Seventeen-lump model for the simulation of an industrial fluid catalytic cracking unit (FCCU)

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Abstract. A 17-lump kinetic model has been developed for the riser–reactor cum regenerator of a fluid catalytic cracking unit (FCCU). This accounts for cracking, hydrogen transfer, aromatization, isomerization, alkylation and dimerization, as well as catalyst deactivation due to the coke deposition in its pores. A model for the industrial combustor–regenerator unit is also developed. The lumping scheme includes the detailed characterization in terms of the paraffins, naphthenes and aromatics (PNAs) for the VGO feed and also the detailed compositions of the two important products: gasoline and LPG. A total of 199 kinetic parameters for the riser–reactor cum regenerator have been fitted (tuned) using 192 sets of plant data (under different operating conditions) from an industrial FCC unit. The tuned model of the integrated FCCU was run for 15 additional operating conditions. The match was found to be quite good.

Keywords. Fluidized bed catalytic cracking (FCC); genetic algorithm; modelling; simulation.

1. Introduction

The fluid catalytic cracking (FCC) process converts low-grade heavy oils into high-value products such as high-octane gasoline, diesel, LPG, propylene and alkylation feed (isobutene and butene). This process involves hundreds of hydrocarbons in the feed as well as the products and is associated with several reactions. Also, the hydrodynamic behaviour of the catalyst and the gaseous hydrocarbons in the riser–reactor poses challenges. Researchers have modelled the process by grouping/lumping the hydrocarbons using a limited number of reactions. Kinetic models have been developed using two [1], three [2], four [3], five [4–9], six and eight [10–17] kinetic lumps. Dasila *et al* [16, 18] have developed an artificial neural network model to characterize the FCC feed in terms of the paraffin, naphthene and aromatic (PNA) composition.

The present study presents a detailed kinetic model with feed and product characterization. This includes a 17-lump kinetic model with detailed naphtha and LPG compositions. Propylene is considered as a separate lump, it being a high-value product. The VGO feed to the fluid catalytic cracking unit (FCCU) was characterized in terms of three kinetic lumps as per the literature [16]. The main advantage of the

present model is the use of a detailed characterization of the products such as gasoline in terms of the PIONA analysis (paraffin, iso-paraffin, olefin, naphthene and aromatics) and detailed LPG compositions in terms of butane, butylene, propane and propylene.

In this study the riser–reactor and regenerator are modelled and the model equations integrated to simulate an industrial FCCU. The industrial regenerator comprises two parts: the lower part is a combustor and the upper part is the regenerator (see figure 1). The combustor is assumed to involve only a dense phase while the regenerator is assumed to involve both dense and dilute phases. The spent catalyst from the riser–reactor is received at the bottom of the combustor, where pre-heated air is supplied. There are two pipes from the regenerator to the combustor. They are used to recirculate the regenerated catalyst. The recirculation helps heat up the incoming spent catalyst. A slide valve is used to control the flow of the spent catalyst. A controller is used to maintain the pressure head across the slide valve to ensure good recirculation of the regenerated catalyst. Recirculation is done to control the pre-combustion mixing temperature, the catalyst bed density, the catalyst flux and the catalyst residence time.

Though the industrial results have been normalized because of proprietary reasons, the model equations given in the “Appendix” can be used to simulate any other

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Figure 1. Schematic of the riser and the combustor-regenerator of the FCCU.

industrial FCCU with re-tuned values of the kinetic parameters using appropriate industrial data. The values in this study can be used as a first guess for this.

2. Model formulation

2.1 Riser-reactor

In the present study, the riser-reactor is modelled as a steady-state transported plug flow reactor, a good assumption considering the high turbulence and mixing of catalyst and vapours. Figure 2 shows the proposed 17-lump kinetic model, in which the VGO feed is characterized in terms of three kinetic lumps, namely HPs, HNs and HAs (heavy paraffins, heavy naphthenes and heavy aromatics, respectively). One of the several products, light cycle oil (LCO), is characterized in terms of three kinetic lumps, namely LPs, LNs and LAs (light paraffins, light naphthenes and light aromatics, respectively). The gasoline (another product) is characterized in terms of five sub-components, gasoline n-paraffin (G-nP), gasoline iso-paraffin (G-iP), gasoline olefins (G-O), gasoline naphthenes (G-N) and gasoline aromatics (G-A), while the LPG (product) is characterized in terms of four sub-components, C_4^- , $C_4^=$, C_3^- and $C_3^=$ (where superscript $-$ indicates saturated C_4 and C_3 compounds and

Figure 2. Seventeen-lump scheme of cracking reactions lines at the same level indicate going to boxes at the same height (for example K2 and K44 are going to G-nP, etc.). The rate constant for the i^{th} reaction in this figure is K_i (same as k_i or k_i later on).

superscript = indicates C₄ and C₃ compounds with a double bond). There are two more kinetic lumps, namely dry gas and coke. There are a total of 94 cracking reactions (after simplification, see details later) involving these 17 lumps. The rate parameters (frequency factors and activation energies) for these 94 cracking reactions have been estimated using a considerable body of *industrial* data, as described later. These rate constants are found to be relatively insensitive to the composition of the several VGO feeds used in this study, which lends credence to this model. The kinetic model also involves the effect of coke on the catalyst activity.

The model was developed with the following assumptions from the literature [7, 16]: (a) in the riser–reactor, the gases and the catalyst are both in transported plug flow, (b) all the cracking reactions follow first-order kinetics, (c) the variation of temperature in the flowing gas and solids is only in the axial direction, (d) the heat capacities and densities are constant throughout the length of the reactor, (e) dry gases produce no coke, (f) the fractional change of the rate constants for all the reactions due to the deactivation of the catalyst is the same, and is related only to the coke deposited and (g) the temperature of the solid catalyst particles at any axial location is the same as that of the gas at the same location. The pressure balance equations of Pugsley and Berruti [19] have been added to account for the fluidization in a better manner.

