DEEP PURIFICATION OF PYROLYSIS GAS STREAMS USING BAY ZEOLITE AND OPPORTUNITIES FOR PRODUCING ACTIVATED CARBON

Davlatova Odina
Namangan davlat texnika universiteti
Tel:+998950092324,
E-mail: DavlatovaO@mail.ru

Abstract. This study analyzed the interaction of BaY zeolite with water and xylenes based on adsorption isotherms, differential heats (Qd), and entropy (ΔS) parameters. The results show that water molecules strongly bind to the hydrophilic sites of the zeolite, releasing a high initial heat (Qd ≈ 88 kJ/mol), whereas xylenes are taken up stepwise on adsorption sites of different energetics. These features demonstrate the effectiveness of BaY in the efficient removal of water from pyrolysis streams and in the selective adsorption of aromatics. In addition, using a catalytic pyrolysis scheme based on Zeolite+$NiFe_2O_4$ composites increased the fractions of H_2 and CO in the gas stream, while the solid carbon residue was converted into activated carbon. This integrated approach not only improves energy efficiency but also enables the production of high-value feedstock for supercapacitor applications.

Keywords: BaY zeolite, adsorption isotherms, differential heat (Qd), entropy (ΔS), aromatic compounds (benzene, toluene, xylenes), pyrolysis streams, zeolite–$NiFe_2O_4$ composite catalyst, gas conditioning, SOFC (solid oxide fuel cell), activated carbon, energy efficiency, renewable fuel from biomass.

Annotatsiya. Ushbu tadqiqot adsorbsion izotermalar, differentsial isitgichlar (Qd) va entropiya (KSILENLAR) parametrlari asosida BaY zeolitining suv va ksilenlar bilan o'zaro ta'sirini tahlil qildi. Natijalar shuni ko'rsatadiki, suv molekulalari seolitning hidrofilik joylariga kuchli bog'lanib, yuqori boshlang'ich issiqlikni chiqaradi (QD va 88 kJ/mol), ksilenlar esa turli energetikaning adsorbsion joylarida bosqichma-bosqich olinadi.bstrakt.avhum. Ushbu tadqiqot adsorbsion izotermalar, differentsial isitgichlar (Qd) va entropiya (KSILENLAR) parametrlari asosida BaY zeolitining suv va ksilenlar bilan o'zaro ta'sirini tahlil qildi. Natijalar shuni ko'rsatadiki, suv molekulalari seolitning hidrofilik joylariga kuchli bog'lanib, yuqori boshlang'ich issiqlikni chiqaradi (QD va 88 kJ/mol), ksilenlar esa turli energetikaning adsorbsion joylarida bosqichma-bosqich olinadi.bstrakt. Ushbu tadqiqot adsorbsion izotermalar, differentsial isitgichlar (Qd) va entropiya (KSILENLAR) parametrlari asosida BaY zeolitining suv va ksilenlar bilan o'zaro ta'sirini tahlil qildi. Natijalar shuni ko'rsatadiki, suv molekulalari seolitning hidrofilik joylariga kuchli bog'lanib, yuqori boshlang'ich issiqlikni chiqaradi (QD

ISSN 3030-3907

va 88 kJ/mol), ksilenlar esa turli energetikaning adsorbsion joylarida bosqichma-bosqich olinadi. Ushbu xususiyatlar Bayning piroliz oqimlaridan suvni samarali olib tashlashda va aromatik moddalarning selektiv adsorbsiyasida samaradorligini namoyish etadi.atijalar shuni ko'rsatadiki, suv molekulalari seolitning hidrofilik joylariga kuchli bog'lanib, yuqori boshlang'ich issiqlikni chiqaradi (QD va 88 kJ/mol), ksilenlar esa turli energetikaning adsorbsion joylarida bosqichma-bosqich olinadi. Ushbu xususiyatlar Bayning piroliz oqimlaridan suvni samarali olib tashlashda va aromatik moddalarning selektiv adsorbsiyasida samaradorligini namoyish etadi. Bundan tashqari, zeolit+Nife$_2$oometrik kompozitlarga asoslangan katalitik piroliz sxemasidan foydalanib, gaz oqimida H_2 va CO fraktsiyalarini olib keldi, qattiq uglerod qoldig'i esa faollashtirilgan uglerodga aylantirildi. Ushbu kompleks yondashuv nafaqat energiya samaradorligini oshiradi, balki superkondensator ilovalari uchun yuqori qiymatli xomashyo ishlab chiqarishni ham dushman qiladi.

