Reinforcement learning for process synthesis with COCO and ChemSep: Distillation Gym

BY LAURENCE MIDGLEY

CONTACT: LAURENCEMIDGLEY@GMAIL.COM

GITHUB REPOSITORY: HTTPS://GITHUB.COM/LOLLCAT/DISTILLATIONTRAIN-GYM

Synopsis

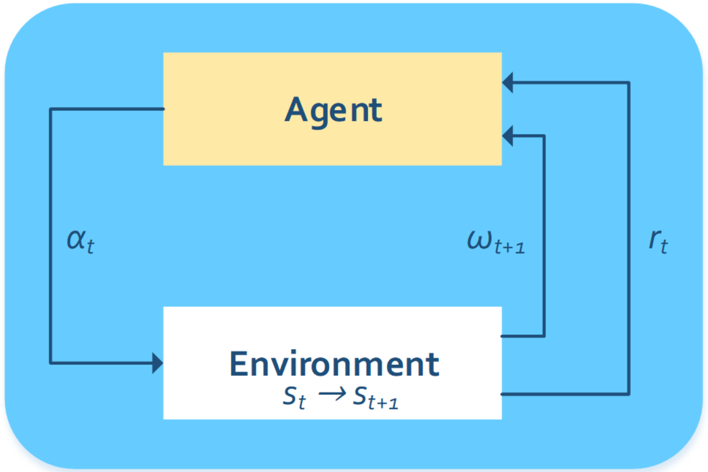
- Brief introduction to reinforcement learning (RL)
- How RL can be applied to process synthesis
- Distillation gym: A set of reinforcement learning environments for the design simple distillation trains
- Chemical Engineering Gym (next step): A general process synthesis reinforcement learning framework
- Recommendations for Co-Lan

Introduction to Reinforcement learning

- Reinforcement learning (RL), is a type of machine learning which involves an agent making decisions within an environment to maximize an expected reward. RL has had many recent successful applications, including mastering games such as chess and go.
- The environment is structured as a Markov Decision Process (MDP), where the following set of steps occurs

Repeat until episode is completed:

1. The agent observes the state (or part of the state) of the environment,
2. The agent takes an action
3. The agent receives a reward
4. Environment transitions to the next state



Reinforcement learning for chemical engineering process synthesis

- Reinforcement learning has been recently applied to chemical engineering problems, notably process control (Nian et al., 2020).
- However, it has not yet been successfully applied to computer aided process synthesis, which is currently dominated by other techniques such as MINLP (Chen and Grossmann, 2017).
- Chemical engineering process design can be framed as an MDP.