The *complete* set of model equations is summarized in the “Appendix”. This model is a slight update of the models of Kasat *et al* [7] and Dasila *et al* [16]. The variation of the yields of the products, the catalyst activity and the riser temperature as a function of the location in the riser can be predicted by the model. Industrial data obtained from an operating unit are (non-linearly) regressed using an evolutionary optimization technique, genetic algorithm (GA) [20, 21], to obtain the rate constants (best-fit or tuned values obtained by minimizing the sum-of-square errors, SSEs {≡ *E*}, between industrial data and model predictions). MATLABTM was used in the present study. The studies of Dave and Saraf [8] and Kasat *et al* [7] are also on industrial FCCUs and are subject to similar proprietary restrictions. Their self-made computer program (in FORTRAN) can be supplied by one of the authors (SKG) but without proprietary values.

The values of the three components of the VGO feed, namely the PNA of the VGO (HP, HN and HA), are estimated using standard API correlations, which require the specific gravity, refractive index, distillation temperatures and viscosity as input parameters to calculate these [22]. The ASTM D1160 vol% data for one sample varies from *about* 355 to *about* 530 K (more information, e.g., density, total S, nitrogen, CCR, etc., are not provided here due to proprietary reasons). The yields of the products are obtained from the model using the best-fit values of the rate constants.

2.2 Combustor–regenerator

The main reactions in the combustor–regenerator are

The coke combustion depends on the amount of carbon in the regenerated catalyst (*C_{reg}*) and the partial pressure of oxygen. The heterogeneous and homogeneous CO combustion reactions depend on the partial pressures of oxygen and CO. A constant weight fraction of hydrogen is assumed with complete combustion [see the “Appendix” for details].

The complete sets of model equations for the combustor (dense phase) as well as in the regenerator are also given in the “Appendix”. Again, these equations are similar to those of Kasat *et al* [7].

A palladium-based combustion promoter is added to the regenerator to promote combustion. The same assumptions are made for the modelling of the combustor–regenerator unit as available in the literature [7, 19, 23, 24]. In addition, the recirculation of catalyst from the regenerator bottom to the combustor bottom is assumed to be 30% [this 30% is reflected in Eqs. (A.16), (A.28), (A.29) and (A.45) of the “Appendix” for the evaluation of *C_{sc}*, the kg of coke per kg of catalyst, etc.].

3. Results and discussion

3.1 Best-fit values of the kinetic parameters

A sensitivity test was done starting with *all* the possible reaction pathways in the 17-lump kinetic scheme. Some of the kinetic parameters were found to be relatively insensitive and hence dropped. Finally, (i) 188 kinetic parameters for the cracking reactions, (ii) 3 (*α*, *β* and *γ*) characterizing the deactivation reactions (assumed to be the same for all the coke formation reactions) and (iii) 8 characterizing the reactions for the regenerator; a total of 199 parameters, were *tuned* using data from an industrial unit (under *several* different operating conditions). Only the (final) 94 reactions in the riser are shown in figure 2. The computed reactor outputs (using the best-fit values of the parameters) are then compared to plant data used for tuning. The tuned model is found to be acceptable.

It may be emphasized that dropping of parameters that are relatively insensitive is a matter of judgment. Indeed, we tuned so many (199) parameters since we had access to a considerable body of industrial data (192 sets, as discussed later).

The detailed kinetic lumping scheme proposed by earlier researchers usually ran into difficulty because of the non-availability of data. Jacob *et al* [10] used a pattern search technique to determine the rate constants using experimental data from an isothermal micro-activity test (MAT) at 482.2°C. However, the validity of these results for an industrial FCCU working under very different and non-isothermal conditions is doubtful.

In the present study, the kinetic parameters were tuned in two stages. The 191 (188 + 3) kinetic parameters of the cracking reactions were first tuned using plant data only for the riser-reactor. This was done using *industrial* values of the temperature and the flow rate of the regenerated catalyst being re-circulated to the riser, coke content in the regenerated catalyst being almost zero). In all, 192 *sets* of industrial data (at different operating conditions) from an operating plant were collected. The feed *compositions* for these runs were somewhat similar, but the reactor operating conditions were *quite* different. Plant data used for tuning the parameters for the *riser-reactor* included the yields, Y_i , of the three components of the unreacted feed, yields of the three components of LCO, five components of gasoline, four components of LPG, dry gas and coke, i.e., 17 *industrial* values of Y_i . The remaining eight kinetic parameters characterizing the combustor-regenerator were *then* tuned using data from the combustor-regenerator unit. For this, the yields of the five flue gas components and the coke on the regenerated catalyst (a total of six) and the temperature of the regenerator were used for fitting the eight kinetic parameters. This was done for each of the 192 sets of plant data. This ensured sufficient redundancy for tuning (optimization) of the values of the parameters.

GA was used for the minimization of the following two objective functions (sum of square errors, E , a function of all the 191 + 8 kinetic parameters, the decision variables):

$$\begin{aligned} \min E(191 \text{ kinetic parameters}) \\ \equiv \sum_{n=1}^{192} \sum_{i=1}^{17} (Y_{i,\text{indus}} - Y_{i,\text{model}})_n^2 + \sum_{n=1}^{192} (T_{n,\text{indus}} - T_{n,\text{model}})^2, \end{aligned} \quad (2)$$

$$\begin{aligned} \min E(8 \text{ kinetic parameters}) \equiv & \sum_{n=1}^{192} \sum_{i=1}^6 (Y_{i,\text{indus}} - Y_{i,\text{model}})_n^2 \\ & + \sum_{n=1}^{192} (T_{\text{rgn},n,\text{indus}} - T_{\text{rgn},n,\text{model}})^2. \end{aligned} \quad (3)$$

In Eqs. (2) and (3), subscripts *indus* and *model* represent the values for the industrial plant and the model-predicted values, respectively. GA is well suited for estimation of the

kinetic parameters [21]. The code available in the MATLAB Optimization Toolbox was used for minimization of the sum of square error, E , in Eqs. (2) and (3). The model equations in the “Appendix” form the equality constraints for the optimization problem. It may be added that normalized errors using $Y_{i,\text{model}}$ and $T_{n,\text{model}}$, etc., and even with different weighting factors for each term, are normally used for ‘tuning’ the parameters [20, 21]. This was, indeed, attempted but the results obtained were quite similar.