Kalit so'zlar: dafna seoliti, adsorbsion izotermalar, differensial issiqlik (QD), entropiya (KSILENLAR), aromatik birikmalar (benzol, toluol, ksilenlar), piroliz oqimlari, zeolit–Nife$_2$oexpress kompozit katalizatori, gazni konditsiyalash, SOFC (qattiq oksidli yonilg'i xujayrasi), faollashgan uglerod, energiya samaradorligi, biomassadan qayta tiklanadigan yoqilg'i.

Анотация. В этом исследовании анализировалось взаимодействие цеолита BaY с водой и ксилолами на основе изотопов адсорбции, дифференциальных теплот (Qd) и энтропийных параметров (ΔS). Результаты показывают, что молекулы воды прочно связываются с гидрофильными участками цеолита, выделяя высокую начальную теплоту (Qd ≈ 88 кДж/моль), в то время как ксилолы поглощаются поэтапно на участках адсорбции с различной энергетикой. В этом исследовании анализировалось взаимодействие цеолита BaY с водой и ксилолами на основе изотопов адсорбции, дифференциальных теплот (Qd) и энтропийных параметров (ΔS). Результаты показывают, что молекулы воды прочно связываются с гидрофильными участками цеолита, выделяя высокую начальную теплоту (Qd ≈ 88 кДж/моль), в то время как ксилолы постепенно поглощаются адсорбционными участками различной энергетики. Эти особенности демонстрируют эффективность BaY в эффективном удалении воды из потоков пиролиза и в селективной адсорбции ароматических соединений. Кроме того, при использовании схемы каталитического пиролиза на основе композитов цеолит+НИФЕ$_2$O$_4$ в газовом потоке были получены фракции H_2 и CO, в то время как твердый углеродный остаток был преобразован в активированный уголь. Такой комплексный

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подход не только повышает энергоэффективность, но и препятствует производству высококачественного сырья для суперконденсаторов.

Ключевые слова: цеолит BaY, изотопы адсорбции, дифференциальная теплоемкость (Qd), энтропия (ΔS), ароматические соединения (бензол, толуол, ксилолы), потоки пиролиза, композитный катализатор цеолит–нифенол, кондиционирование газа, ТОТЭ (твердооксидный топливный элемент), активированный уголь, энергоэффективность, возобновляемое топливо из биомассы.

I. Introduction

Improving energy efficiency and making rational use of renewable resources remains one of today's most urgent scientific and practical challenges. In many countries, converting agricultural and forestry residues—such as cotton stalks, sunflower husks, sawdust, and wheat straw—into energy has become a priority from both ecological and economic perspectives. Pyrolysis—thermochemical decomposition in an oxygen-free environment—is among the most promising routes and simultaneously yields three product streams: a gas, a liquid bio-oil fraction, and a solid carbon residue (char). However, the "raw" pyrolysis stream is not immediately suitable for direct use in energy devices: it typically contains excessive moisture, heavy high-molecular organic fractions ("tar"), aromatics, and even trace sulfur and halogens. This demands additional steps for cleaning, conditioning, and fine-tuning the composition before the streams can be fed into high-performance energy systems. In this context, selective sorbents and tailored catalysts—especially BaY zeolite and $NiFe_2O_4$ composites—can transform a basic pyrolysis line into a highly efficient, integrated energy platform.

