Mineral-Controlled Vapor Quality and Feedstock Operating Window for HZSM-5 Aromatization of Oil-Shale Pyrolysis Vapors

Mengliyev Sh. Sh.
Gulomov Sh. T.
Khabipov R. S.
Tashkent Institute of Chemical Technology
Khabipovruslan@gmail.com

Background and Rationale

The catalytic response of HZSM-5 during oil-shale conversion is governed not only by catalyst acidity and pore architecture but also by the composition of the vapor stream generated upstream. Minerals can modify heat transfer, primary decomposition, secondary cracking, adsorption of intermediates, and the partitioning of sulfur- and nitrogen-containing species. Consequently, two shale batches with similar total organic carbon can produce vapors with different catalytic suitability. For metalliferous shales from Uzbekistan, a practical feedstock qualification criterion is therefore needed before catalyst optimization. The central question is not simply how much oil a shale yields, but whether its organo-mineral matrix generates a vapor composition that lies inside a reproducible operating window for HZSM-5 aromatization.

Keywords

oil shale; HZSM-5; pyrolysis vapors; mineral matrix; feedstock operating window; aromatization.

Objective and Experimental Basis

The objective is to establish the relationship 'organo-mineral composition → thermolysis behavior → primary vapor quality → expected catalytic suitability'. At least three independent feedstock batches from one deposit are characterized by XRD, XRF, CHNS/O, TOC/TIC, moisture, and ash content. TGA-DSC is performed at 5, 10, 20,

and 30 °C min-1, while TG-FTIR tracks the temperature-resolved evolution of CO2, CO, hydrocarbon groups, and heteroatom-containing vapors. Bench reactor pyrolysis is used for material-balance closure and chromatographic characterization of condensable and gaseous products.

All batches are prepared under the same particle-size and drying protocol. Reactor experiments are normalized to dry feed mass and fixed thermal history. Material-balance closure of 95-105% is used as a minimum quality criterion before a batch is included in the feedstock-to-vapor model.

Methodological Principle

An apparent activation energy obtained from thermoanalysis is not interpreted directly as technological efficiency. Isoconversional analysis is used to identify transformation windows, whereas reactor measurements establish the actual vapor distribution under defined conditions. Mineral descriptors are interpreted together with TOC and vapor evolution rather than as isolated predictors.

A feedstock operating window is proposed instead of a universal 'best shale' ranking. The window is defined by a combination of carbon potential, carbonate-to-silicate balance, temperature of hydrocarbon-vapor release, heteroatom-vapor burden, and material-balance closure. Batches inside the window are considered suitable for subsequent HZSM-5 contact tests under a common catalytic protocol.

Proposed Scientific Contribution 1

The first contribution is a vapor-quality descriptor that couples feedstock composition with the temperature-resolved formation of catalytically relevant vapors. This avoids ranking a shale by total oil yield alone. A batch with high organic content but excessive COx or heteroatom release may be less suitable for direct aromatization than a lower-yield batch with a more favorable hydrocarbon-vapor profile.

Proposed Scientific Contribution 2

The second contribution is an operating-window validation strategy. Two independent batches are used to establish the composition-to-vapor relationship, while a third batch is reserved for transferability testing. The reserved batch is not used to tune the descriptor. Agreement between predicted suitability and measured vapor composition provides a stronger basis for deciding whether the framework is transferable beyond one pooled sample.

Block	Key parameter	Method	Use in operating window
Organic matter	TOC, H/C, CHNS/O	TOC/TIC + elemental analysis	Carbon and hydrogen potential
Minerals	Carbonates, silicates, sulfides	XRD/XRF	Mineral-control descriptor
Kinetics	T peaks, E_a(α)	TGA-DSC	Thermolysis window
Vapors	HC groups, COx, S/N species	TG-FTIR + reactor GC	Catalytic feed quality

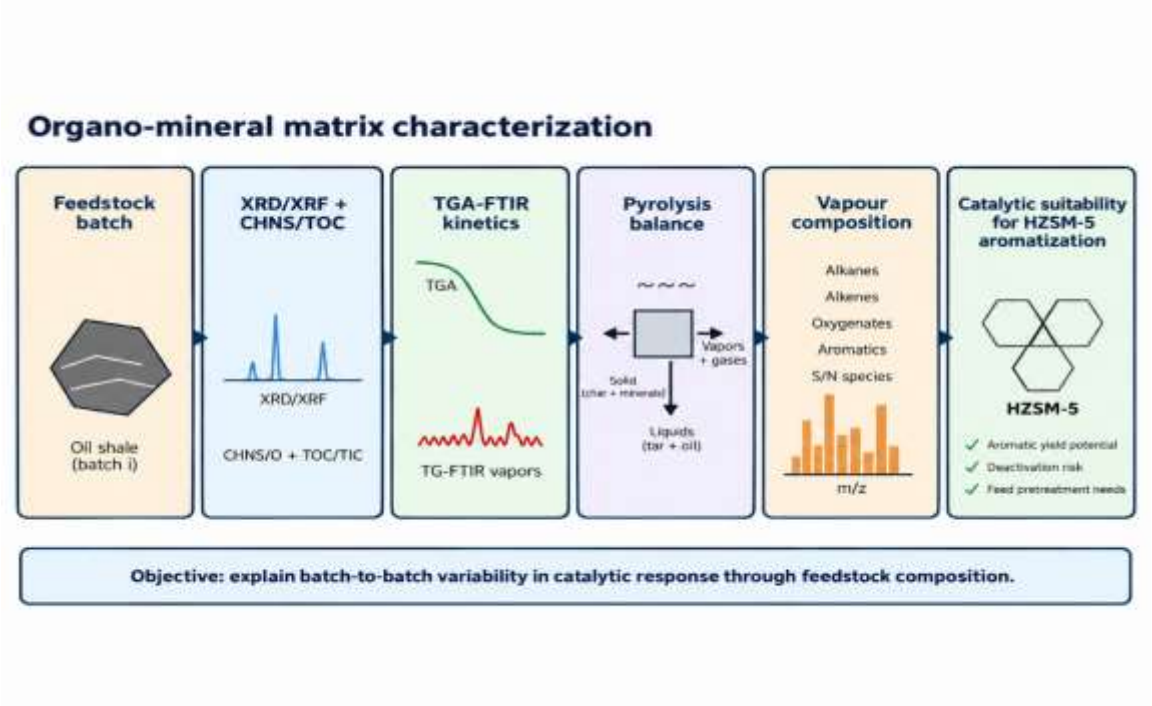


Figure 1. Feedstock-to-vapor workflow for defining a reproducible oil-shale operating window before HZSM-5 aromatization.

Expected Scientific Value

The expected value is a feedstock qualification step that precedes catalyst optimization. Instead of assigning one HZSM-5 condition to all shale batches, catalytic testing can be focused on batches whose measured vapor characteristics fall inside the defined operating window. This improves comparability between catalyst tests and reduces the risk of attributing feedstock variability to catalyst performance.

Conclusion

A reproducible oil-shale aromatization study should first qualify the primary vapor feed generated by the organo-mineral matrix. Combining independent feedstock batches, thermoanalytical kinetics, reactor material-balance closure, and vapor composition provides a causal route for defining a feedstock operating window and selecting appropriate HZSM-5 contact conditions.

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