The best-fit values of the rate parameters are shown in tables 1 and 2 for the riser and the regenerator. These values of the rate constants are then used for simulation and validation of an industrial FCCU. Again, the tuned values of the rate parameters should be looked upon as pure curve-fit values and physical meanings should not be attributed to them. The values of the activation energies (in kJ/kmol) are similar in magnitude to values of about 40 kcal/gmol (160,000 kJ/kmol) given in the literature.

3.2 Solution procedure for the model equations

The following procedure is used for solving the equations for the regenerator given in the “Appendix”, so as to obtain the model-predicted values required in Eqs. (2) and (3). This procedure is slightly different from that used by Kasat *et al* [7]

- Initial *guess* values of the temperature, T_{sc} , at the top of the riser and the temperature, T_{rgn} , of the regenerated catalyst are assumed.
- The combustor-regenerator calculations are performed to obtain the values of the temperature of the regenerated catalyst, and the composition of the flue gas at the end of the regenerator dense bed. Using the assumed value of T_{rgn} , Eqs. (A.23)–(A.27), (A.35)–(A.38) and (A.50) are integrated using the Runge–Kutta technique [25], with a step size of 0.01 of the total height of the combustor-regenerator. This gives the *calculated* value of the temperature of the regenerated catalyst, T_{rgncheck} .
- If the calculated value of T_{rgn} does not match with the assumed value, iterations (step b) are carried out till convergence. The successive substitution method [25] (Picard iteration) was used for this, with a tolerance of 1°C for T_{rgn} .
- Using the converged value of T_{rgn} , values of the flue gas composition at the outlet and C_{rgc} are calculated using Eqs. (A.51)–(A.55) and (A.68).
- The riser calculations are then performed by integrating Eqs. (A.1)–(A.12), again using the Runge–Kutta technique with a step size, dh , of 0.01, the dimensionless axial location in the riser, to obtain the *calculated* value of the temperature, T_{sc} , at the top of the riser. Iterations need to be performed for the riser, too (see the

Table 1. Estimated kinetic parameters (riser reactions).

k_i	Frequency factor (m ³ /kg cat s)	Activation energy (kJ/kmol)	k_i	Frequency factor (m ³ /kg cat s)	Activation energy (kJ/kmol)	k_i	Frequency factor (m ³ /kg cat s)	Activation energy (kJ/kmol)
k_1	8.0	60000.0	k_{35}	0.3	60000.0	k_{69}	1.6	10011.0
k_2	5.2	10004.5	k_{36}	4.4	10006.8	k_{70}	4.5	60000.0
k_3	12.0	10003.9	k_{37}	5.4	60000.0	k_{71}	5.4	38053.3
k_4	2.4	10009.0	k_{38}	6.4	60000.0	k_{72}	4.3	60000.0
k_5	3.3	10002.6	k_{39}	10.3	10007.3	k_{73}	10.8	45535.5
k_6	4.4	10007.3	k_{40}	4.8	10010.5	k_{74}	4.5	60000.0
k_7	11.5	38967.3	k_{41}	1.9	21605.2	k_{75}	3.0	60000.0
k_8	4.4	34413.3	k_{42}	4.1	60000.0	k_{76}	0.4	10006.3
k_9	2.8	13749.5	k_{43}	6.5	10007.5	k_{77}	4.4	57470.5
k_{10}	5.8	60000.0	k_{44}	2.5	26732.1	k_{78}	2.0	60000.0
k_{11}	6.6	24341.8	k_{45}	1.2	10007.7	k_{79}	15.6	28470.7
k_{12}	2.0	10010.4	k_{46}	5.5	60000.0	k_{80}	6.7	60000.0
k_{13}	4.6	60000.0	k_{47}	0.3	60000.0	k_{81}	6.3	60000.0
k_{14}	5.3	10006.3	k_{48}	8.1	60000.0	k_{82}	6.3	60000.0
k_{15}	4.0	60000.0	k_{49}	5.7	10006.6	k_{83}	3.0	60000.0
k_{16}	6.4	10004.6	k_{50}	4.3	60000.0	k_{84}	0.1	10005.0
k_{17}	17.0	24238.6	k_{51}	5.3	60000.0	k_{85}	0.9	42415.5
k_{18}	1.9	10005.9	k_{52}	1.2	57355.4	k_{86}	3.7	60000.0
k_{19}	0.1	60000.0	k_{53}	6.5	60000.0	k_{87}	3.3	60000.0
k_{20}	1.4	10007.0	k_{54}	5.8	60000.0	k_{88}	7.5	56309.3
k_{21}	3.6	10008.9	k_{55}	10.0	10003.7	k_{89}	3.7	60000.0
k_{22}	4.6	24138.8	k_{56}	4.4	60000.0	k_{90}	7.3	60000.0
k_{23}	1.0	10006.3	k_{57}	4.1	60000.0	k_{91}	7.5	60000.0
k_{24}	3.4	60000.0	k_{58}	3.2	51102.2	k_{92}	0.4	60000.0
k_{25}	4.1	60000.0	k_{59}	3.3	29973.6	k_{93}	1.3	10007.4
k_{26}	1.8	10005.9	k_{60}	8.5	60000.0	k_{94}	9.2	60000.0
k_{27}	0.0	32245.1	k_{61}	3.5	60000.0			
k_{28}	0.3	10006.8	k_{62}	3.5	60000.0			
k_{29}	0.1	10005.9	k_{63}	7.6	60000.0			
k_{30}	5.7	60000.0	k_{64}	1.7	10007.7			
k_{31}	0.6	10004.4	k_{65}	3.7	60000.0			
k_{32}	5.3	60000.0	k_{66}	6.2	60000.0			
k_{33}	7.2	60000.0	k_{67}	3.0	49926.3			
k_{34}	1.4	10007.3	k_{68}	1.0	10004.8			

$56 \leq \alpha \leq 68$, $2.5 \leq \beta \leq 3.5$ and $2.5 \leq \gamma \leq 3$; exact values not supplied for proprietary reasons.