The proposed concept unifies three consistent directions into a single technological chain. First, catalytic pyrolysis over a (Zeolite + $NiFe_2O_4$) composite is used to enrich the H_2/CO profile in the gas fraction, suppress the liquid fraction's tar and heavy aromatics via cracking–reforming, and increase the carbonization degree of the solid residue by carefully choosing process parameters (temperature, residence time, heating rate). Here, the active centers of the $NiFe_2O_4$ spinel promote dehydrogenation and partial steam/CO_2 reforming reactions, while the zeolite's strong acidity and ordered pore system provide synergy: tar molecules are trapped in micropores and cleaved into lighter fragments; aromatic rings are encouraged to convert into short-chain gaseous products. Second, the resulting gas stream is conditioned by mechanical and thermal means: aerosols are removed in cyclones, condensable droplets are knocked out in heat exchangers and condensers, and inertial/fibrous filters capture larger particulates. At this stage, the liquid bio-fraction is diverted either to fuel blends or to further chemical processing

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(hydrodeoxygenation, fractionation), while the solid char is collected separately for subsequent activation. Third, the gas undergoes final "polishing" on a BaY zeolite bed: the supercages and strongly localized Ba cations generate a high electrostatic field that deeply dehydrates the gas and selectively retains aromatic hydrocarbons, thereby preserving the gas's H_2/CO ratio while bringing impurity levels down to the specifications required by sensitive devices such as solid oxide fuel cells (SOFCs). BaY succeeds here because its faujasite-Y framework, large supercages, and Ba-cation adsorption sites create strong interactions with water (via solvation-like complexes) and with π-systems (via cation–π interactions).

Integration with an SOFC is the heart of this platform. The SOFC anode, typically a Ni–YSZ composite, is susceptible to poisoning by tars and heavy aromatics; excessive moisture can also perturb the anode's equilibrium reactions. Deep dehydration on BaY and selective removal of aromatics to trace levels are thus not merely "fine tuning," but key to long-term cell stability and to preventing coke formation on electrode surfaces. Within this chain, the $NiFe_2O_4$ composite's role upstream is equally important: it "lightens" the gas, reduces tar at its source, and adjusts the H_2 and CO content toward a favorable window. As a result, the excessive burden on internal reforming inside the SOFC is mitigated, the core components that set the Nernst potential are kept more stable, and the heat balance is more even at the cell/stack level.

The "second life" of the solid residue is a techno-economic amplifier of the platform. Pyrolysis char—a carbon-rich material—can be converted into high-surface-area activated carbon through physical activation with steam or CO_2, or through chemical activation using reagents such as KOH or H_3PO_4. The resulting micro/mesoporous architecture establishes efficient transit pathways for electrolyte ions, enabling high power density and good cycle stability in supercapacitor electrodes. Moreover, heat integration across the platform—the reuse of high-temperature heat from the pyrolyzer, condensers, and SOFC exhaust—reduces the energy demand of activation. In this way, a single line co-produces electricity (via the SOFC), heat (partly recycled within the process), and a valuable solid product—activated carbon—turning waste into a value chain and realizing the idea of "green carbon" in practice.

Such integration naturally demands balanced process engineering. For example, lower pyrolysis temperatures tend to increase the liquid fraction but also the tar content; raising the temperature increases the gas yield but reduces char output. The amount and dispersion of $NiFe_2O_4$, the zeolite type and acidity, particle size, and residence time—all strongly influence the product spectrum. In gas conditioning, pressure drops must be controlled; in the condensation stage, the heat

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"pinch point" must be chosen well; and for BaY the regeneration cycles must be planned (e.g., swing strategies, mild heating, or inert-gas purging) to enable continuous operation. On the SOFC side, the anode-gas temperature profile, fuel utilization, steam/hydrocarbon equilibria at the anode, and oxygen supply at the cathode are jointly tuned; the BaY stage functions as an external "buffer," delivering a steady, clean, and compositionally stable fuel gas to the cell.