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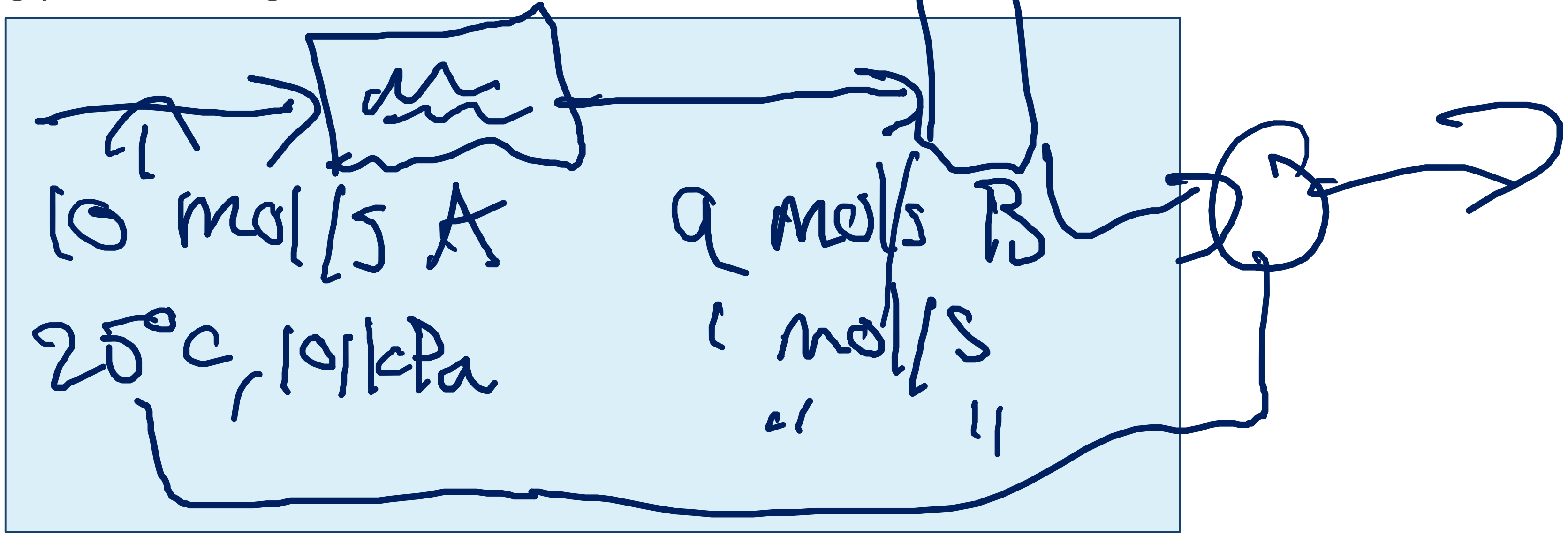
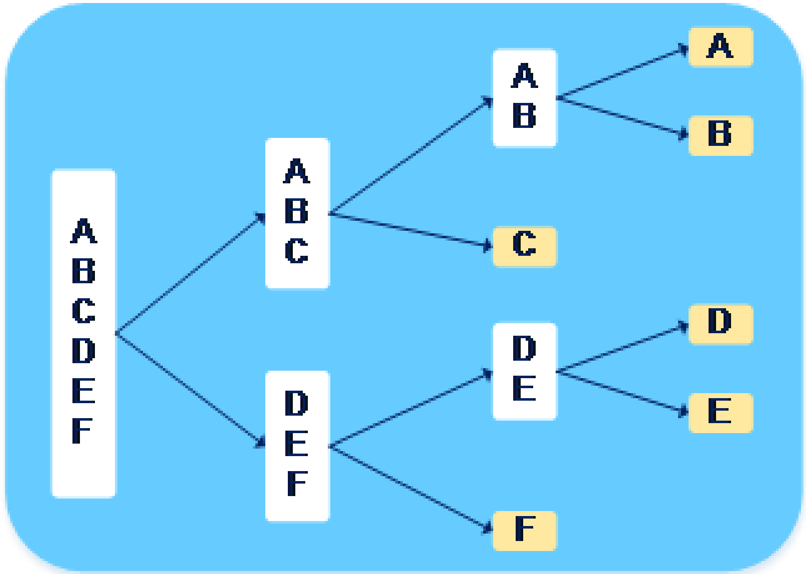
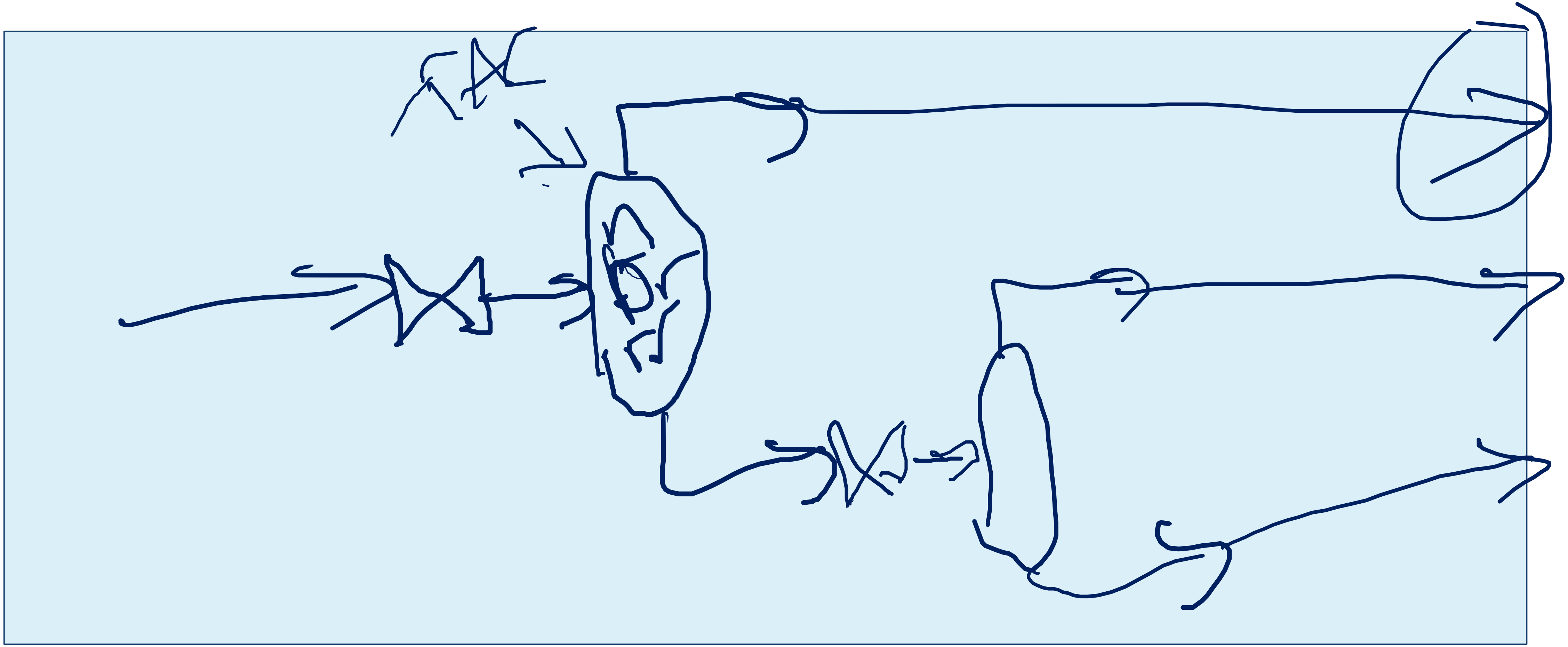


Distillation Gym with COCO and ChemSep

- Design of a simple distillation train sequence
- User defined
  - starting stream
  - simulator thermophysical properties
  - product definition (selling prices and required purity)
- Agent selects
  - To separate a stream or not
  - Column specification (pressure, reflux ratio, reboil ratio, number of stages)
- Reward: Revenue - Total Annual Cost
- Unit simulation using COCO and ChemSep
- Agent & environment coded in python
  - Controlling unit simulation using COM interface