Table 2. Estimated kinetic parameters (regenerator).

Rate constant	Frequency factor [16] (unit, values)	Activation energy (kJ/ kmol)
β_c	—	10.48
$k_{\text{reg},c}$	1/atm s	570.43
$k_{\text{reg},13c}$	kmol/kg cat atm ² s	4.43
$k_{\text{reg},13h}$	kmol/m ³ atm ² s	4.06

“Appendix” for details), to obtain the converged value of ε , the void fraction in the riser–reactor at *each* value of $i(\text{dh})$, $i = 1, 2, \dots, 100$.

f. If the assumed and calculated values of the riser top temperature do not match, iterations are carried out (starting from step a) till convergence. The successive substitution technique [25] with a tolerance for T_{sc} of

1°C was used. It is clear that there are several iterative loops in the numerical procedure.

3.3 Simulation of the industrial FCCU and validation of the model

The code for the industrial FCCU (riser and combustor–regenerator) with actual values of the feeds is used to simulate the industrial unit and obtain the best-fit values of the kinetic parameters obtained. They are given in tables 1 and 2 (other thermodynamic parameters are given in table 3) along with the ranges for the parameters, α , β and γ , characterizing the deactivation of the catalyst. The detailed compositions of the feed are obtained from a validated API model. The results of the tuned model matched the 192 sets of plant data used for tuning quite well.

Table 3. Thermodynamic data used for simulation.

Parameters	Unit	Value
C_{pfl}	$\text{kJ kg}^{-1} \text{K}^{-1}$	3.38
C_{pfv}	$\text{kJ kg}^{-1} \text{K}^{-1}$	3.34
C_{pC}	$\text{kJ kg}^{-1} \text{K}^{-1}$	1.003
C_{pO_2}	$\text{kJ kg}^{-1} \text{K}^{-1}$	32.28
C_{pCO}	$\text{kJ kg}^{-1} \text{K}^{-1}$	30.85
C_{pCO_2}	$\text{kJ kg}^{-1} \text{K}^{-1}$	47.4
$C_{pH_2O} \equiv C_{pst}$	$\text{kJ kg}^{-1} \text{K}^{-1}$	36.932
C_{pN_2}	$\text{kJ kg}^{-1} \text{K}^{-1}$	30.53
H_{pCO}	kJ kmol^{-1}	1.078×10^5
H_{pCO_2}	kJ kmol^{-1}	3.933×10^5
H_{pH_2O}	kJ kmol^{-1}	2.42×10^5
ΔH_{vap}	kJ kg^{-1}	150
$MW_{HP} = MW_{HN} = MW_{HA}$	kg kmol^{-1}	380
$MW_{LP} = MW_{LN} = MW_{LA}$	kg kmol^{-1}	182
$MW_{GNP} = MW_{GiP} = MW_{GO}$	kg kmol^{-1}	108
$MW_{C_4^-}$	kg kmol^{-1}	58
$MW_{C_4^=}$	kg kmol^{-1}	56
$MW_{C_3^-}$	kg kmol^{-1}	44
$MW_{C_3^=}$	kg kmol^{-1}	42
MW_{drygas}	kg kmol^{-1}	20
MW_c	kg kmol^{-1}	12
x_{pt}	–	0.1

Fifteen *additional* sets of operating data were obtained for this FCCU, and the simulated results with these tuned parameters were found to match industrial values satisfactorily. Of these, a sub-set of three, Cases 1–3, is presented in table 4 in normalized form (details of normalization are provided in this table), due to proprietary reasons. The design and operating conditions for these three cases involving different catalyst-to-oil ratios, feed flow rates and regenerator temperatures are given for these three cases in table 4. The performance of the model has been evaluated by comparing the model-predicted values of the conversion and yields of the various components to plant data at the riser and regenerator outlets. The match is quite good (in terms of the *actual* values, which is not very clear from the normalized values in the table) as shown in table 5 (in each case, plant values are normalized to unity, as described in this table). It may be added that the model values for Cases 2 and 3 in table 5 have been normalized using plant values for Case 1, so that they can be compared to normalized plant values for these two cases easily. It may also be mentioned that these three industrial cases do not represent variation of *any* single operating condition, and several operating conditions are varied simultaneously, these being *actual* operating runs.

Table 4. Plant operating conditions and design data used for simulation.*

Description	Case 1	Case 2	Case 3
Feed (VGO) composition (mol%) from API model (all normalized with respect to Case 1)			
Paraffins, HP (mol%)	1.0	0.9216	1.0316
Naphthenes, HN (mol%)	1.0	1.0057	1.0067
Aromatics, HA (mol%)	1.0	1.0482	0.9709
Operating parameters (all normalized with respect to Case 1)			
Fresh feed rate (kg/s)	1.0	0.9290	0.9957
Steam flow rate (kg/s)	1.0	1.1430	1.1363
Feed preheat temperature, T_{feed} (K)	1.0	0.9979	0.9958
Feed steam temperature, T_{st} (K)	1.0	1.0	1.0
Riser outlet temperature (ROT) (K)	1.0	1.0012	1.0037
Catalyst/oil ratio (kg/kg)	1.0	1.0490	0.9478
Catalyst circulation rate (kg/s)	1.0	0.9746	0.9437
Catalyst density, ρ_s (kg/m ³)	1.0	1.0	1.0
Catalyst diameter, D (μm)	1.0	1.0	1.0
Reactor bottom pressure (kPa)	1.0	0.9654	0.7034
Riser height (m)	1.0	1.0	1.0
Riser cross-sectional area (m ²)	1.0	1.0	1.0
Combustor height (m)	1.0	1.0	1.0
Combustor diameter (m)	1.0	1.0	1.0
Regenerator height (m)	1.0	1.0	1.0
Regenerator diameter (m)	1.0	1.0	1.0
Combustor–regenerator pressure (kPa)	1.0	0.9563	0.8224
Air flow rate, f_{air} (m ³ /s)	1.0	0.8790	0.7654
Air preheat temperature, T_{air} (K)	1.0	0.9941	0.9686
Hydrogen/carbon ratio in coke, C_h (kg/kg)	1.0	1.0147	1.0294