There are, of course, challenges and risks. Variable, small-scale feedstock (moisture, ash content, alkalis, and chlorides) can affect the lifetimes of both catalyst and zeolite; even trace sulfur species may poison Ni centers; BaY's structural stability must be verified under long-term humid conditions. But there are robust technological responses: pre-drying and partial ash washing; sulfur capture via dedicated sorbents; strengthening the zeolite matrix through controlled crystal growth and post-synthetic modification; doping the catalyst (e.g., with Cu or Co); and deploying monoliths and lightweight foams to reduce pressure drop. Deeper heat integration—reusing the SOFC's high-grade exhaust heat for pre-heating in pyrolysis or for BaY regeneration—lowers overall exergy losses.

A major strength of this platform is its modularity and contextual adaptability. It can be deployed in small-scale units (for rural districts or satellite industrial sites) and mid-scale clusters (for centralized hubs). Proximity to feedstock reduces logistics costs, while on-site heat reuse boosts overall efficiency. In Uzbekistan, residues from cotton processing, horticulture and wood industries, and food-processing organics offer a natural feedstock base for such a platform. Instead of open-air burning or landfilling, the waste is converted into electricity, heat, and a high-value solid—activated carbon. Domestic demand for supercapacitor materials, filtration media, and electrochemical devices can be met locally.

Future research will deepen along several lines: controlling the nano-architecture of $NiFe_2O_4$ composites; exploring hybrid micro–mesoporous zeolite variants; optimizing mass and heat transfer in monolithic and 3D-printed structures; fine-tuning the thermal profile via microwave or plasma pyrolysis; and digitizing the entire chain with smart sensors and machine-learning-based control. In particular, real-time GC or NDIR sensors, online dew-point monitoring, and indicators for adsorbent bed "breathing" (breakthrough) can feed data into predictive control to raise reliability. At the same time, the electrochemical properties of char-derived activated carbon—surface chemistry, ion-transport pathways, and the electrode–electrolyte interface—unlock significant value in hybrid energy systems (for example, supercapacitor banks that shave short peak loads) operating alongside the SOFC.

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By combining catalytic pyrolysis on (Zeolite + $NiFe_2O_4$), adsorptive polishing on BaY, and SOFC conversion, this platform tailors "raw" pyrolysis streams to the needs of energy devices: moisture and heavy organics are deeply reduced, aromatics are selectively removed, and the H_2/CO profile is preserved. The result is a single chain that reliably produces electrical power, recycles process heat internally, and converts the solid residue into high-value activated carbon. This solution is not only technologically coherent but also economically and environmentally beneficial, opening new horizons for transforming agricultural and forestry residues into high-value products. In the energy transition, it offers a practical way to turn waste from a liability into an opportunity.

II.Experimental Methods

The study was conducted in five main stages:

1) Synthesis and modification of BaY zeolite: BaY was prepared by ion exchange in $Ba(NO_3)_2$ solutions, followed by calcination at 550 °C to ensure structural stability. Next, a bimetallic composite catalyst (Zeolite + $NiFe_2O_4$) was prepared by binding metal oxide particles to the zeolite matrix.

2) Structural and property analysis. The structure and phase composition of the prepared zeolite and composite catalyst were examined by the following spectroscopic methods:

XRD (X-ray diffraction): crystal structure and phase purity;

FTIR (infrared spectroscopy): functional groups in the zeolite matrix and signatures of ion exchange;

SEM/TEM (scanning/transmission electron microscopy): particle morphology, size, and distribution;

BET: surface area and porosity;

TPR/TGA: thermal stability and redox behavior of the catalyst; adsorption calorimetry under high vacuum: adsorption characteristics of BaY.

