Simulation of a Steam Cracking Reactor with Ethane-propane Mixtures using COMSOL Multiphysics®

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INTRODUCTION: The Colombian Petroleum Company (ECOPETROL) needs to increase the production of ethylene and propylene from diverse feedstocks. Therefore, this simulation studied the pyrolysis of ethane-propane mixtures in an existing steam-cracking reactor (SCR) which was originally designed for ethane cracking.

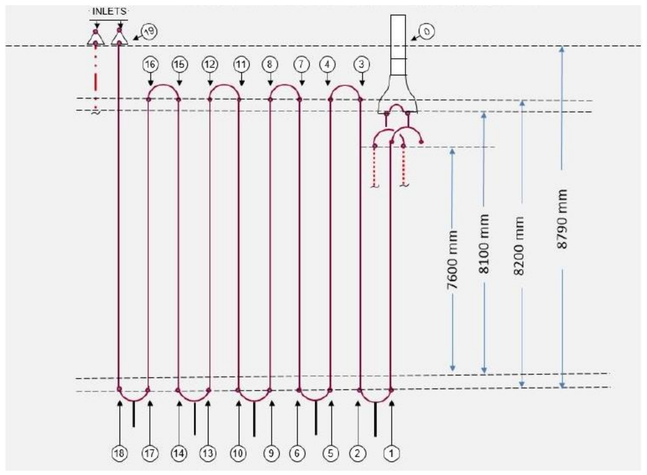


Figure 1. The SCR geometry

Parameter		Value	Unit
Flow		787.65	g/s
Steam/Fluid		0.4	kg/kg
Temperature in		913.2	K
Temperature out		1118.15	K
Average velocity outlet		206.65	m/s
Tube	Internal diameter	108	mm
	Length straight tube	8.2	m
	Total lenght	90.4	m

Table 1. Some SCR datasheet

COMPUTATIONAL METHODS: The radiant section of the SCR was simulated as a plug flow reactor. The coil geometry and its datasheet are shown in Figure 1 and Table 1. A 0D,1D and 2D models have been developed using COMSOL Multiphysics®. The Chemical Reaction Engineering module was used for the definition of chemical species and reaction kinetics. A modified molecular kinetic model proposed by Froment[1] was used. The thermodynamic properties were calculated using the TEA COCO simulator. For the 0D case, the following balance equations were set up:

Mass Balance

$$\frac{dF_i}{dV} = \sum_{j=1}^{NR} \gamma_{ij} r_j (V) \qquad c_i = \frac{P}{RT} \frac{F_i}{\sum_i F_i}$$

Energy Balance

$$\sum_i F_i C_{p,i} \frac{dT}{dV} = Q + Q_{ext} \qquad Q = -\sum_j H_j r_j$$

RESULTS: An example of an ethylene concentration profile for the 2D model is shown in Figure 2 for a 50/50w ethane-propane mixture. A validation of the models were carried out with results obtained by Froment[1] and Galán[3]. The absolute errors for these results were less than 4% for the reactions products.

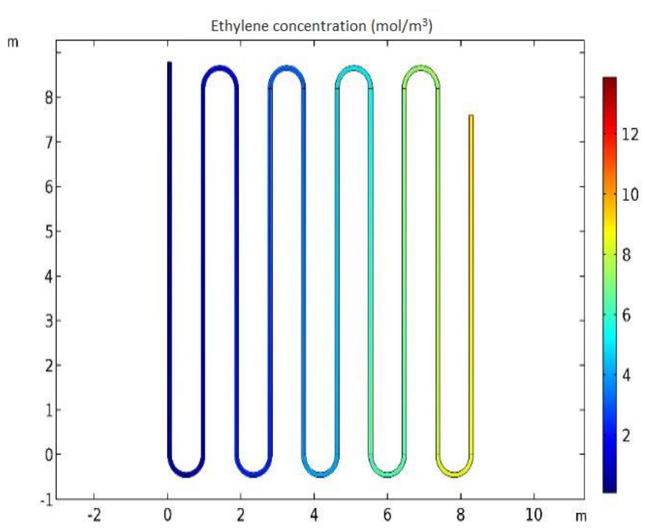


Figure 2. Ethylene concentration profile

Species	%w		
	0D COMSOL	1D Matlab	Froment
H_2	2.95	2.69	3.00
CH_4	13.61	13.75	12.00
C_2H_4	43.38	41.55	38.00
C_2H_6	18.42	21.85	26.00
C_3H_6	8.77	8.80	8.00

Table 2. Comparison of 0D COMSOL model with other models

For the 0D model, the model was investigated with a 0/100, 25/75, 50/50 75/25 and 100/0 mass relation of ethane/propane.