* Normalized values being provided for proprietary reasons. The values for Case 1 are individually normalized to unity for Case 1, e.g., the entry in the table for T_{feed} (K) for Case 1 means $T_{feed, actual, Case 1} (K) / T_{feed, actual, Case 1} (K) = 1$. Values for Cases 2 and 3 are normalized using *actual* values for Case 1, e.g., the entry in the table for T_{feed} for Case 2 means $T_{feed, actual, Case 2} (K) / T_{feed, actual, Case 1} (K)$, etc. The units shown in column 1 are for the actual values, and have no other meaning.

Table 5. Comparison of model calculated values with plant data for Cases 1–3 in table 4. Predictions with the five-lump model of Kasat *et al* [7] are also shown.*

Data	Case 1			Case 2			Case 3		
	Pnt.	Mod.	[7]	Pnt.	Mod.	[7]	Pnt..	Mod.	[7]
Riser results (all normalized with respect to corresponding values for Case 1)									
Unconverted (clubbed) VGO (wt%)	1.0	1.0773	1.45	1.0459	1.0170	1.4395	1.0642	0.9305	1.0822
LCO (clubbed) yield (wt%)	1.0	0.9477		0.9819	0.9735		0.9833	0.9178	
Gasoline n-paraffin yield (wt%)	1.0	0.8944	1.08	0.9056	0.9056	1.0812	0.9444	0.8056	1.2186
Gasoline iso-paraffin yield (wt%)	1.0	0.9941		0.9327	0.9054		0.8907	0.9854	
Gasoline olefins yield (wt%)	1.0	1.0396		1.0022	1.0154		0.9945	0.9868	
Gasoline naphthenes yield (wt%)	1.0	0.8920		0.9724	0.9447		0.8744	0.8945	
Gasoline aromatics yield (wt%)	1.0	0.9832		0.9951	1.0238		0.9916	1.0049	
C ₄ [−] yield (wt%)	1.0	0.9386	0.61	0.8872	0.8734	0.5394	1.0000	0.9799	0.5956
C ₄ [−] yield (wt%)	1.0	1.0327		1.0214	1.0655		1.0088	1.1196	
C ₃ [−] yield (wt%)	1.0	1.0413		1.0254	1.0000		1.0857	1.1651	
C ₃ [−] yield (wt%)	1.0	0.9661		1.0106	1.0074		0.9926	0.9651	
Dry gas yield (wt%)	1.0	1.1111	0.97	1.2137	1.3590	1.1894	1.1560	1.3889	1.2831
Coke yield (wt%)	1.0	1.0650	0.89	1.0704	1.0000	0.9955	1.0993	0.9621	1.0443
Regenerator Results (all normalized with respect to corresponding values for Case 1)									
O ₂ (mol%)	1.0	1.0372	1.16	0.9202	0.9840	1.0490	0.9787	1.0426	1.0864
CO (mol%)	0	0	0	—	—	—	—	—	—
CO ₂ (mol%)	1.0	0.9560	0.93	0.9174	0.9387	0.8348	0.9346	0.9511	0.8598
H ₂ O (mol%)	1.0	1.0115	0.90	0.9958	0.9478	0.9560	0.9467	0.8986	0.9183
N ₂ (mol%)	1.0	1.0153	1.01	1.0188	1.0190	1.0086	1.0207	1.0213	1.0309
Coke-on-regenerated catalyst (kg/kg-catalyst)	1.0	1.2	1.31	0.8000	1.0000	0.9040	1.0000	1.2000	1.1800
Dense phase temperature (K)	1.0	0.9990	1.01	0.9898	0.9908	1.0492	0.9786	0.9806	1.0666

*: Pnt.: plant; Mod.: model.

* Normalized values being provided for proprietary reasons. The values for Case 1 are individually normalized to unity for Case 1, e.g., the entry in the table for the plant value of Unconverted VGO (wt%) for Case 1 means Unconverted VGO_{Case 1} (wt%)/Unconverted VGO_{Case 1} (wt%) = 1. Plant values for Cases 2 and 3 are normalized using *actual* (plant) values for Case 1, e.g., the entry in the table for Dry gas yield (wt%) for Case 2 means Dry gas yield_{plant, Case 2} (wt%)/Dry gas yield_{plant, Case 1} (wt%), etc. Model values are defined in a similar manner for Cases 1–3, using corresponding *plant* values for Case 1 for normalization. For example, the entry in the table for Dry gas yield (wt%) for Case 2 means Dry gas yield_{model, Case 2} (wt%)/Dry gas yield_{plant, Case 1} (wt%), etc. The units shown in column 1 are for the *actual* values.

Table 5 also compares the normalized simulation results obtained using the kinetic parameters of the earlier five-lump kinetic scheme [7] for the three operating cases of the *present* industrial FCCU. The kinetic parameters of the five-lump scheme were tuned using data on a *different* industrial FCCU. It is difficult to say which is better of the two, since for some cases the predictions of the five-lump parameters are superior while for others, those of the 17-lump scheme are better. However, the earlier five-lump model cannot give as detailed a set of predictions as the present 17-lump scheme. For example, the less detailed five-lump model *cannot* give the yields of C₃ and C₄ alkanes and alkenes, e.g., propylene, etc. Present-day FCCUs attempt to maximize the yields of propylene, etc., due to their higher values.