3)Adsorbent design and purification of pyrolysis streams: an adsorber-column concept was developed to selectively separate moisture (H_2O vapor) and aromatic fractions using BaY zeolite; isotherm ($a = f(P/P_0, T)$), differential heat (Qd), entropy (ΔSd), and equilibration time $\tau(a)$ were used as design inputs; equilibrium models (TOZM) and saturation equations were used in calculations.

4)Catalytic pyrolysis and gasification scheme: a technological roadmap was developed to obtain electric power in an SOFC and, by selective removal of high-molecular-weight organics, to obtain activated carbon via catalytic pyrolysis over Zeolite/$NiFe_2O_4$; sizing considered reactor volume, residence time, temperature ranges, and catalyst loading; laboratory tests were used to determine

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H_2, CO, and CH_4 fractions in the product gas and to assess its suitability for SOFC operation.

5)Experimental verification of adsorption properties: adsorption isotherms of water and xylenes on BaY were measured; differential heats (Qd) and entropies (ΔSd) were determined to evaluate selectivity and stability; these results were used to demonstrate the applicability of BaY to biofuel purification.

3. Process Schemes

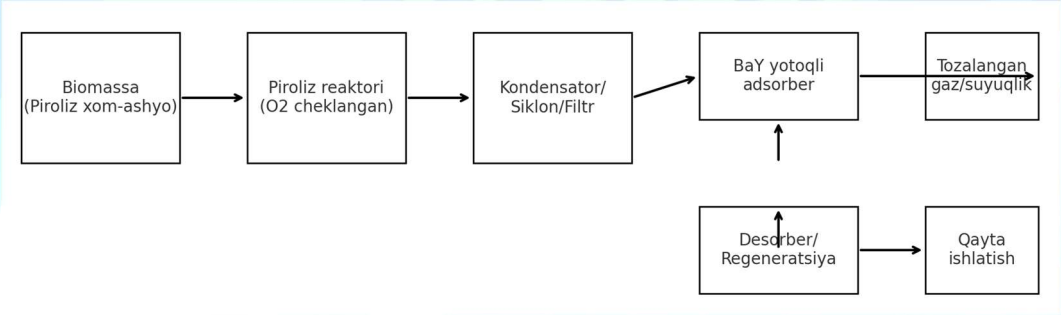


Figure 1. Process scheme for cleaning pyrolysis streams using BaY zeolite.

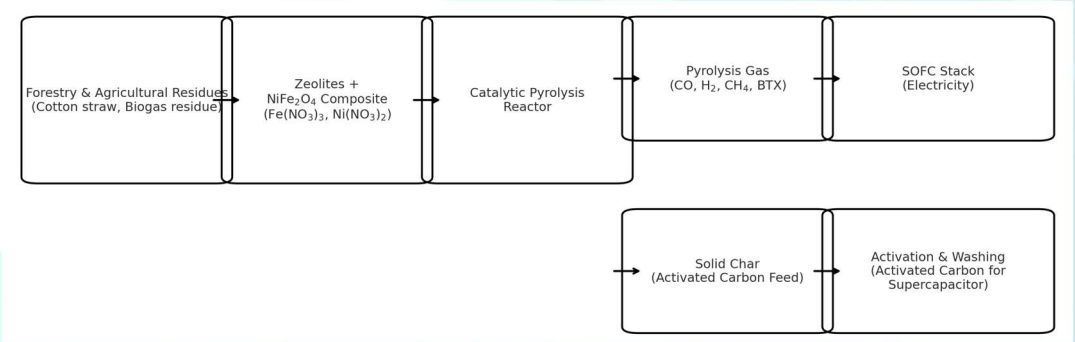


Figure 2. Process scheme for the Biomass → Zeolite/$NiFe_2O_4$ catalytic pyrolysis → SOFC and activated carbon pathway.