Distillation Gym Visualisation



Note – text in order of appearance reads:

n (number of stages), br (boil-up ratio), rr (reflux ratio), TAC (total annual cost)

Example Problems

Problem 1: Benzene - Toluene - p-Xylene:

- Equimolar starting stream: 3.35 mol/s, 25 °C, 1 atm
- Price ($/tonne): $488, $488, $510

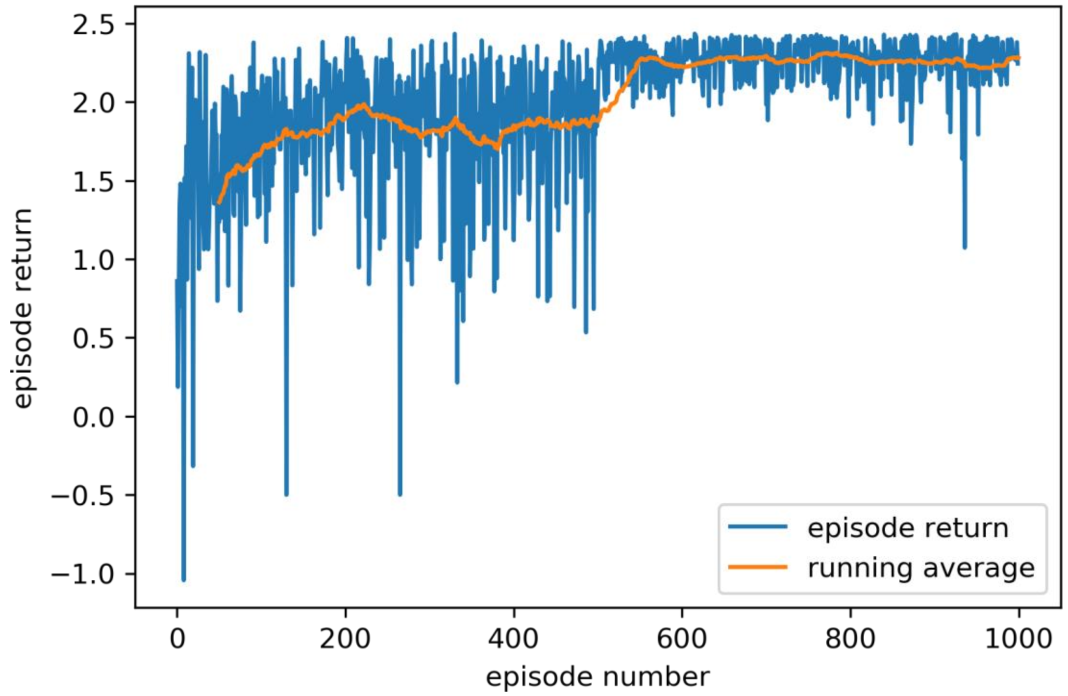
Problem 2: Hydrocarbons:

- Initial conditions: 105 °C, 17.4 atm

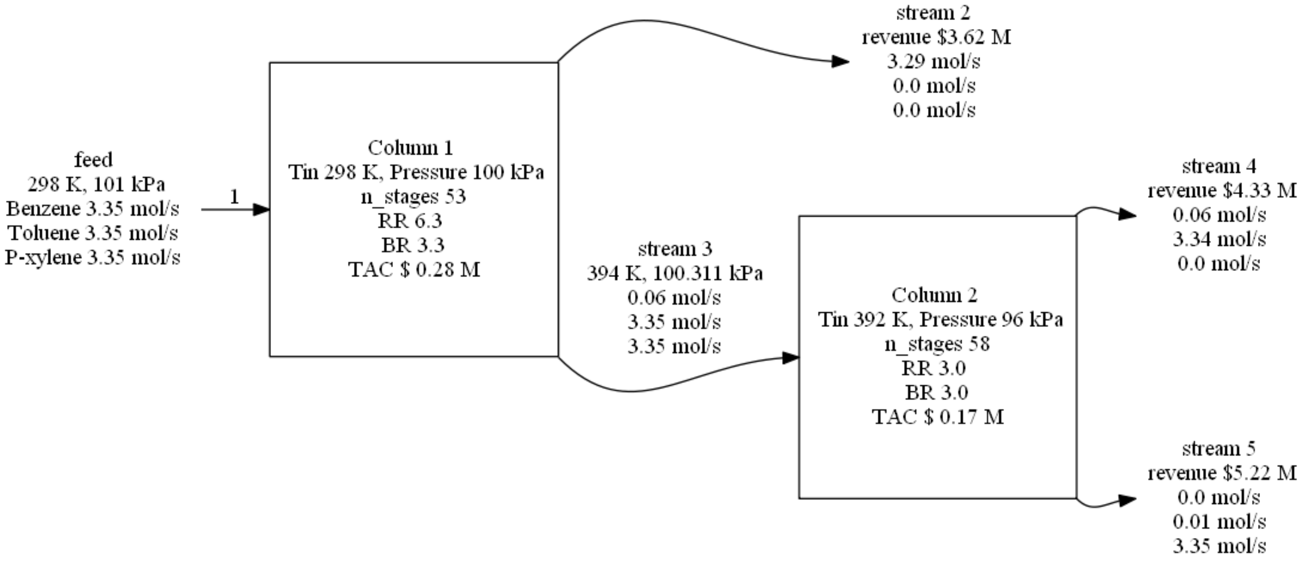
Compounds	Starting stream flowrate (mol/s)	Price ($/tonne)
Ethane	17	125
Propane	1110	204
Isobutane	1198	272
N-butane	516	249
Isopentane	344	545
N-pentane	173	545

