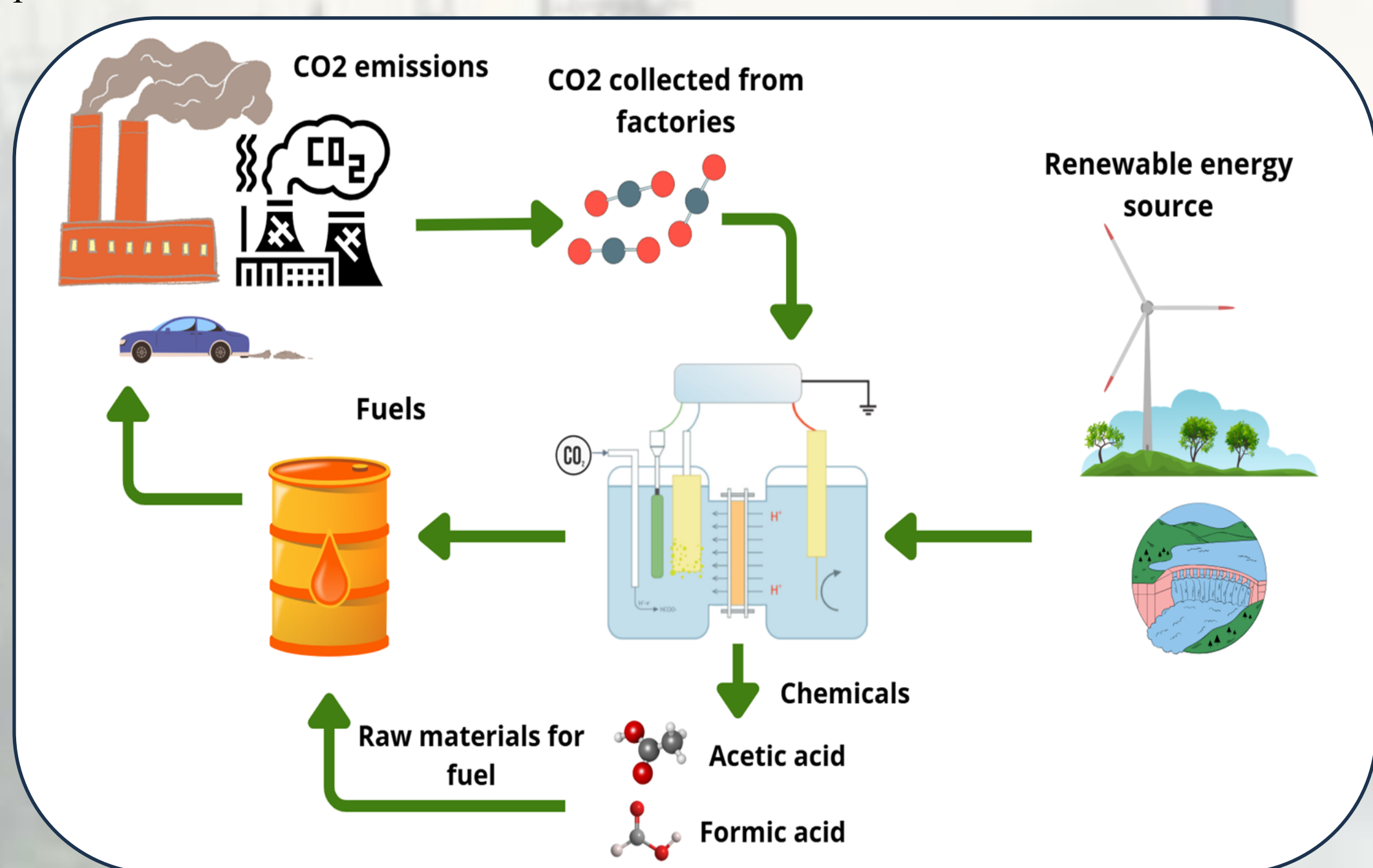


Electrochemical Synthesis of Ortho- and Para-Hydroxybenzoic Acids Using CO₂: Experimental and Simulation-Based OptimizationRuzimurod Jurayev^{a,*}, Bekzod Eshkulov^b^aDepartment of “Chemical Engineering and Quality Management”, Karshi State Technical University Shahrizabz Faculty of Food Engineering, 20, Shakhrisabz str., Shakhrisabz 181306, Uzbekistan; jurayevorganikqdu-1992@mail.ru (J.R.);^bStudent of “Chemical technology”, Karshi State Technical University Shahrizabz Faculty of Food Engineering, 20, Shakhrisabz str., Shakhrisabz 181306, Uzbekistan; bekzodeshqulov49@gmail.com (E.B.);*Correspondence: jurayevorganikqdu-1992@mail.ru

