

Supplementary Materials - Unraveling the Capability of an Open-Source Process Simulator as a Deterrent to Cracked Commercial Simulators: “A Correlation Analysis of Their Predictions for Ethane Dehydrogenation”

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I. Results for the enthalpy & entropy balances across the reaction at 400 °C and 1 bar

II. Sensitivity of change in temperatures at low (0.5 bar) pressure

III. Sensitivity of change in temperatures at normal (1.0 bar) pressure

IV. Sensitivity of change in temperatures at high (10.0 bar) pressure

I. Results for the enthalpy & entropy balances across the reaction at 400 °C and 1 bar

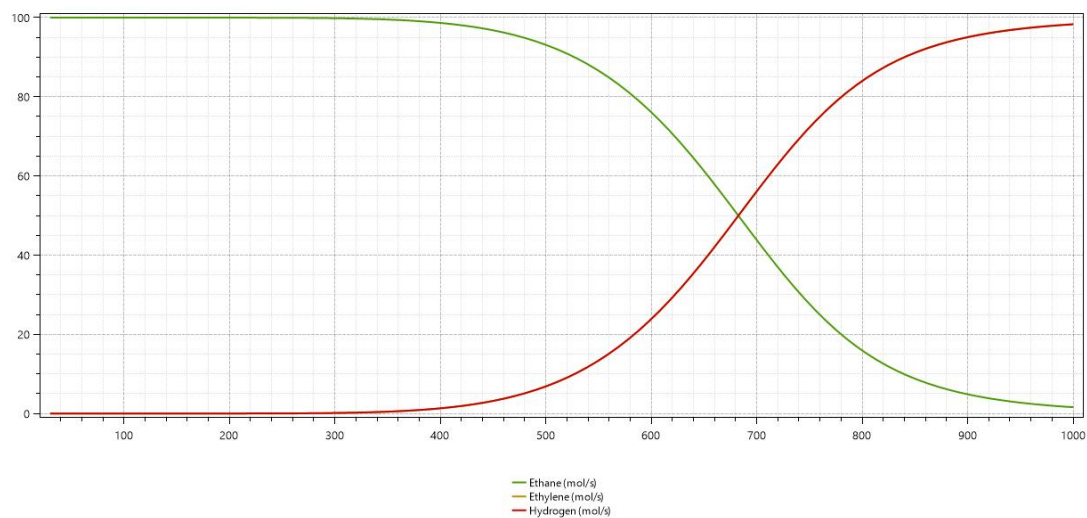
Table A1 – Plant enthalpy balances across the process simulators at 400°C

Stream Enthalpy, H	Symbol	Aspen HYSYS	DWSim	COCO	A/C	D/C	A/D
In/1 (kJ/mol)	Hf Hnf	-56.41 N/A	N/A 28.34	-55.48 28.34	1.0	1.0	-2.0
Out/9 (kJ/mol)	Hf Hnf	-54.66 N/A	N/A 28.12	-53.64 28.12	1.0	1.0	-1.9
Out-In (kJ/mol)	Hf Hnf	1.75 N/A	N/A -0.22	1.84 -0.21	1.0	1.0	-8.0

