Simulation of Methanol Production from Biogas: Impact of Feedstock Composition and Stoichiometric Number Adjustment

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Muhammad Zulkefal[1], Magne Hillestad[2], Truls Gundersen[1], and Bjørn Austbø[1]

[1]Department of Energy and Process Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway

[2]Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway

NTNU
Norwegian University of Science and Technology

INTRODUCTION

- Biogas-to-methanol production requires synthesis gas quality close to the methanol stoichiometric target.
- In biogas reforming, variations in the CH_4/CO_2 ratio and reformer conditions can shift the stoichiometric number (SN), reducing synthesis gas suitability for methanol synthesis.
- SN is a key indicator of synthesis gas suitability for methanol synthesis. Maintaining SN at the target value is essential to maximize conversion and productivity.

$$SN = (H_2 - CO_2) / (CO + CO_2) \qquad \text{Target SN} = 2.01$$

METHODS

- Steady-state Aspen Plus model of integrated biogas-to-methanol process.
- eSMR for synthesis gas production followed by synthesis gas conditioning.
- Methanol synthesis loop with recycle/purge, flash separation, and two-column purification.
- Parametric analysis: CH_4/CO_2 ratio, reformer temperature and pressure, and H_2O/CH_4 ratio – required H_2/CO_2 adjustment for targeted SN.
- Thermodynamic models: PR for reforming, RKSMHV2 for high-pressure methanol synthesis, and NRTL for low-pressure separation.

BASE-CASE SPECIFICATIONS

Feed	145 tonne/day biogas, 60% CH_4 and 40% CO_2
Steam-to-carbon ratio (S/C)	3
eSMR	950 °C, 25 bar (△p = 1 bar)
Methanol reactor (BWR)	230 °C, 75 bar, 1100 tubes, length 7 m, diameter 0.04 m, catalyst density 1775 kg/m³, catalyst diameter 5.5 mm
Recycle-to-feed ratio	4
Purification target	Fuel-grade methanol 99.85 wt%