INTRODUCTION & AIM

In industrial organic synthesis, the Kolbe-Schmitt reaction is essential because it yields aromatic hydroxybenzoic acids employed in fine chemicals, dyes, and medications. Under some circumstances, it involves alkali metal phenoxides and CO₂, and its mechanism is attracting much study interest for optimization. The reaction emphasizes the dual advantage of using CO₂ as a feedstock and producing valuable products, promoting carbon neutrality as sustainability becomes a priority. Developments in computational chemistry, including molecular dynamics and density functional theory, have improved knowledge of its kinetics and mechanism, opening the door to creative process enhancements



METHOD

The optimization of the electrochemical synthesis of ortho- and para-hydroxybenzoic acids in the presence of CO₂ is achieved through a combination of experimental studies and process simulation. The goal is to minimize energy consumption and byproduct formation while maximizing the yield and selectivity of the desired products. The approach includes an experimental setup for electrochemical synthesis, modeling and optimizing reaction conditions using Aspen Plus, and validating and refining the process by integrating experimental data with simulation results.

Parameter	Ortho-HBA Yield (%)	Para-HBA Yield (%)	Selectivity (%)
-1.0 V, 1 atm CO ₂ , 25°C	Not specified	Not specified	Not specified
-1.2 V, 1 atm CO ₂ , 25°C	52.3	35.4	Not specified
-1.5 V, 1 atm CO ₂ , 25°C	Not specified	Not specified	Not specified
-1.2 V, 5 atm CO ₂ , 25°C	57.8	40.1	Not specified
-1.2 V, 3 atm CO ₂ , 50°C	60.2 (maximum)	42.3	102.5 (maximum)
-1.2 V, 3 atm CO ₂ , 25°C	55.6	38.2	Not specified

Yields of ortho-HBA and para-HBA under Various Conditions

(The highest yield of ortho-HBA (60.2%) and highest selectivity (102.5%) were achieved at -1.2 V, 3 atm CO₂, and 50°C.)

The Arrhenius equation was applied to anticipate the electrochemical production of ortho- and para-hydroxybenzoic acids.

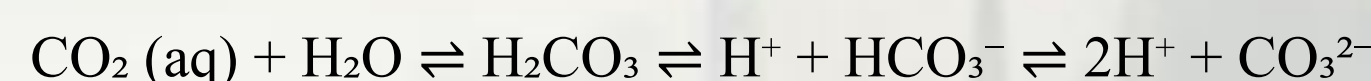
$$\text{Kinetic factor} = k \left(\frac{T}{T_0} \right)^{n*} e^{-\frac{E}{R} \left(\frac{1}{T} - \frac{1}{T_0} \right)}$$

where k is the pre-exponential factor, E is the activation energy, n is the temperature exponent, and T₀ is the reference temperature. The process flowsheet included an electrochemical reactor (RCSTR) to simulate the synthesis of ortho- and para-hydroxybenzoic acids, a neutralization reactor (RCSTR) to convert the products to their sodium salts using NaOH, and a flash separator to separate the products from unreacted reactants and by-products.

