Production of Benzene, Toluene, and Xylenes from Natural Gas via Methanol: A Process Synthesis and Global Optimization Approach

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Introduction & Motivation

- Natural gas is an abundant, inexpensive, and versatile feedstock for conversion into valuable products, such as aromatics
- Several competing and commercial technologies exist for natural gas conversion
- Objective: Determine novel processes for aromatics production from natural gas using a global optimization algorithm that maximizes the profit from these refineries.
- The optimal processes are economically competitive with the current state-of-the-art
- The optimal processes are environmentally sustainable
- Optimization algorithm is completed using the Ada supercomputer at Texas A&M University

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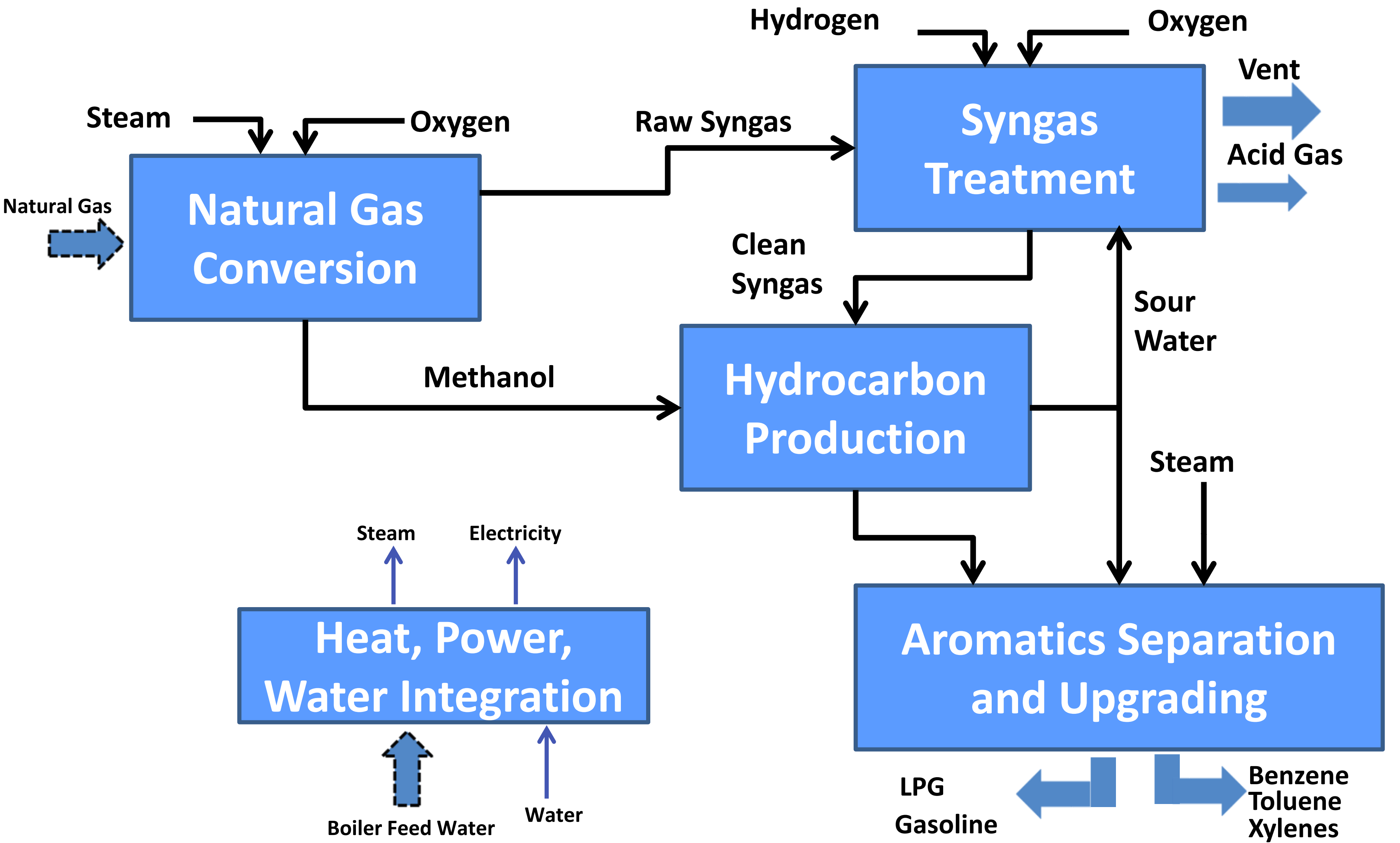
Natural Gas to Aromatics Processes: Block Flow Diagram



