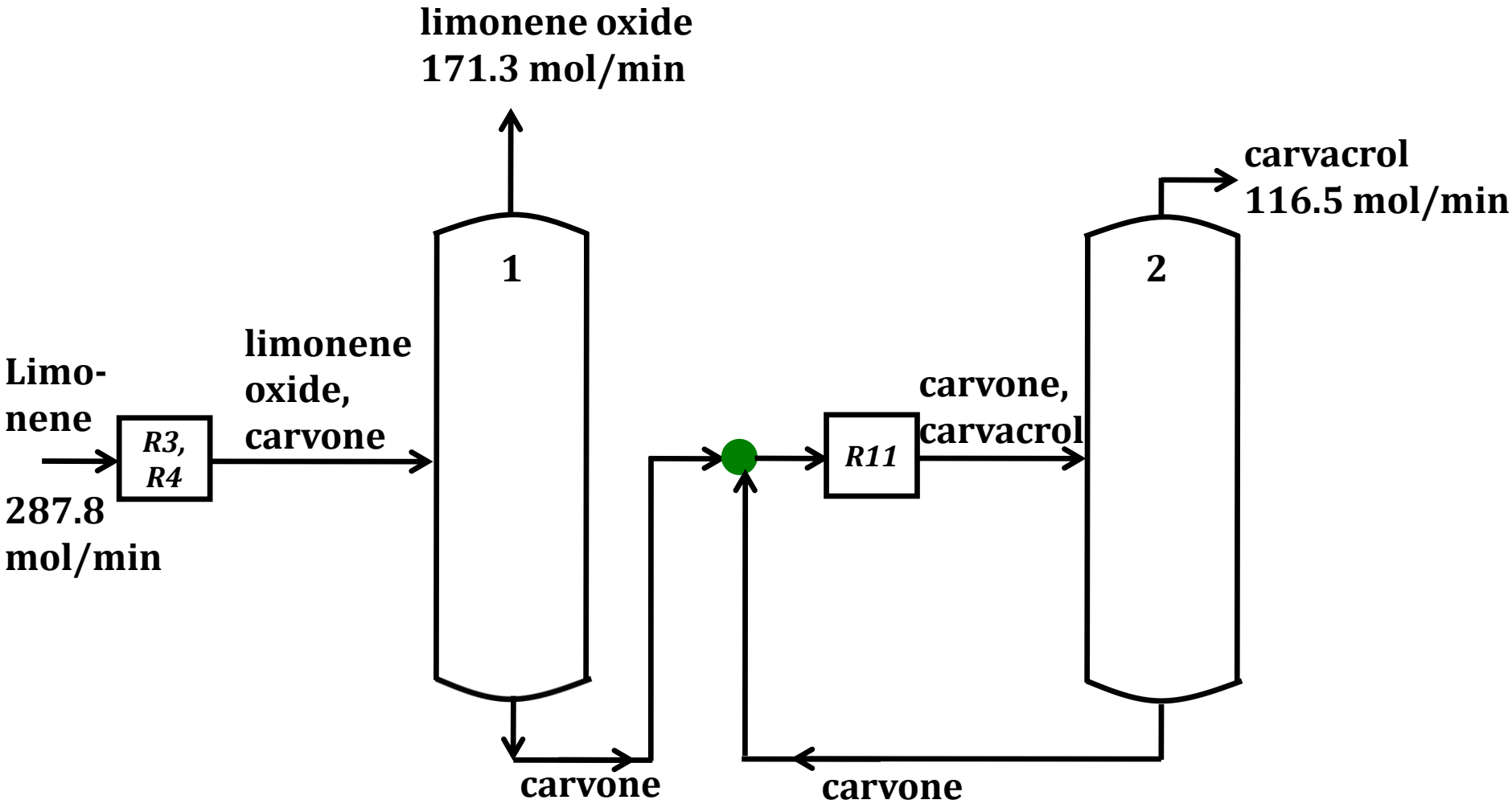

Profit: $20.8 million per annum

Conclusions

-Process synthesis from reaction networks: a superstructure-based approach

-Reactor model

-Distillation sequence model

-Splitter model

-Demonstrated the framework on a case study

Thank You!