Benzene, Toluene P-xylene

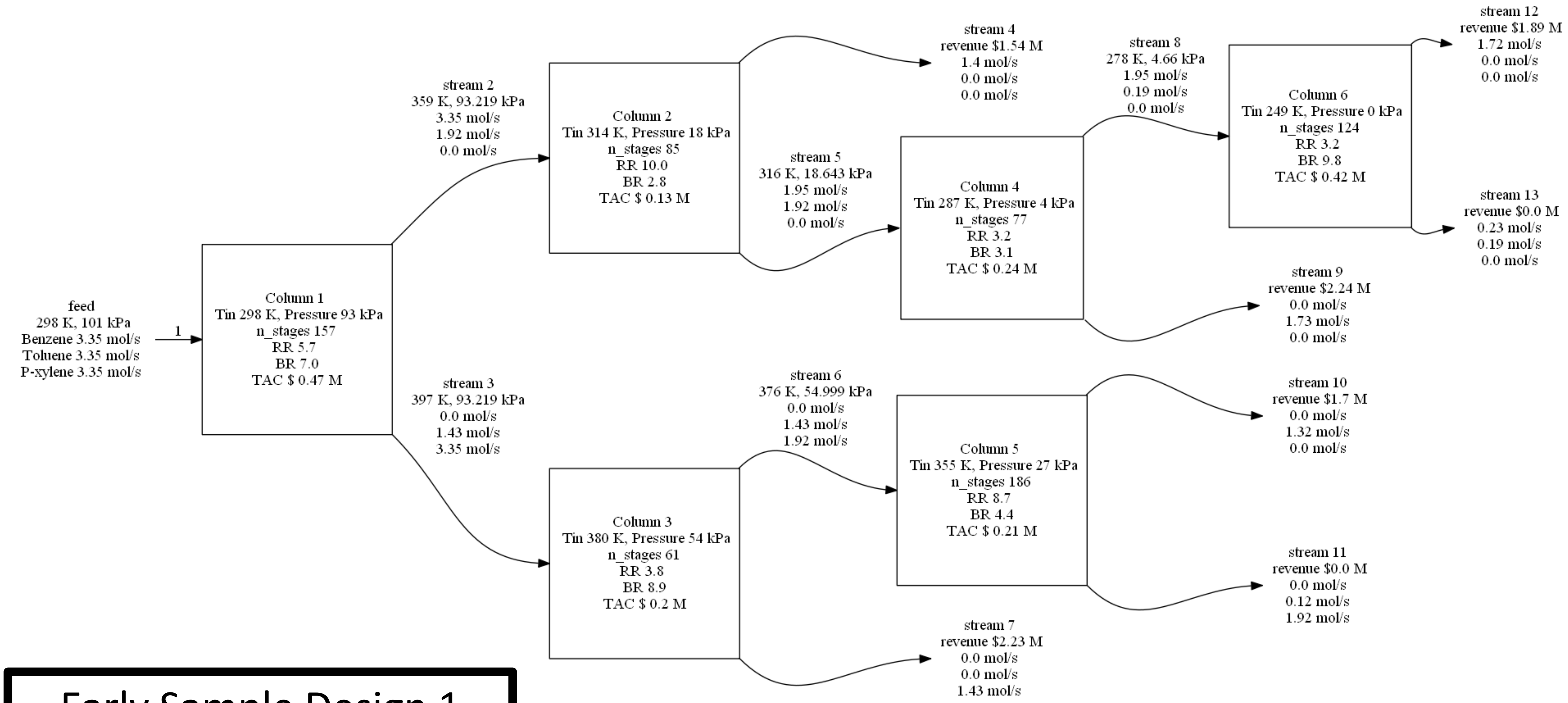
Agent performance during training



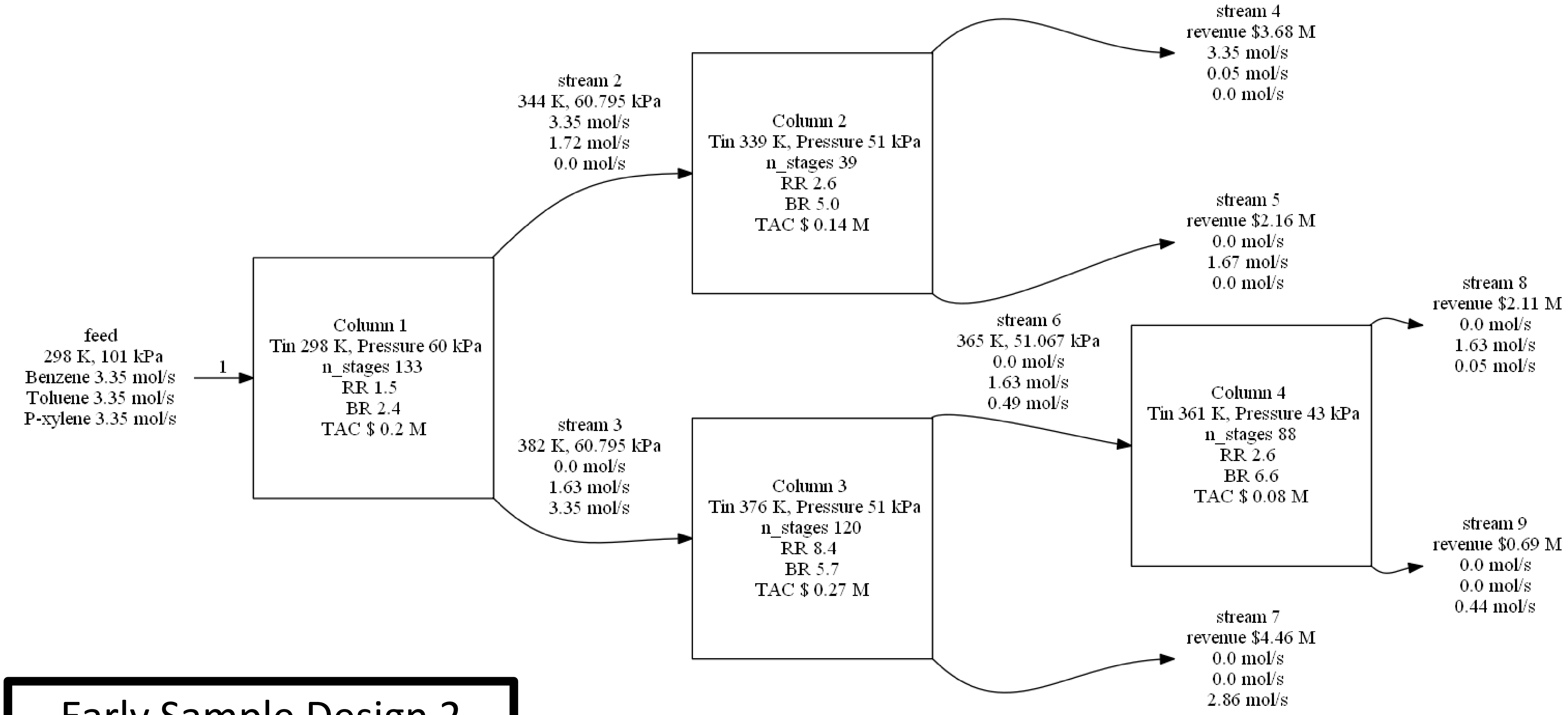