Adsorption on BaY: Isotherm, Differential Heats, and Entropy

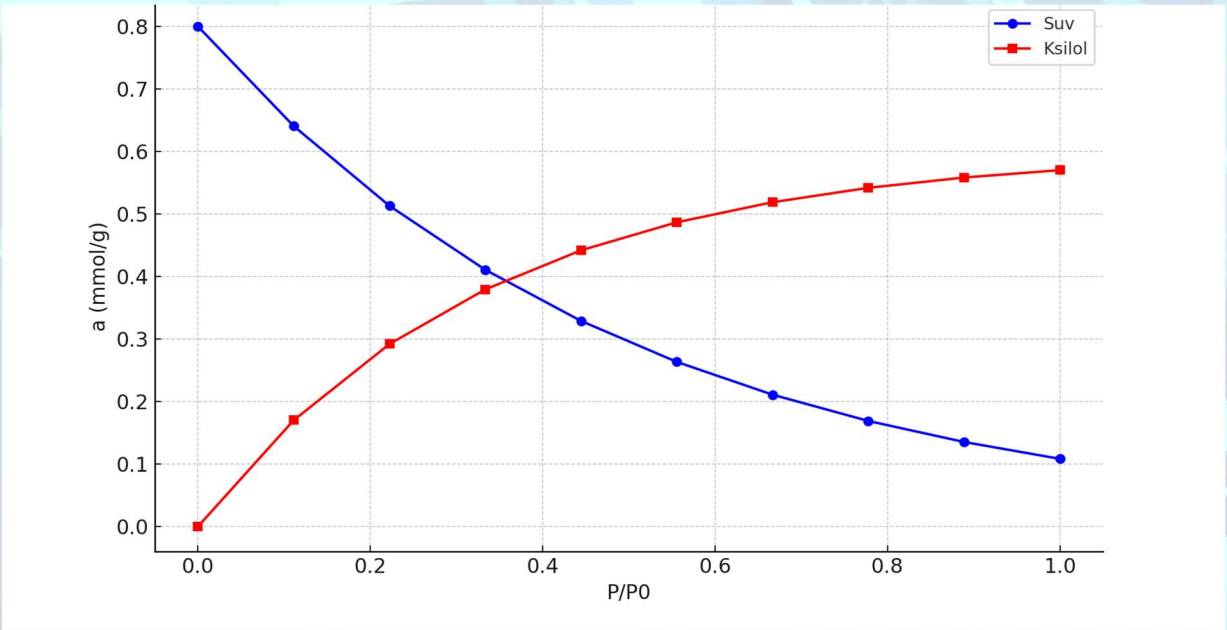


Figure 3. Adsorption isotherms of water and xylenes on BaY.