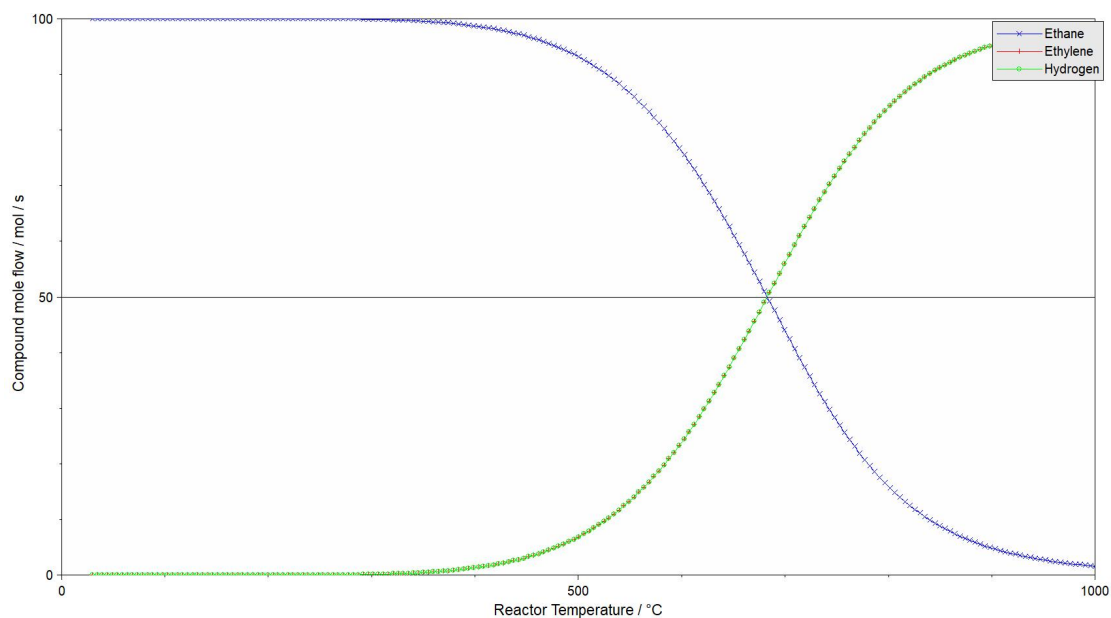
TableA2 – Plant entropy balances across the process simulators at 400°C

Stream Entropy, S	Symbol	Aspen HYSYS	DWSim	COCO	A/C	D/C	A/D
In/1 (J/mol/K)	Sf Sfn	254.49 N/A	N/A 59.24	288.37 59.25	0.9	1.0	4.3
Out/9 (J/mol/K)	Sf Sfn	254.11 N/A	N/A 64.75	287.79 59.69	0.9	1.1	3.9
Out-In (J/mol/K)	Sf Sfn	-0.39 N/A	N/A 5.51	-0.57 0.44	0.7	12.5	-0.1

II. Sensitivity of change in temperatures at low (0.5 bar) pressure



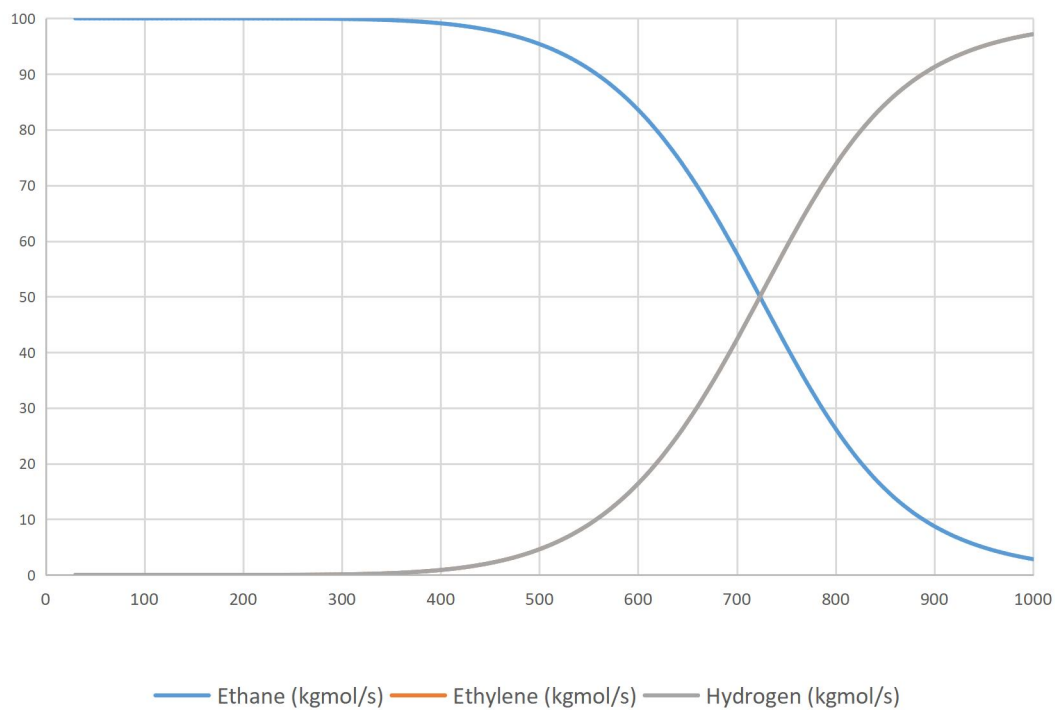
(a)