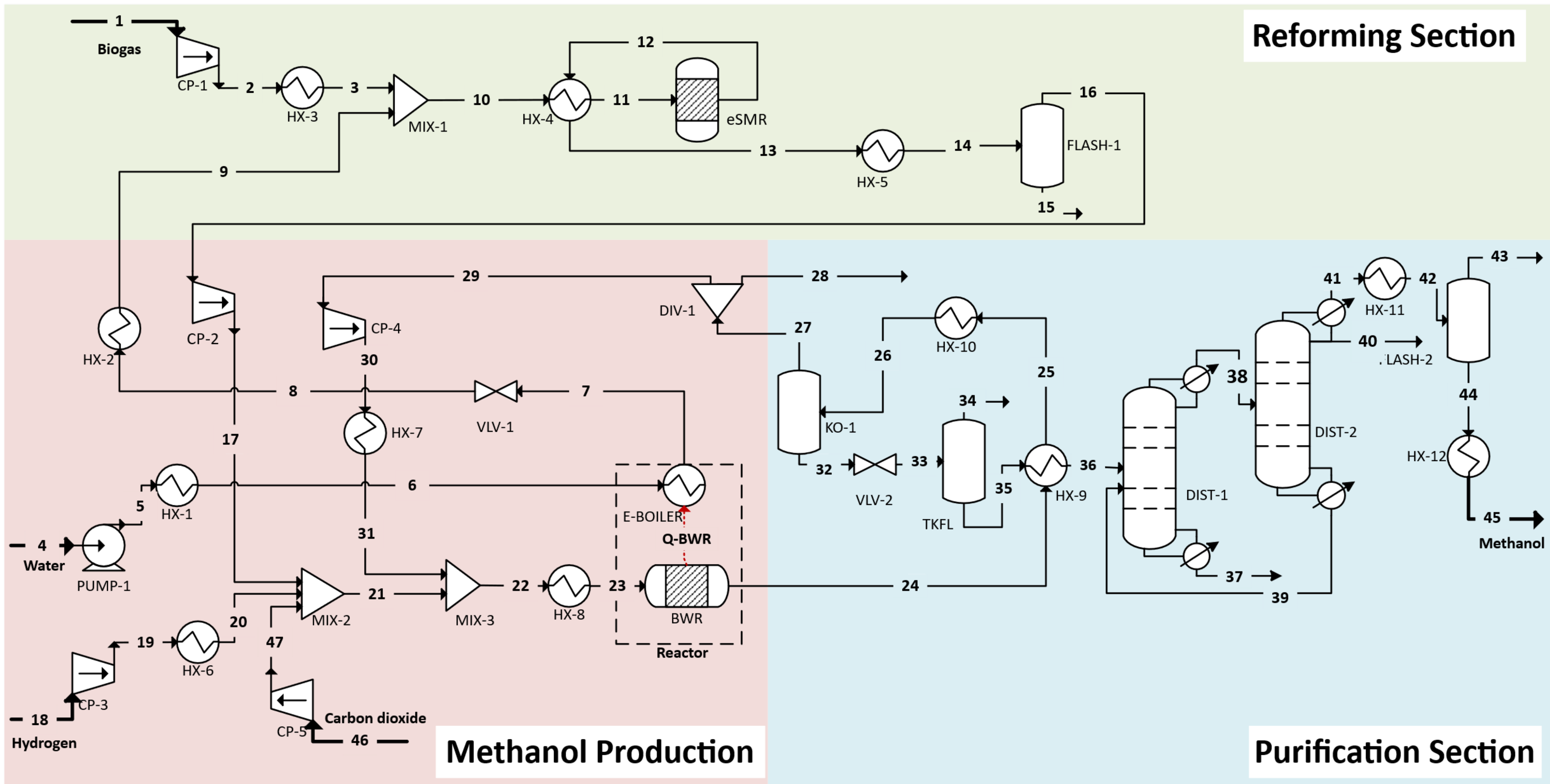
BASE-CASE RESULTS

CH_4 conversion (%)	96.2	CO conversion (%)	98.8
Reformer-outlet SN	1.36	CO_2 conversion (%)	87.9
H_2 addition (green)	6.8 tonne/day	H_2 conversion (%)	93.6
Final methanol production	151 tonne/day	Biogas to methanol conversion (%)	92.9

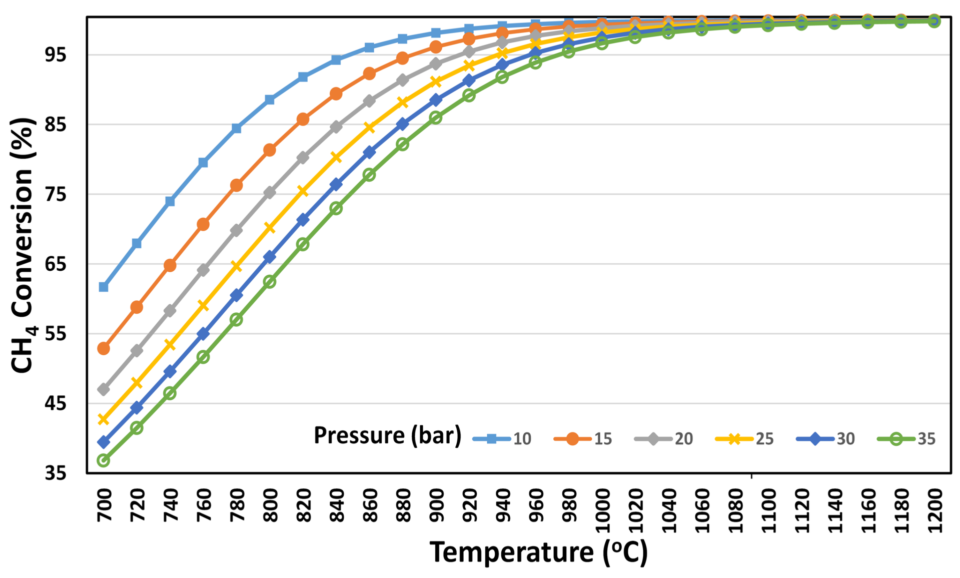
KEY TAKEAWAYS AND CONCLUSIONS

- CH_4/CO_2 ratio is the dominant factor controlling reformer-outlet SN and the transition between H_2-deficient and H_2-excess synthesis gas.
- Higher reformer temperature increases CH_4 conversion and SN.
- Pressure reduces CH_4 conversion and SN, but its effect becomes smaller at high reformer temperature.
- Increasing H_2O/CH_4 can improve SN, but CO_2-rich feeds may still require H_2 addition or CO_2 removal to reach the target.
- A crossover occurs near CH_4/CO_2 ≈ 3.21 for given reformer parameters, where the reformer outlet meets the target SN without any stoichiometric correction.
- Maintaining SN close to 2.01 supports high and efficient methanol production.