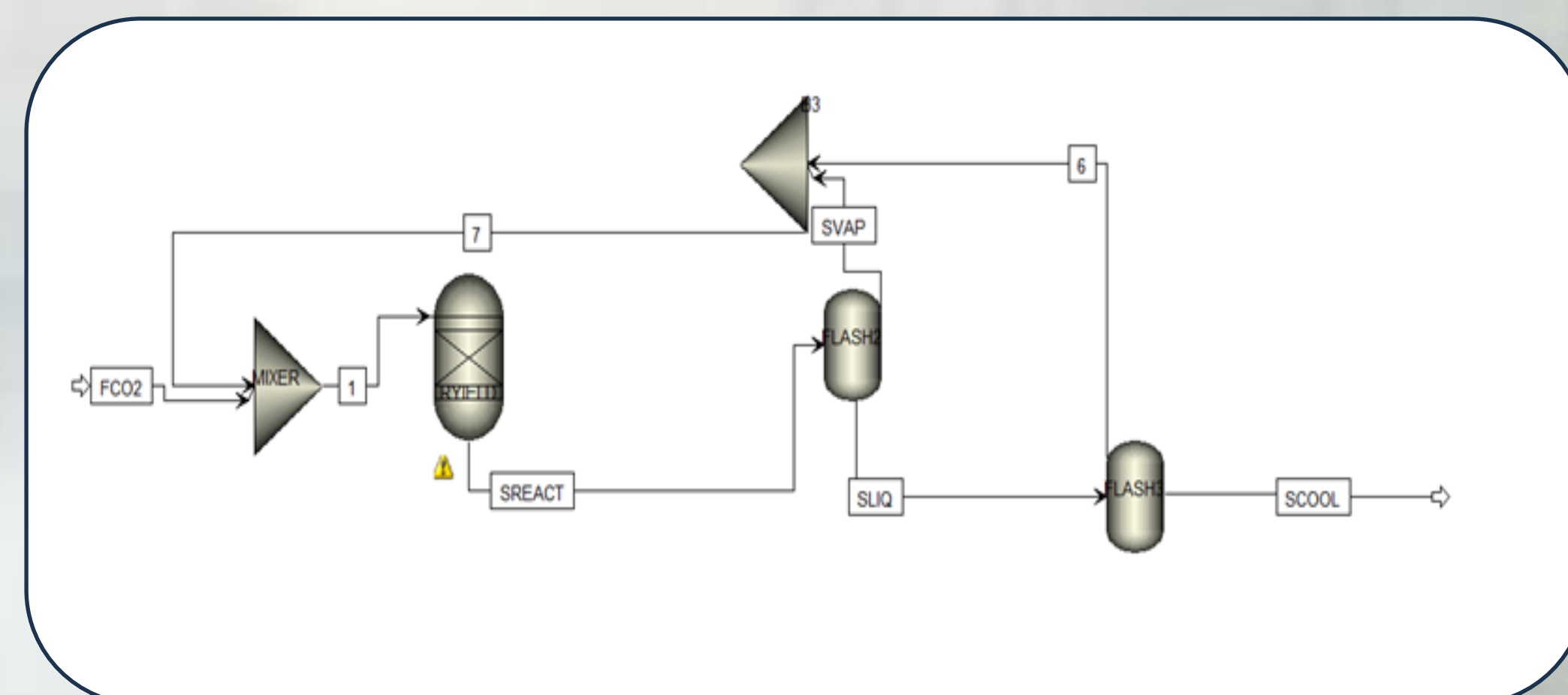
RESULTS & DISCUSSION

The electrochemical synthesis of ortho- and para-hydroxybenzoic acids (o-HBA and p-HBA) from carbon dioxide (CO₂) involves a combination of physical dissolution, ionic equilibrium, and electrochemical reduction pathways. In the simulated model constructed using Aspen Plus, the reaction network is implemented as a yield-based process under mild operating conditions: 25 °C, 1 bar, and an aqueous electrolyte medium. After generating the Stream Summary table, I first compared the CO₂ input flow in *FCO2* with the recycled CO₂ flow in *SVAP*. For example, the CO₂ flow in *FCO2* appeared as 1.000 kmol/hr, while in *SVAP* about 0.232 kmol/hr of CO₂ was recycled. Using these values, I calculated the CO₂ conversion according to the following formula:

$$\text{Conversion} = \frac{FCO2 - SVAP}{FCO2} = \frac{1 - 0.232}{1} = 0.768$$

Upon entering the aqueous phase, CO₂ participates in the following equilibria:

These equilibria are handled through the ELECNRTL thermodynamic property method in Aspen Plus, which accurately models ionic dissociation, ion-ion and ion-molecule interactions, and acid-base behavior in electrolyte systems.



Following the simulated reaction, a two-stage separation process is applied. The first flash (Flash2) separates unreacted CO₂ (SVAP stream) from the product mixture, enabling its reuse. The second flash (Flash3) cools the liquid to 5 °C to induce selective crystallization, exploiting the differing solubilities of o-HBA and p-HBA. This is modeled via the SSPLIT block, where 90% of o-HBA and 50% of p-HBA precipitate into the solid phase (SSOLID), with the remaining fractions retained in the mother liquor (SMOTHER).

By integrating the electrolyte model, component dissociation, yield-based reaction block, and recycle-enhanced conversion, the simulation provides a macro-scale representation of the electrochemical synthesis. These simulation insights correspond closely with experimental yields and validate the mechanistic feasibility of converting CO₂ into high-value hydroxybenzoic acids under sustainable conditions.

CONCLUSION

The electrochemical synthesis of ortho- and para-hydroxybenzoic acids (HBAs) from CO₂ was successfully optimized through an integrated approach combining laboratory experimentation and Aspen Plus process simulation. This study highlights how electrochemical synthesis, which uses CO₂ gas as a reactant to create useful compounds while lessening its impact on the environment, has the potential to be a green chemistry strategy. The results open the door for large-scale applications, supporting the circular carbon economy and the advancement of sustainable chemical processes. To further improve efficiency and economic feasibility, future research should concentrate on scaling the procedure, improving electrode materials, and investigating the integration of complementing technologies. All things considered, this effort is a big step toward more sustainable and environmentally friendly chemical manufacturing methods.

FUTURE WORK / REFERENCES

G.Sabia, ‘ASPEN dynamics simulation for combined cycle power plant – Validation with hot start-up measurement’,
R.S.Jurayev, ‘Effect and Spectroscopic Analysis of Solutions in Trychloratsetylpyrogallol Synthesis’.