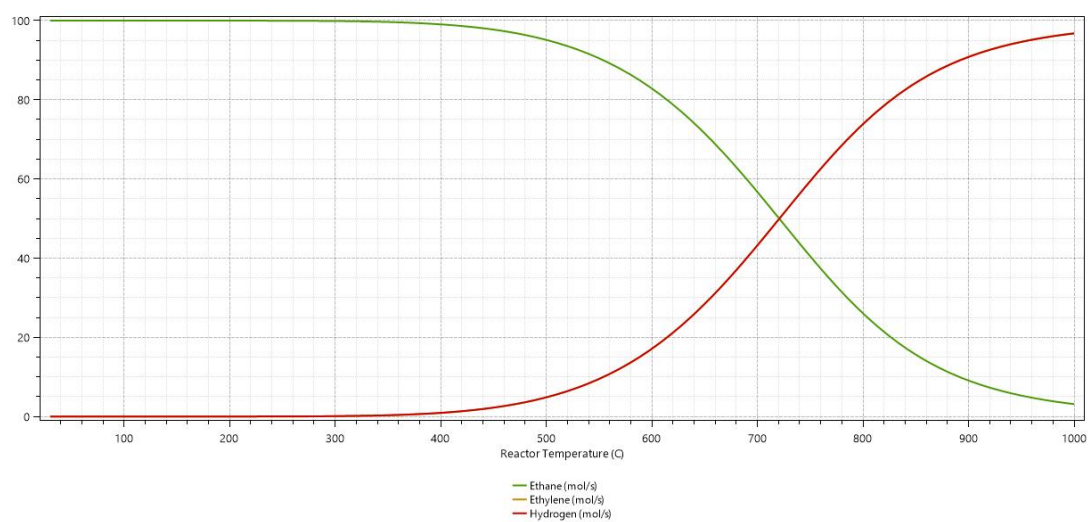
(b)

Fig. A1. Effect of temperature change at low pressure (0.5 bar) on ethane conversion and ethylene yield: (a) DWSim and (b) COCO process simulator.