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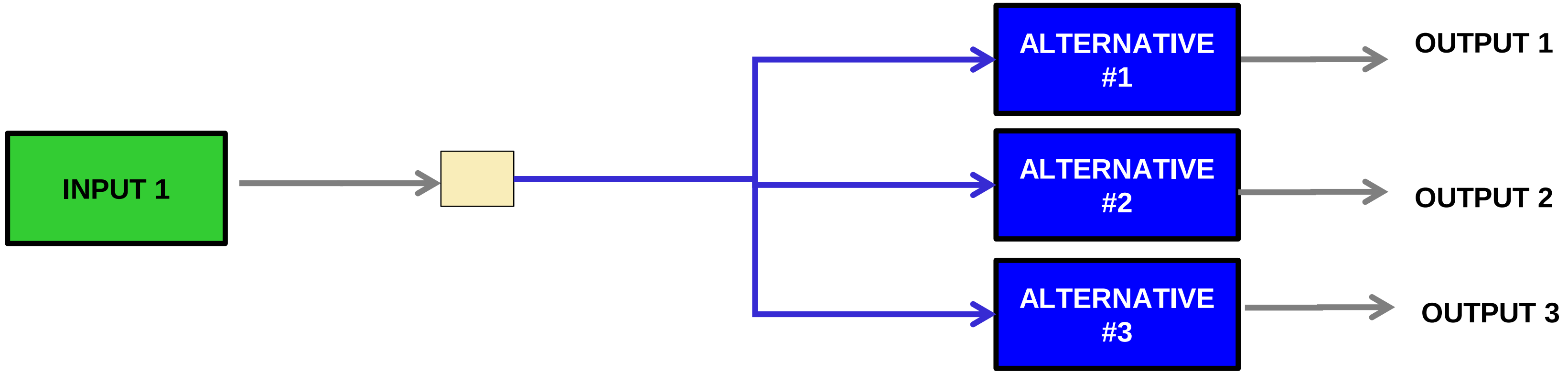
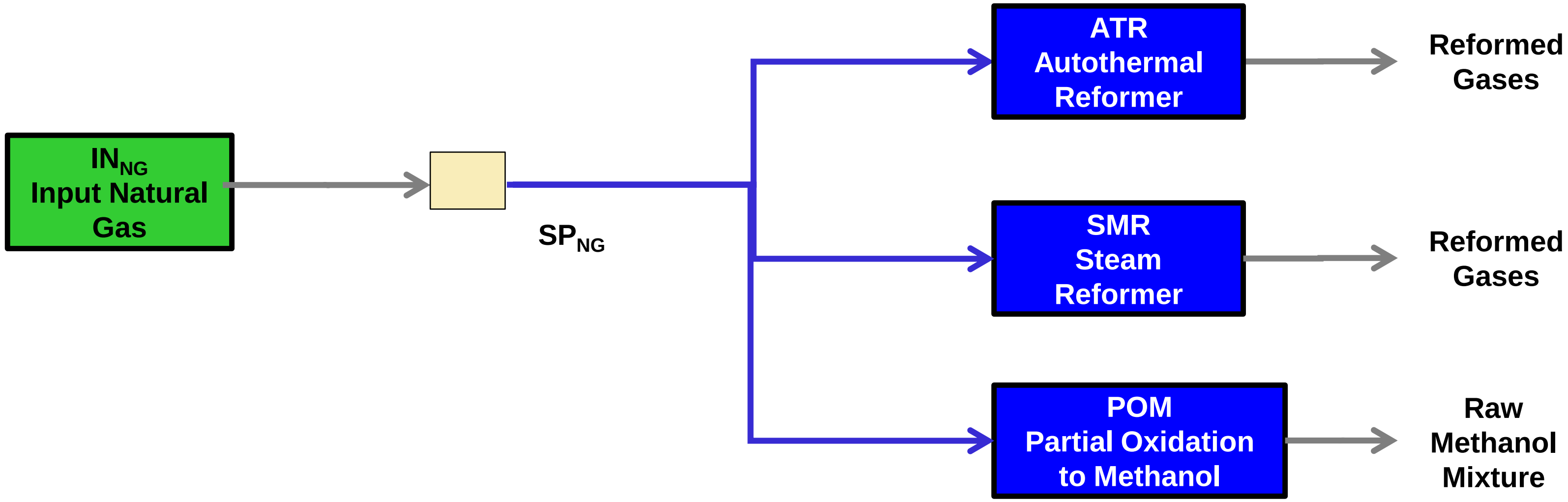
Mathematical Modelling of Large-Scale Process Superstructure

Each alternative modelled rigorously using chemical engineering first principles



Example: Natural Gas Conversion



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Overall Strategy

Process superstructure of alternatives ⇔ Rigorous input-output relationships for each unit ⇔ Obtain accurate cost functions and scaling factors ⇔ Obtain accurate feedstock & product costs