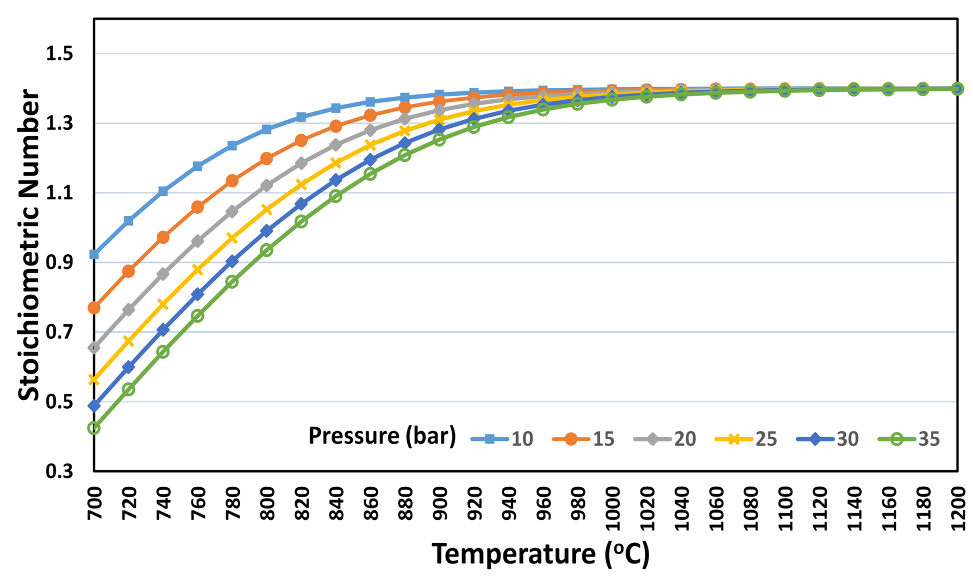
PROCESS FLOWSHEET



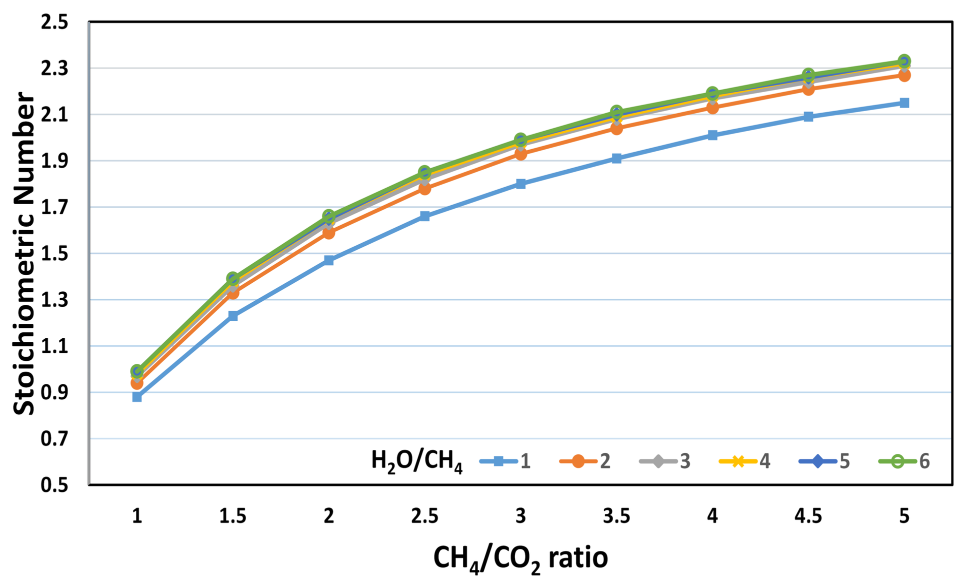
RESULTS



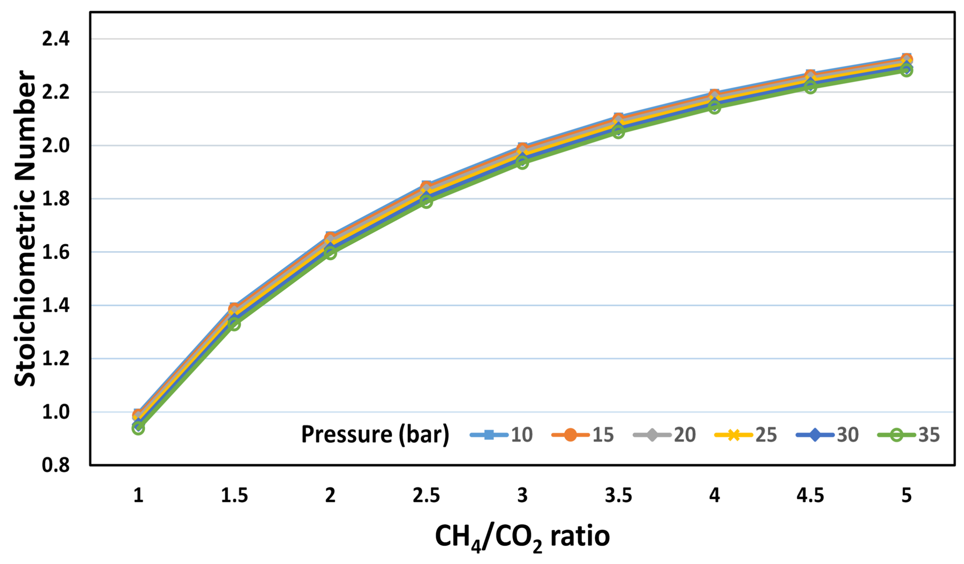
CH_4 conversion vs. temperature at different reformer pressures (CH_4/CO_2 = 1.5, H_2O/CH_4 = 3).