Best Design Outcome



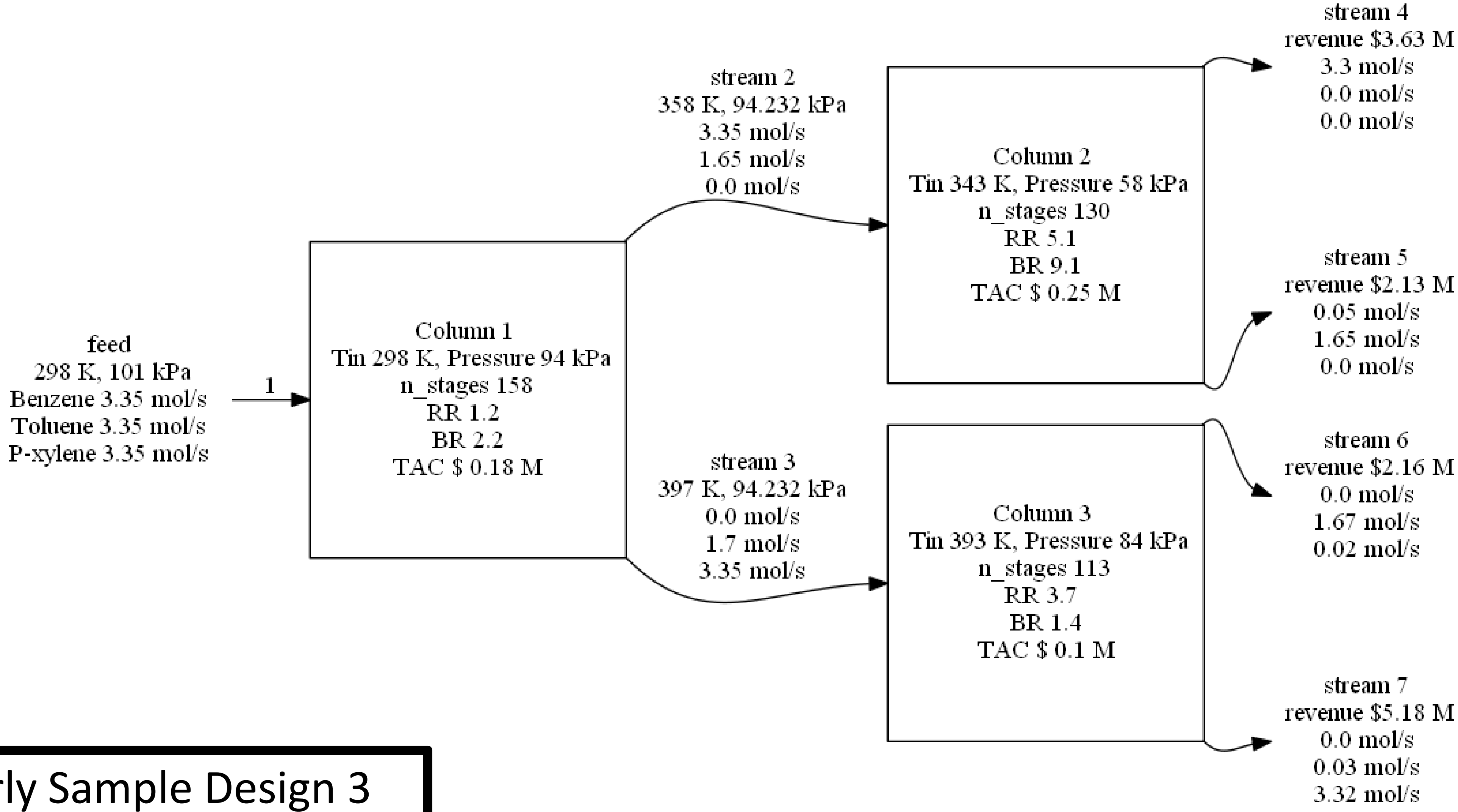
Revenue	$ 13.17 million
Column TAC	$ 0.45 million