Figures 3–6 show the axial profiles of the concentrations of the several products in the riser for Case 1 (in normalized form; clearly, actual values, e.g., of the gasoline concentration, are not 100% at the top of the riser–reactor). Figure 3 shows the gas–oil conversion. The conversion increases rapidly near the bottom of the riser, and slows down as one proceeds along the flow direction. There are a number of

Figure 3. Product profiles in the riser (Case 1).

reasons for this. First, the bottom zone of the riser has a higher catalyst concentration. In addition, this catalyst has just been introduced from the regenerator and therefore has a higher

Figure 4. Profiles of the gasoline components in the riser (Case 1).

Figure 6. Coke and dry gas profiles in the riser (Case 1).

Figure 5. Profiles of the LPG components in the riser (Case 1).

Figure 7. Profiles of the regenerator components (Case 1).

activity than at higher axial locations in the riser. Finally, the concentration of the gas-oil vapour is the highest at the base of the riser compared with that at higher axial locations, where reaction and molar expansion decrease the gas-oil concentration. Figure 3 shows that gasoline becomes almost constant at about a fifth of the riser height. This is because of over-cracking of the gasoline.

The variation of the O_2 , CO_2 and coke in the regenerator (for Case 1) is shown in figure 7. It can be observed from this diagram that the amount of oxygen and coke decreases and carbon dioxide increases along the height of the combustor, as the combustion of coke (in the presence of air) takes place in this section. The amount of carbon monoxide formed is very small as the rate of reaction for the formation of carbon monoxide is extremely low, due to the

presence of promoters. At a non-dimensional height of around 0.56 there is a sudden change in the slope of the graphs. This is because from here onwards the dense bed of the regenerator section begins. Here, the rate of consumption of oxygen and of the combustion of coke increases (and that of the formation of carbon dioxide increases) as palladium-based combustion begins. Promoters are added, which promote the combustion of coke. At the non-dimensional height of around 0.68, again, a sudden change in the rate is observed as from here the dilute bed of the regenerator starts. By this point almost all the coke is burnt off and the amount of carbon monoxide is almost zero. This section is used primarily as a chamber for separating the catalyst and the flue gases, and almost no reaction takes place. Thus, the rate of combustion of coke, consumption of oxygen and formation of carbon dioxide decreases. Again, similar non-dimensional plots for Cases 2 and 3 are not presented since the trends are similar, and it will not make

much sense unless proprietary details are provided in tables 4 and 5.

It may be added that ASPEN PLUSTM also has a program to simulate/design FCCUs, but they use fewer lumps than the 17 used here in this *first-principle* model, with the parameters tuned using an *extremely* large amount of industrial data. Also, this work focuses on the *detailed* composition of gasoline and LPG, which helps in predicting the quality of both these products better, something that the present version of ASPEN PLUSTM does not predict.

4. Conclusions

The model developed incorporates a detailed 17-lump kinetic model for the riser–reactor–regenerator unit. The feed is described in terms of hydrocarbon types (PNAs) for the input VGO. A total of 199 kinetic parameters were estimated (tuned) for the industrial FCCU, using 192 *sets* of plant data. The model is then used to *predict* the gas oil conversion as well as the detailed product composition for gasoline and LPG, and the coke and flue gas compositions for 15 *additional* sets of industrial conditions (validation). Good agreement was observed between model predictions and plant data.

One can use this model and the techniques described herein to simulate any other industrial FCCU with a feed that is different, but a re-tuning of the kinetic parameters will be needed. This will involve a substantial amount of work, but the model and the procedures used in our study can be used for other FCCUs, and orders of magnitude of the kinetic parameters obtained in the present study can be useful starting points for estimating kinetic parameters for other units. Indeed, *all* optimization studies, including GA, could use excellent starting points for the parameters, and tuning of parameters is, indeed, an optimization exercise.

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Appendix (adapted from [7, 19] and extended)

Riser–reactor model equations and procedure

Guess a value ε at $h = 0$ (use F_{feed} , F_{st} , F_{rgc} , ρ_v , ρ_{steam} , ρ_c , etc., for estimation).

Calculate U_0 at $h = 0$ using F_{feed} , F_{st} , F_{rgc} , A_{ris} , ρ_v , MW_g and ε (see Eq. (A.9)).

Integrate the following ODEs using the Runge–Kutta technique (using a step size dh).

Material balance for the j^{th} lump over a differential element of (dimensionless) height, dh :

$$\frac{dF_j}{dh} = A_{\text{ris}} H_{\text{ris}} (1 - \epsilon) \rho_s \sum_{i=1}^{94} (\alpha_{kj})_i r_i; j = 1, 2, \dots, 17; i = \text{reaction no.} \quad (\text{A.1})$$

$(\alpha_{kj})_i$ = stoichiometric coefficient for $k \rightarrow j$ in the i^{th} reaction.

Rate equations for each of the 94 reactions are as follows (k is the reactant in the i^{th} reaction):

$$r_i = k_{i0} \exp\left(-\frac{E_i}{RT}\right) C_k \varphi. \quad (\text{A.2})$$

Catalyst deactivation function:

$$\varphi = \frac{\alpha}{1 + \beta C_c^{\gamma}} \quad (\text{same factor for all 94 reactions}) \quad (\text{A.3})$$

with $C_k = \frac{P_{\text{ris}} F_k}{RT [F_{\text{st}}/x_{\text{st}} + \sum_{i=1}^{16} F_i/x_i]}$;

summation over i does not involve coke;

$$x_j = \frac{F_j}{F_{\text{st}} + \sum_{i=1}^{16} F_i}; x_{\text{st}} = \frac{F_{\text{st}}}{F_{\text{st}} + \sum_{i=1}^{16} F_i} \quad (\text{coke excluded}).$$

