

SUPPORTING INFORMATION

Continuous Age Distribution Method

for Catalytic Cracking

2. Understanding non-idealities

*David M. Stockwell**

BASF Corporation

25 Middlesex-Essex Turnpike

Iselin, NJ 08830, USA

david.stockwell@basf.com

+1-732-205-7035

S1 Methods

S1.1 Rate constants and activation energies

The equation 3 provided earlier¹ describes ideal first order decay for Si_T during hydrothermal treatment. Experimental values of first order Si_T decay rate constants, k_1 , can be found by solving that equation for k_1 , as seen below in eq S1, where Z_2 and Z_1 represent measures of the crystallinity of the Si_T portion of the zeolite at times t_2 and t_1 .

$$k_1 = \frac{-\ln(Z_2 / Z_1)}{(t_2 - t_1)} \quad (\text{S1})$$

In this work, Z_2 and Z_1 are calculated by multiplying the respective steamed zeolite micropore surface areas by $(192 - N_{Al})/192$, where N_{Al} is the number of framework aluminums per unit cell, as determined from the respective steamed unit cell size (UCS) and the Jorik correlation, eq S2.²

$$N_{Al} = 101.2*(a_o - 24.211) \quad (\text{S2})$$

Activation energies were determined from plots of $\ln(k_1)$ vs $1/T$, the classical Arrhenius method,³ where the slopes are interpreted as $-E_a/R$ and the intercepts are $\ln(k_o)$. Fittings of the kinetic models to experimental data were obtained by least squares optimization of the kinetic parameters, and in the case of the two zeolite model, also the mass fraction parameter.

S2 Results

S2.1 Effect of 0-5% front end on selectivity

The abscissa of Figure 10 in the main paper is now re-scaled to allow all of the cracking data for the 0-5% NPS catalyst to show in the plots.

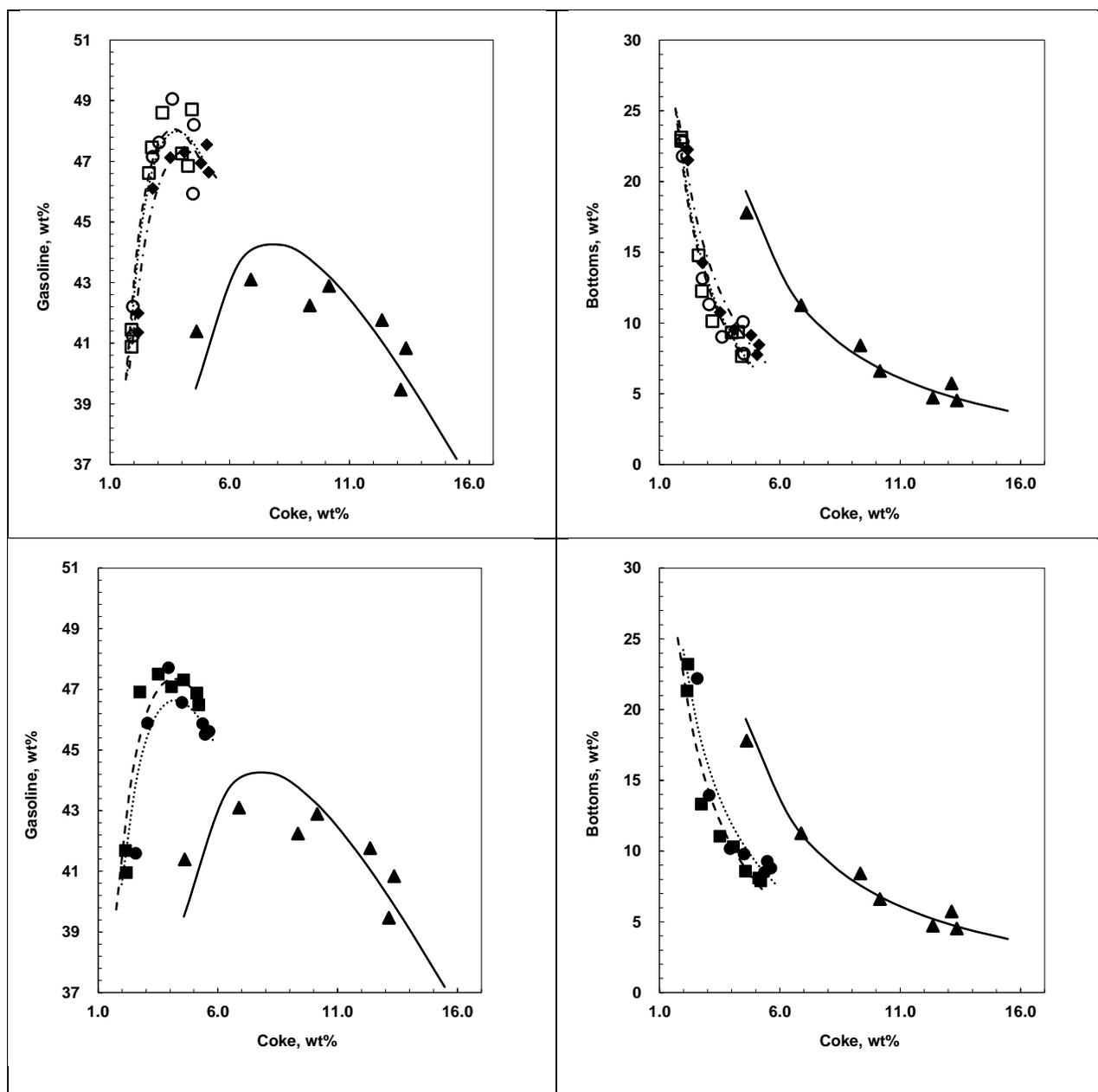


Figure S1. ACE gasoline and bottoms vs coke for cat. E CADM age fractions 0-100% (\circ , \bullet , \cdots), 5-100% (\square , \blacksquare , $-\ - -$) and 0-5% (\blacktriangle , $—$; 24.45 Å) with (open symbols) and without (full symbols) presteaming. Also shown: 0-5% NPS + 5-100% PS (\blacklozenge , $-\ - \cdot \cdot -$).

S3. References

- (1) Stockwell, D. M. Continuous Age Distribution Method for Catalytic Cracking 1 Proof of Principle. *Ind. Eng. Chem. Res.* **2015**, *54*, (22), 5921.
- (2) Jorik, V. Semiempirical Approach to Determination of Framework Aluminum Content in Faujasite-Type Zeolites by X-Ray-Powder Diffraction. *Zeolites*. **1993**, *13*, (3), 187.
- (3) Levenspiel, O. *Chemical Reaction Engineering*. Second ed.; Wiley: New York, 1972.