Early Sample Design 1

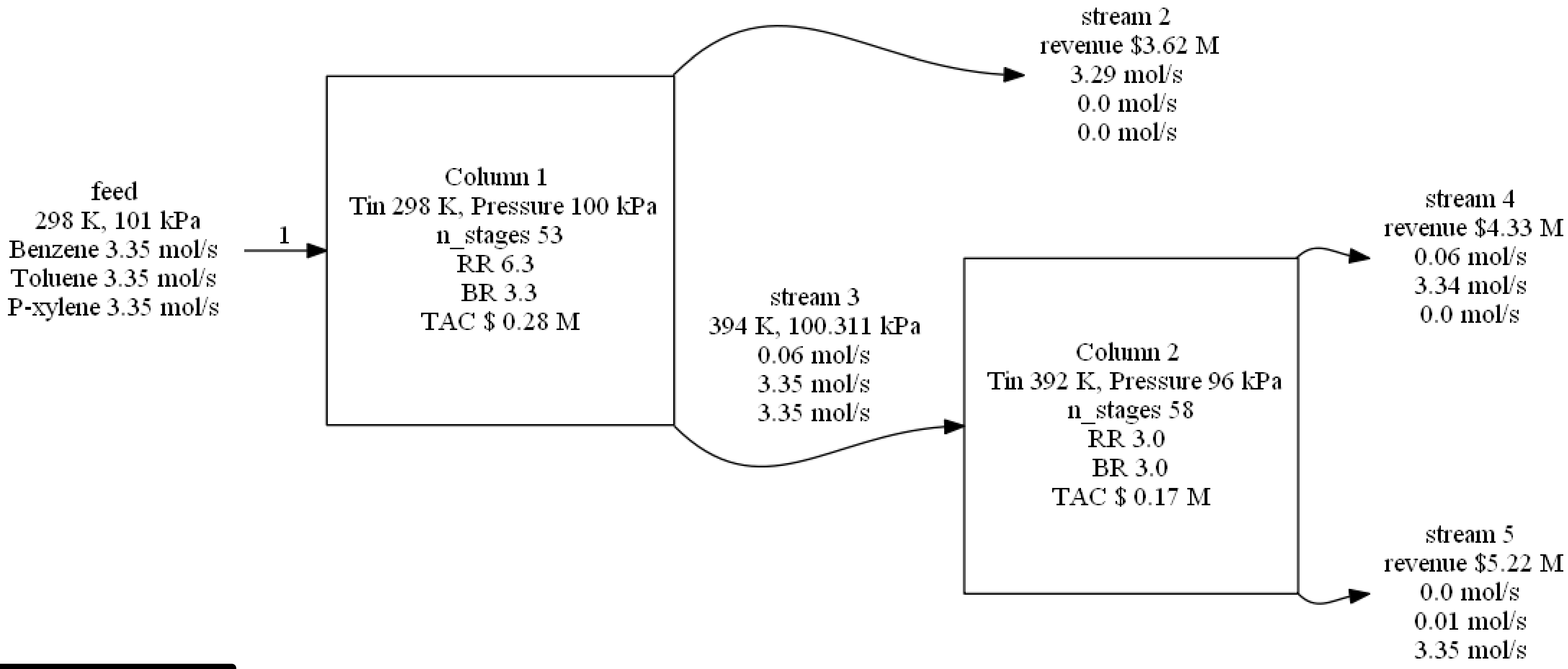


Early Sample Design 2



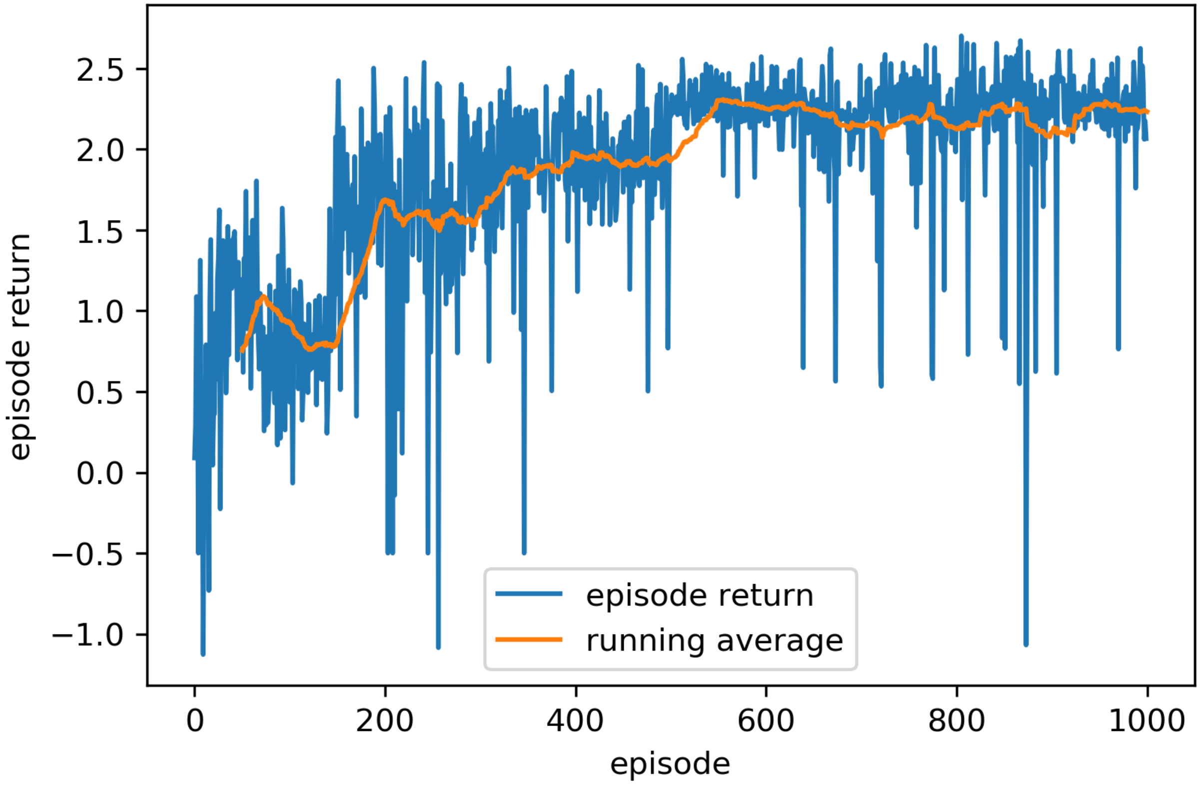
Early Sample Design 3

Final Design



Hydrocarbon Problem

Agent performance during training