Energy balance across dh :

$$\frac{dT}{dh} = \frac{A_{\text{ris}} H_{\text{ris}} (1 - \epsilon) \rho_s}{F_{\text{rgc}} C_{\text{pC}} + F_{\text{feed}} C_{\text{pFV}} + MW_{\text{st}} F_{\text{st}} C_{\text{pst}}} \sum_{i=1}^{94} r_i (-\Delta H_i) \quad (\text{A.4})$$

$$T(h=0) = \frac{F_{\text{rgc}} C_{\text{pC}} T_{\text{rgn}} + F_{\text{feed}} C_{\text{pFV}} T_{\text{feed}} + MW_{\text{st}} F_{\text{st}} C_{\text{pst}} T_{\text{st}} - \Delta H_{\text{evap}} F_{\text{feed}} - Q_{\text{loss,ris}}}{F_{\text{rgc}} C_{\text{pC}} + F_{\text{feed}} C_{\text{pFV}} + MW_{\text{st}} F_{\text{st}} C_{\text{pst}}} \quad (\text{A.5})$$

$$Q_{\text{loss,riser}} = 0.0012 (F_{\text{rgc}} C_{\text{pC}} T_{\text{rgn}} + F_{\text{feed}} C_{\text{pFV}} T_{\text{feed}} + MW_{\text{st}} F_{\text{st}} C_{\text{pst}} T_{\text{st}} - \Delta H_{\text{evap}} F_{\text{feed}}).$$

Pressure balance across dh

$$-\frac{dP_{\text{ris}}}{dh} = H_{\text{ris}} \rho_s g (1 - \epsilon). \quad (\text{A.6})$$

Vapour properties in the riser–reactor at any h are calculated by the following equations:

$$MW_g = x_{\text{st}} MW_{\text{st}} + \sum_{i=1}^{15} x_j MW_j \quad (\text{A.7})$$

$$\rho_v = \frac{P_{\text{ris}} \text{MW}_g}{RT} \quad (\text{A.8})$$

$$U_0 = \frac{\text{MW}_g (F_{\text{st}} + \sum_{j=1}^{16} F_j)}{\rho_v A_{\text{ris}}} \text{ (coke excluded).} \quad (\text{A.9})$$

Slip factor [13]

$$\psi = 1 + \frac{5.6}{\text{Fr}} + 0.47 \text{Fr}_t^{0.41} \quad (\text{A.10})$$

$$\text{Here Fr} = \text{Froude number} = \frac{U_0}{(gD)^{0.5}},$$

Fr_t is the Froude number at the terminal velocity of the single catalyst particle and

$$G_s = \text{solid mass flux} = \frac{F_{\text{rgc}}}{A_{\text{ris}}} \quad (\text{A.11})$$

Compute ε (at i dh) using

$$\varepsilon = 1 - \frac{G_s \psi}{U_0 \rho_s + G_s \psi};$$

then check whether this matches with ε (at i dh) using $\varepsilon = \frac{U_0}{V_p \psi}$, where

$$V_p = \frac{G_s}{\rho_s (1 - \varepsilon)}; \quad (\text{A.12})$$

else, iterate using Picard's iteration (successive substitution [25]). After convergence (tolerance on ε is taken as 0.01), repeat till $h = 1$ is reached.

Rate equations in the combustor-regenerator

The rate expressions for the combustion reactions in the regenerator in $\text{kmol}/(\text{m}^3 \text{ s})$ are given as follows [19]:

$$r_{11} = \rho_s (1 - \varepsilon) k_{\text{reg},11} \frac{C_{\text{sc}} f_{\text{O}_2}}{\text{MW}_C f_{\text{tot}}} (0.009869) P_{\text{rgn}} \quad (\text{A.13})$$

$$r_{12} = \rho_s (1 - \varepsilon) k_{\text{reg},12} \frac{C_{\text{sc}} f_{\text{O}_2}}{\text{MW}_C f_{\text{tot}}} (0.009869) P_{\text{rgn}} \quad (\text{A.14})$$

$$\begin{aligned} r_{13} &= k_{\text{reg},13} P_{\text{O}_2} P_{\text{CO}} \\ &\equiv (\rho_s x_{\text{pt}} (1 - \varepsilon) k_{\text{reg},13c} + \varepsilon k_{\text{reg},13h}) \frac{f_{\text{O}_2} f_{\text{CO}}}{f_{\text{tot}}^2} P_{\text{rgn}}^2 \end{aligned} \quad (\text{A.15})$$

$$C_{\text{sc}} = \frac{12F_C}{1.3F_{\text{rgc}}} \text{ (30\% recirculation rate assumed)} \quad (\text{A.16})$$

$$\left(\frac{\text{CO}}{\text{CO}_2} \right)_{\text{surface}} = \frac{k_{\text{reg},11}}{k_{\text{reg},12}} \equiv \beta_c = \beta_{c0} \exp \left(-\frac{E_\beta}{RT} \right) \quad (\text{A.17})$$

$$k_{\text{reg}} \equiv k_{\text{reg},11} + k_{\text{reg},12} = k_{c0} \exp \left(-\frac{E_c}{RT} \right) \quad (\text{A.18})$$

$$k_{\text{reg},11} = \frac{\beta_c k_{\text{reg},c}}{\beta_c + 1} = \frac{\beta_c k_{c0} \exp \left(-\frac{E_c}{RT} \right)}{\beta_c + 1} \quad (\text{A.19})$$

$$k_{\text{reg},12} = \frac{k_{\text{reg},c}}{\beta_c + 1} = \frac{k_{c0} \exp \left(-\frac{E_c}{RT} \right)}{\beta_c + 1} \quad (\text{A.20})$$

$$k_{\text{reg},13c} = k_{13c0} \exp \left(-\frac{E_{13c}}{RT} \right) \quad (\text{A.21})$$

$$k_{\text{reg},13h} = k_{13h0} \exp \left(-\frac{E_{13h}}{RT} \right). \quad (\text{A.22})$$