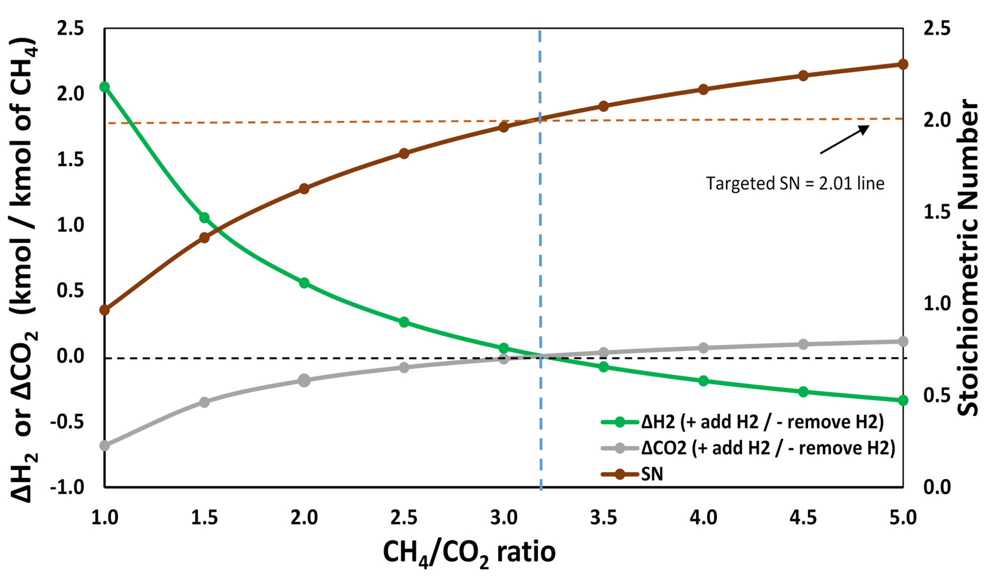
Reformer-outlet SN vs. temperature at different reformer pressures (CH_4/CO_2 = 1.5, H_2O/CH_4 = 3).



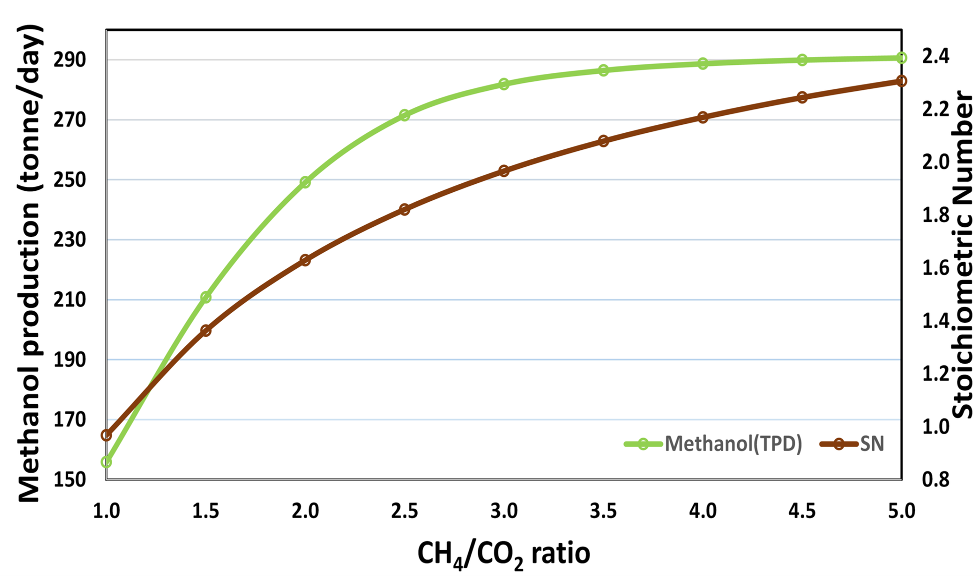
SN vs. CH_4/CO_2 ratio for different H_2O/CH_4 ratios (950 °C, 25 bar).



SN vs. CH_4/CO_2 ratio for different reformer pressures (950 °C, H_2O/CH_4 = 3).



H_2 and CO_2 adjustment required to reach SN = 2.01 (950 °C, 25 bar, H_2O/CH_4 = 3).



Methanol production rate and SN vs. CH_4/CO_2 ratio (950 °C, 25 bar, H_2O/CH_4 = 3).

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Contact:
muhammad.zulkefal@ntnu.no