Best Design Outcome

Total Revenue	$ 1588 million
Total Column TAC	$ 119 million

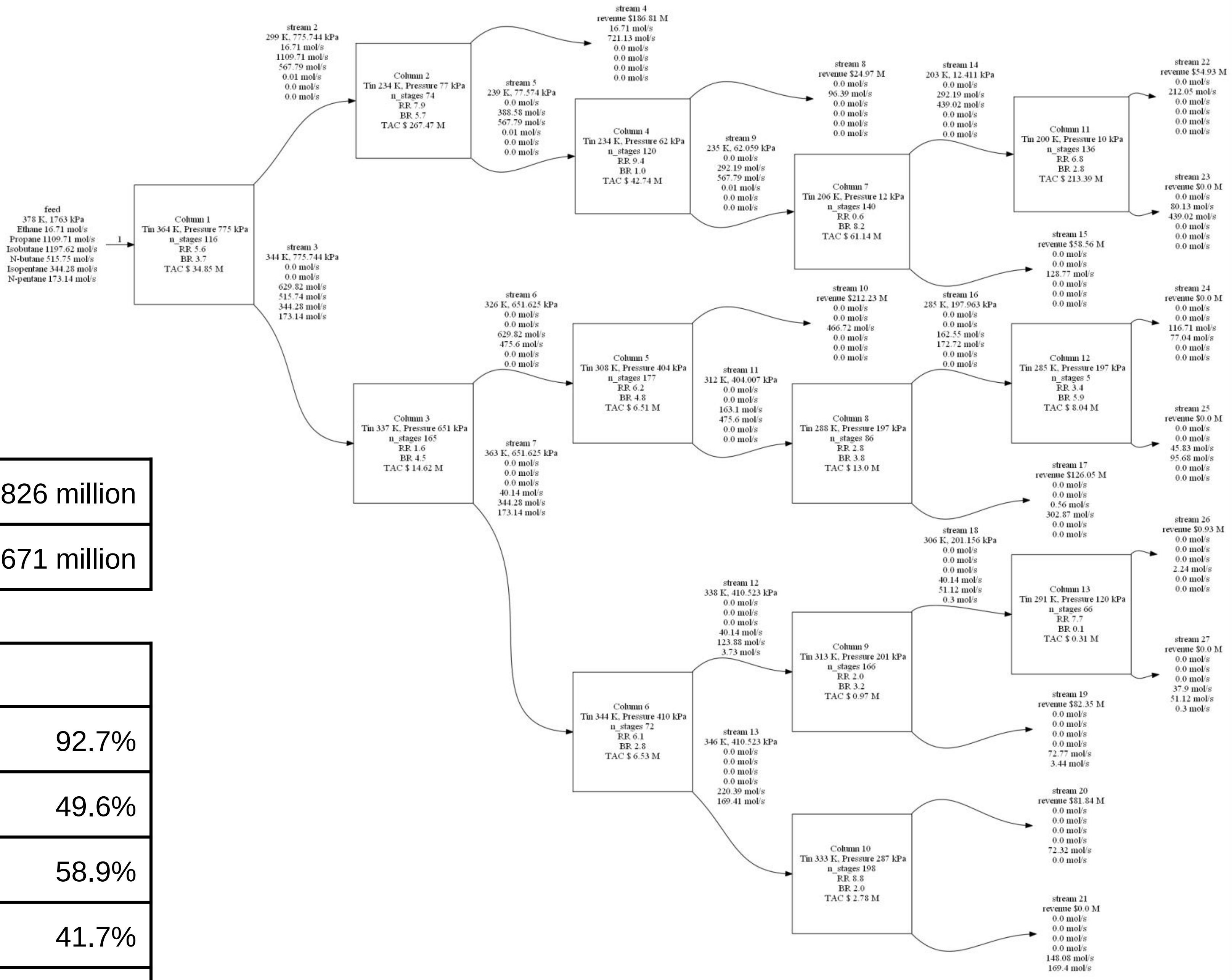
	Recovery
Propane	98.9%
Isobutane	97.3%
N-butane	91.1%
Isopentane	99.6%
N-pentane	97.0%