→ **Process Synthesis Mathematical Model** ←

Large scale mixed integer nonlinear, nonconvex program (MINLP)

~20,000 continuous variables	Molar flow of species, extents of reaction
~30 binary variables	Existence of units
~23,500 constraints	Environmental constraints, plant scale
~500 nonconvex terms	Bilinear terms, trilinear term, quadrilinear terms, power functions

Solved using a global optimization branch-and-bound framework using the Ada supercomputing capabilities at Texas A&M University

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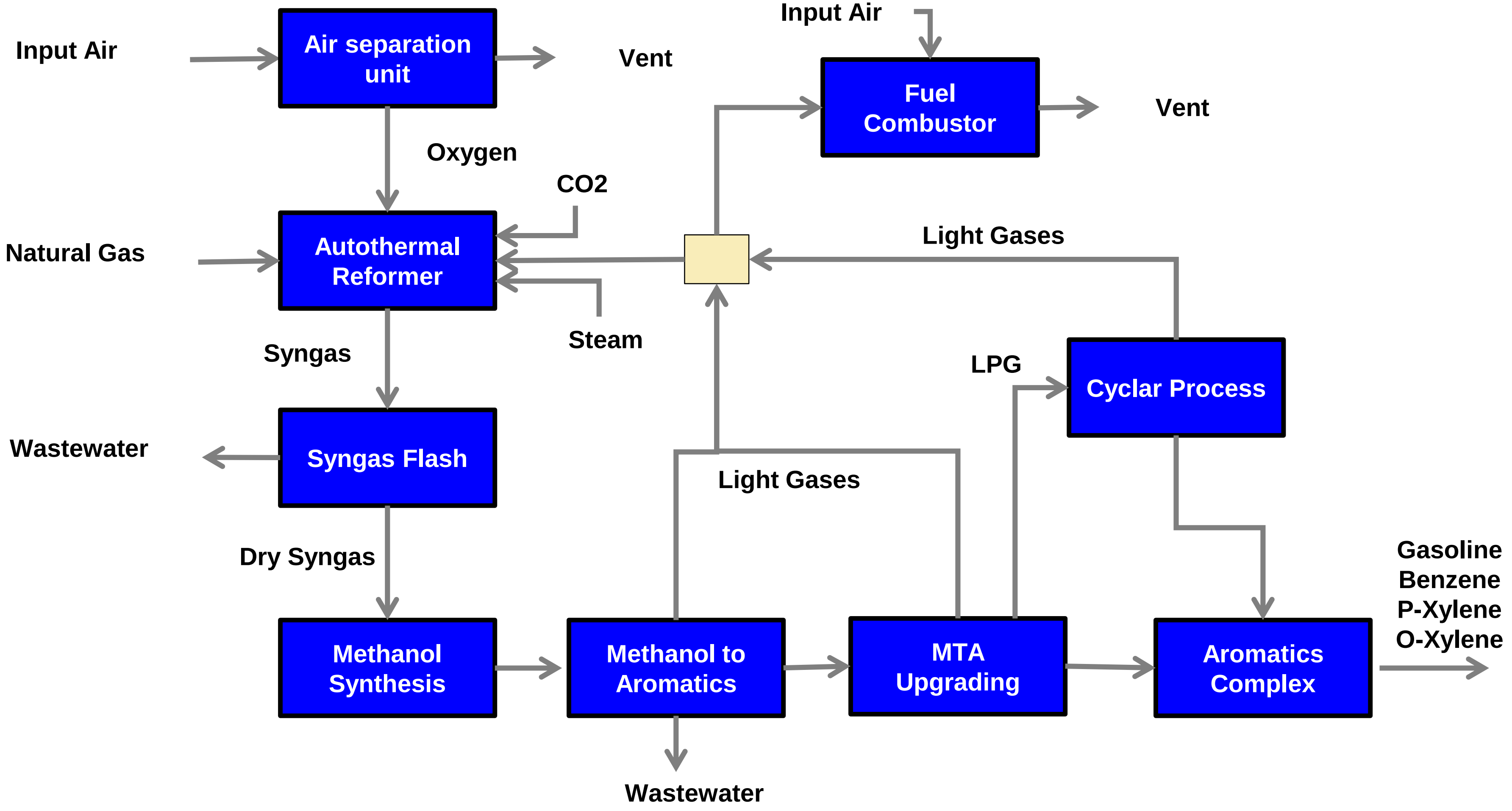
Results: Optimal Natural Gas to Aromatics Topology

Global optimization algorithm run for 120 hours to determine optimal processes (shown below) for aromatics production from natural gas



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Resource Requirement

- Runtime wall-clock limit: 120 hours
- Cores: 8 cores for execution
- 2500 MB per process/CPU
- Software used: GAMS (General Algebraic Modeling System)