ISSN 3030-3907

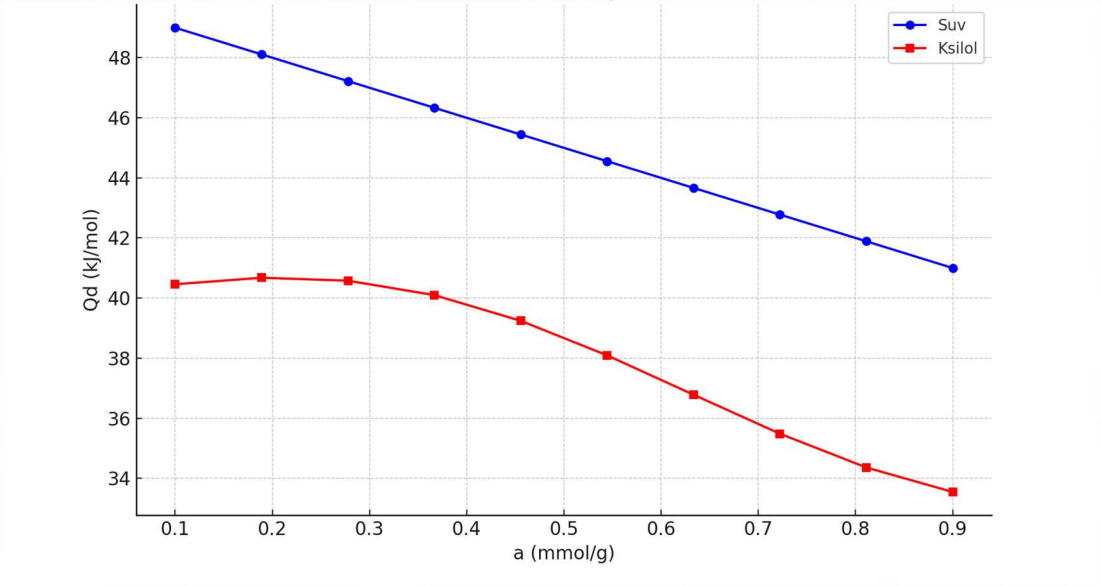


Figure 4. Comparison of differential heats of adsorption for water and xylenes.

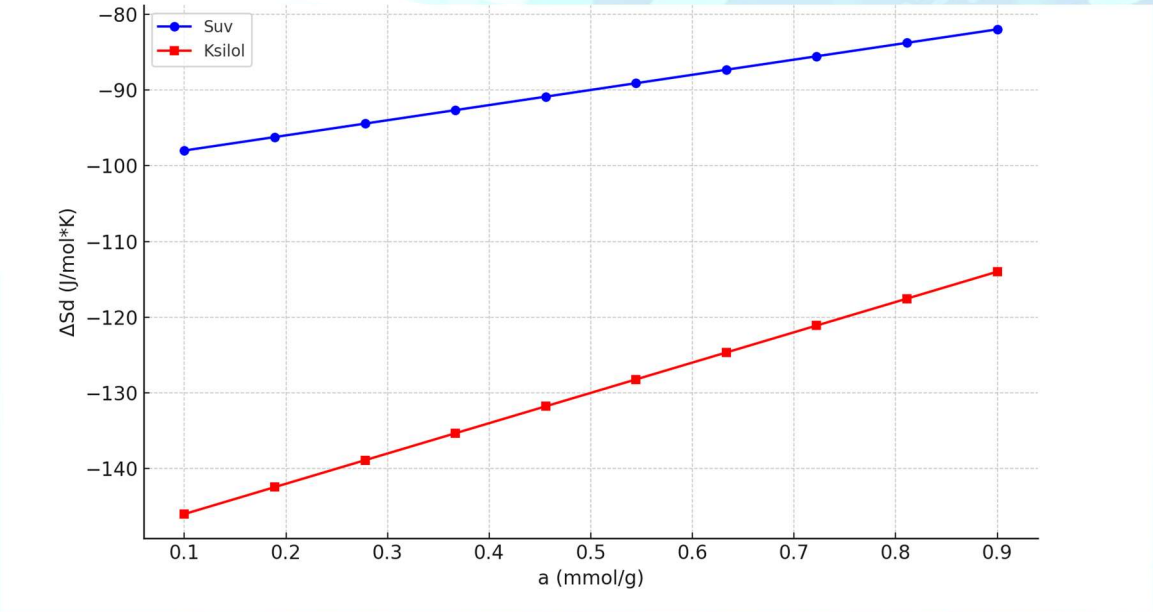


Figure 5. Differential entropy of adsorption for water and xylenes.

IV.Discussion

Large-scale studies in recent years on energy recovery from solid biomass residues regard the efficient organization of pyrolysis and the conditioning of the resulting gas stream for fuel-cell operation as priority tasks. Work with HZSM-5 and Y-type zeolites has achieved high performance in reducing tar and heavy aromatics and in optimizing the H_2/CO ratio. There is also international experience in combining Ni-based catalysts with pyrolysis and gasification to produce gas mixtures suitable for SOFCs. However, gas conditioning has not been fully resolved in many studies. Incomplete removal of condensable heavy organics and aromatic fractions causes electrode carbonization in SOFCs and other catalytic

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systems, reduces stability, and leads to long-term operational issues. Deep removal of water vapor has also been overlooked in many cases.