Early Sample Design

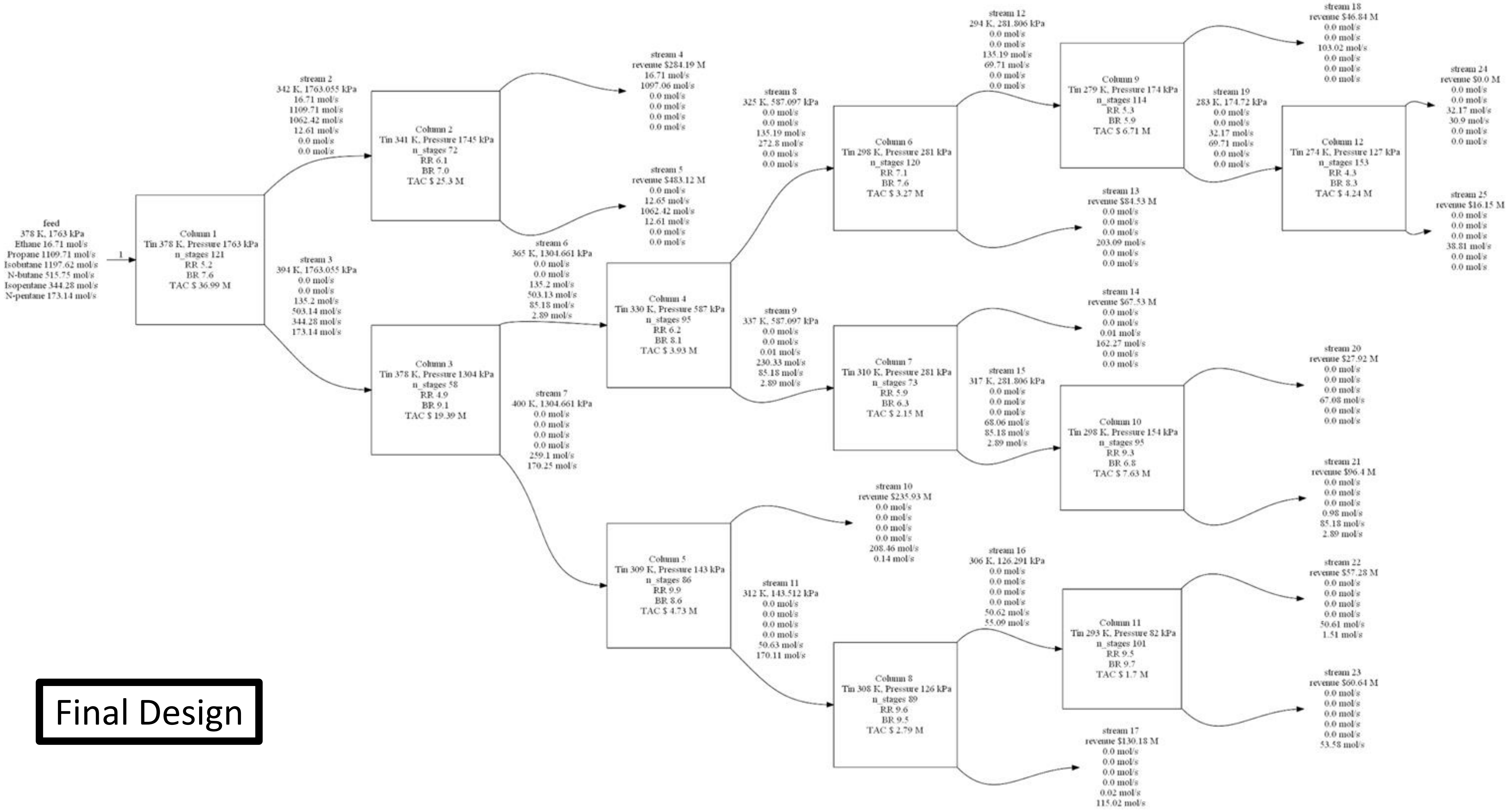
Design Outcome

Total Revenue	$ 826 million
Total Column TAC	$ 671 million

	Recovery
Propane	92.7%
Isobutane	49.6%
N-butane	58.9%
Isopentane	41.7%
N-pentane	0.0%



Final Design



Next steps: Build Chemical Engineering Gym

A general all-purpose reinforcement learning framework for chemical engineering process synthesis

Recommendations to Co-Lan

- Create an interface for external programs (e.g. python) to easily manipulate flowsheets.
  - Try make as much functionality that is accessible from GUI accessible from external program
  - i.e. add new units/streams, deleting units/streams, changing flowsheet topology etc…
  - Multithreading support
- This would give computational chemical engineering in simulators a far larger scope, extending from being able to edit existing flowsheet structures (e.g. changing unit conditions), to creating complete flowsheets from scratch

Thank you

Jasper van Baten (COCO) & Harry Kooiman (ChemSep) for answering endless emails with lots of help

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