III. Sensitivity of change in temperatures at normal (1.0 bar) pressure



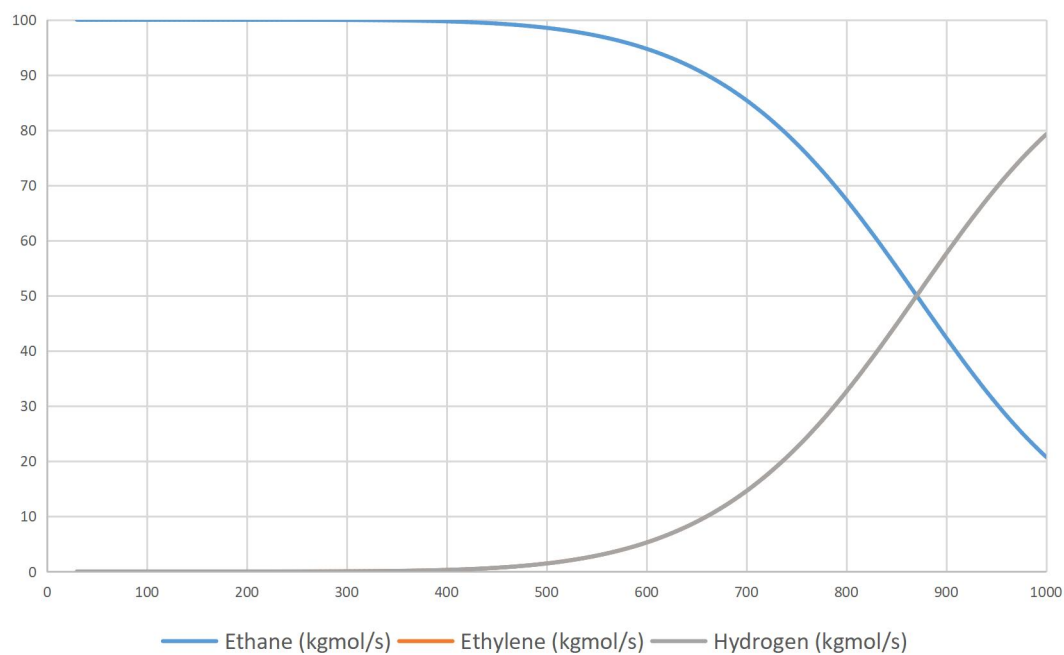
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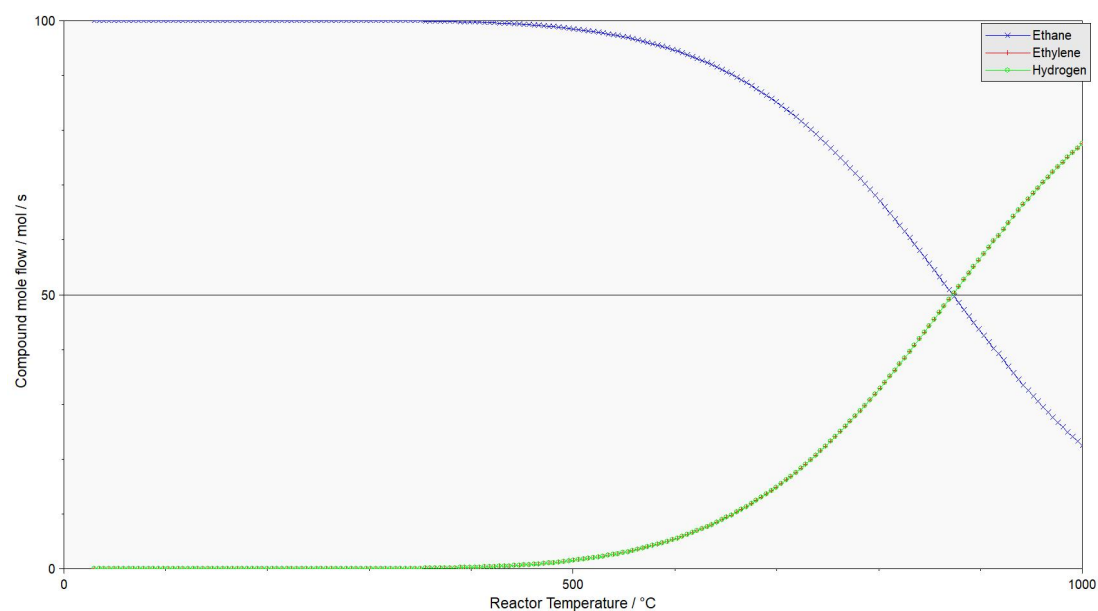
(b)

Fig. S2. Effect of temperature change at normal (1 bar) pressure on ethane conversion and ethylene yield: (a) Aspen HYSYS and (b) DWSim process simulator.

IV. Sensitivity of change in temperatures at high (10.0 bar) pressure



(a)



(b)

Fig. S3. Effect of temperature change at high pressure on ethane conversion and ethylene yield: (a) Aspen HYSYS and (b) COCO process simulator.