The present results indicate that BaY zeolite offers significant potential for deep drying of pyrolysis streams and selective uptake of aromatic fractions. BaY's strong hydrophilicity and π-electron interactions with aromatics provide an advantage in preparing SOFC-grade gas. Additionally, the Zeolite–$NiFe_2O_4$ composite catalyst increases the fractions of H_2 and CO during pyrolysis, and the solid char can be converted into activated carbon, adding economic value.

V.Conclusion

The interaction between BaY zeolite and polar/non-polar sorbates embodies the core of why this material is such a powerful "finishing" adsorbent for biomass-derived gas streams. In the presence of water, BaY presents strongly hydrophilic, high-field sites—Ba^{2+} cations localized within the faujasite-Y supercages—where water molecules anchor through intense ion–dipole interactions and cooperative hydrogen bonding within the confined pore network. This manifests as a large initial differential heat of adsorption (Qd ≈ 88 kJ/mol), a signature of high-affinity uptake at low surface coverage. As loading increases, the differential heat typically declines toward a plateau, reflecting progressive filling of weaker sites and the onset of lateral interactions among adsorbates. By contrast, xylenes (o-, m-, and p-isomers) engage BaY via π-complexation (cation–π interactions) and dispersive forces in the supercages, but their adsorption proceeds in a stepwise fashion across sites of different energetics and steric accessibility. This "tiered" uptake reveals both site heterogeneity (e.g., SII/SIII cation locations) and molecular-shape effects at 12-ring windows connecting sodalite cages and supercages, which is why isomer selectivity can emerge under suitable conditions.

These thermodynamic fingerprints directly translate into process utility. In mixed "raw" pyrolysis streams, water competes strongly for the highest-energy sites and is therefore removed first and most deeply—precisely what is required upstream of sensitive energy-conversion devices. Once the gas is dehydrated, the same BaY bed can continue to "polish" the stream by selectively capturing aromatic hydrocarbons, including xylenes that otherwise promote coke formation and electrode poisoning. The result is a gas whose impurities are driven to trace levels while the desired H_2/CO profile is preserved, enabling reliable downstream operation (for example, in solid oxide fuel cells).

Raising the quality of the incoming gas in the first place further reduces the burden on the polishing step. A catalytic pyrolysis scheme based on Zeolite+$NiFe_2O_4$ composites does exactly that. The spinel $NiFe_2O_4$ phase provides redox-active sites that favor dehydrogenation and tar cracking, while the acidic,

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shape-selective zeolite scaffolds trap and fragment heavy organics within their pore network. This synergy suppresses high-molecular-weight "tar," nudges equilibria toward lighter gases, and increases the share of H_2 and CO in the product. Because the gas leaves the reactor "lighter," the subsequent separations (cyclones, condensers, filters) become simpler and less energy-intensive, and the BaY adsorber can focus on deep dehydration and selective aromatic removal rather than bulk cleanup.

Importantly, the solid carbon residue from pyrolysis is not waste but a feedstock for value creation. With either physical activation (steam or CO_2) or chemical activation (e.g., KOH, H_3PO_4), the char can be transformed into activated carbon featuring a tailored micro/mesoporous architecture. Such carbons are well-suited for supercapacitor electrodes, where high accessible surface area, short ion-transport paths, and robust cyclability are prized. Integrating this valorization step with heat recovery from the pyrolysis/conditioning train improves overall exergy efficiency and strengthens the project economics by co-producing an electrochemically valuable solid alongside a cleaned synthesis-gas-like fuel.

Designing the BaY-based adsorber hinges on a consistent thermodynamic and kinetic description of uptake. In your approach, equilibrium isotherms are represented by the TOZM model, which captures site heterogeneity and temperature effects; the temperature dependence of affinity is resolved through differential heat and entropy data, while the equilibration time $\tau(a)$ encodes the dominant mass-transfer resistances. Practically, these ingredients combine as follows:

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ISSN 3030-3907