Figure 4 shows the concentration profiles for the main reactants and products at outlet temperature of 1110 K and a 50/50w ethane propane mixture. The ethane and propane conversions are 0.75 and 0.90. Ethylene yield is 0.58 (mol ethylene/ mol ethane + mole propane). Industrial data yield is 0.60.

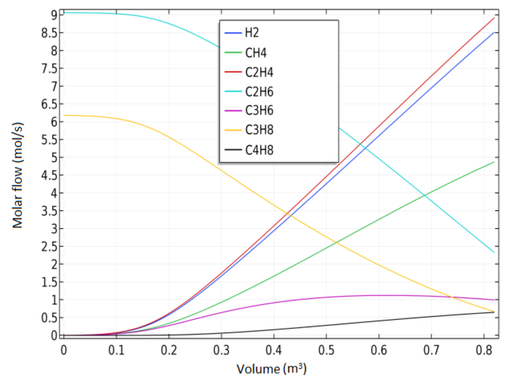


Figure 4. Concentration profiles at T = 1110K

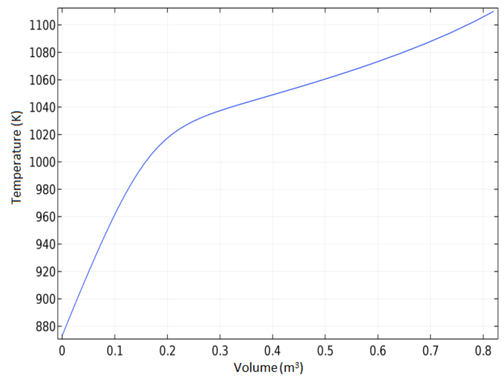
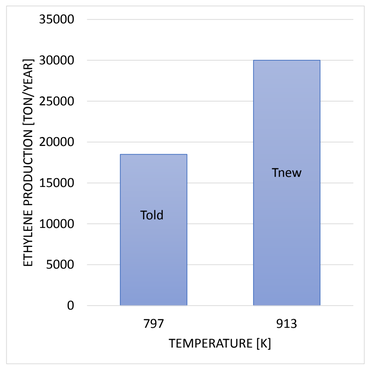


Figure 5. Temperature profile with a 50/50w ethane-propane mixture



The models revealed a potential increase in ethylene production when the old inlet temperature of 797 K is increased to a new temperature of 913 K.

Figure 6. Influence of inlet temperature on ethylene production

A fractional factor analysis was performed to study the selectivity to ethylene as a function of outlet temperature and mass fraction of propane. Results show that propane mass fraction do not overcome 0.4. Reaction temperature does not influence ethylene selectivity.

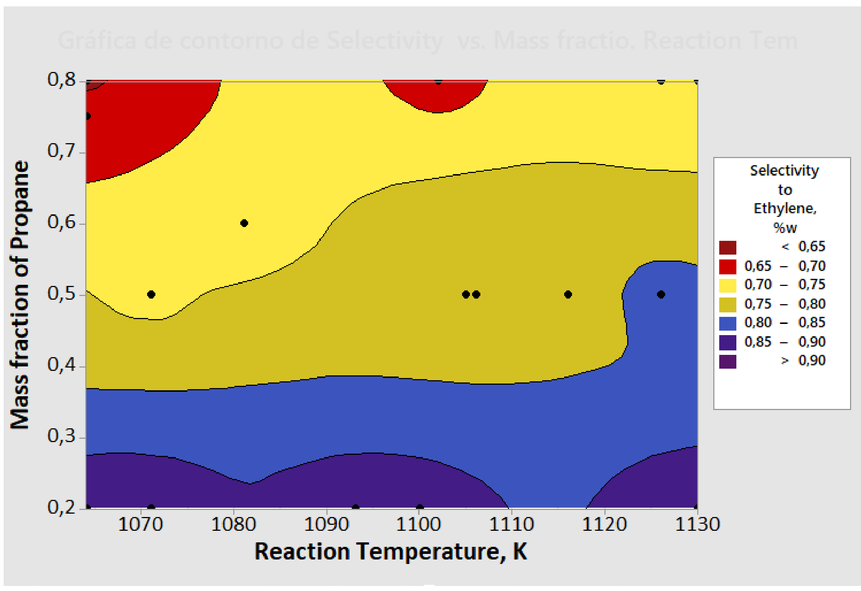


Figure 5. Respond surface for ethylene selectivity as a function of propane mass fraction and reaction temperature

CONCLUSIONS: The results of 0D COMSOL vs industrial data and other models show that absolute errors are less than 4%.
All models were used to detect operational conditions below optimal conditions.
Factor Analysis shows that the propane concentration at the feed has a strong influence on the ethylene selectivity.

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