Combustor model equations

Material balances across the differential element of height, dz , of the combustor

$$\frac{df_{\text{O}_2}}{dz} = -A_{\text{comb}} \left(\frac{r_{11}}{2} + r_{12} + \frac{r_{13}}{2} \right) \quad (\text{A.23})$$

$$\frac{df_{\text{CO}}}{dz} = -A_{\text{comb}} (r_{13} - r_{11}) \quad (\text{A.24})$$

$$\frac{df_{\text{CO}_2}}{dz} = A_{\text{comb}} (r_{12} + r_{13}) \quad (\text{A.25})$$

$$\frac{df_C}{dz} = -A_{\text{comb}} (r_{11} + r_{12}) \quad (\text{A.26})$$

$$\frac{df_{\text{N}_2}}{dz} = 0. \quad (\text{A.27})$$

Initial conditions for the combustor, at $z = 0$

$$C_{\text{sc},i} = \frac{12f_{C,i}}{1.3F_{\text{rgc}}} \quad (\text{A.28})$$

$$f_{\text{H}_2\text{O}} = 1.3C_{\text{sc},i} \left(\frac{C_h}{\text{MW}_{\text{H}_2}} \right) F_{\text{sc}} \quad (\text{A.29})$$

$$f_{\text{O}_2} = 0.21f_{\text{air}} - \frac{1}{2}f_{\text{H}_2\text{O}} \quad (\text{A.30})$$

$$f_{\text{CO}} = f_{\text{CO}_2} = 0 \quad (\text{A.31})$$

$$f_C(z=0) = F_{c,\text{ris}} \quad (\text{A.32})$$

$$f_{\text{N}_2} = 0.79f_{\text{air}} \quad (\text{A.33})$$

$$f_{\text{tot}} = f_{\text{O}_2} + f_{\text{CO}} + f_{\text{CO}_2} + f_{\text{H}_2\text{O}} + f_{\text{N}_2} \quad (\text{A.34})$$

Regenerator dense phase model equations

The material balances across a differential elemental of height, dz , of dense bed are as follows:

$$\frac{df_{O_2}}{dz} = -A_{\text{rgn}} \left(\frac{r_{11}}{2} + r_{12} + \frac{r_{13}}{2} \right) \quad (\text{A.35})$$

$$\frac{df_{CO}}{dz} = -A_{\text{rgn}}(r_{13} - r_{11}) \quad (\text{A.36})$$

$$\frac{df_{CO_2}}{dz} = A_{\text{rgn}}(r_{12} + r_{13}) \quad (\text{A.37})$$

$$\frac{df_C}{dz} = -A_{\text{rgn}}(r_{11} + r_{12}). \quad (\text{A.38})$$

Initial conditions are the same as at the end of the combustor.

Evaluation of dense bed characteristics

$$\varepsilon = \frac{0.305u_1 + 1}{0.305u_1 + 2} \quad (\text{A.39})$$

$$u_1 = \frac{f_{\text{air}}}{0.3048\rho_g A_{\text{rgn}}} \quad (\text{A.40})$$

$$\rho_g = \frac{P_{\text{rgn}}}{RT_{\text{rgn}}} \quad (\text{A.41})$$

$$Z_{\text{bed}} = 0.3048\text{TDH} \quad (\text{A.42})$$

$$\text{TDH} = \text{TDH}_{20} + 0.1(D_{\text{reg}} - 20) \quad (\text{A.43})$$

$$\log_{10}(\text{TDH}_{20}) = \log_{10}(20.5) + 0.07(u_1 - 3) \quad (\text{A.44})$$

$$F_{\text{sc}} = 1.3F_{\text{rgc}} + 12F_{\text{c,ris}}; (f_{\text{c,ris}} = f_{\text{c,i}}). \quad (\text{A.45})$$

Equation (A.45) gives the flow rate of spent catalyst along with recirculated catalyst from the regenerator at the entrance of the combustor.

Energy balance

The temperature throughout the combustor–dense bed of the regenerator is constant (and the same) since the catalyst is well mixed. The overall heat balance is given by

$$\frac{dT_{\text{rgn}}}{dz} = 0. \quad (\text{A.46})$$

Heat balance across the regenerator dense bed

$$a \equiv [f_{CO}(Z_{\text{bed}})H_{CO} + f_{CO_2}(Z_{\text{bed}})H_{CO_2} + f_{H_2O}H_{H_2O} + f_{\text{air}}C_{\text{pair}}(T_{\text{air}} - T_{\text{base}}) + F_{\text{sc}}C_{\text{pC}}(T_{\text{sc}} - T_{\text{base}})] \quad (\text{A.47})$$

$$b \equiv 0.2[f_{CO}(Z_{\text{bed}})H_{CO} + f_{CO_2}(Z_{\text{bed}})H_{CO_2} + f_{H_2O}H_{H_2O} + f_{\text{air}}C_{\text{pair}}(T_{\text{air}} - T_{\text{base}}) + F_{\text{sc}}C_{\text{pC}}(T_{\text{sc}} - T_{\text{base}})] \quad (\text{A.48})$$

$$c \equiv [F_{\text{sc}}C_{\text{pC}} + f_{CO_2}(Z_{\text{bed}})C_{\text{pCO}_2} + f_{O_2}(Z_{\text{bed}})C_{\text{pO}_2} + f_{H_2O}C_{\text{pH}_2O} + f_{N_2}C_{\text{pN}_2}] \quad (\text{A.49})$$

$$T_{\text{rgn}}(z = 0) = T_{\text{base}} + [(a - b)/c] \quad (\text{A.50})$$

with $f_i(Z_{\text{bed}})$ being the value of f_i at the end of the regenerator dense bed.

Regenerator dilute phase model equations

Material and energy balance equations in the dilute phase of the regenerator are given by

$$\frac{df_{O_2}}{dz} = -A_{\text{rgn}} \left(\frac{r_{11}}{2} + r_{12} + \frac{r_{13}}{2} \right) \quad (\text{A.51})$$

$$\frac{df_{CO}}{dz} = -A_{\text{rgn}}(r_{13} - r_{11}) \quad (\text{A.52})$$

$$\frac{df_{CO_2}}{dz} = A_{\text{rgn}}(r_{12} + r_{13}) \quad (\text{A.53})$$

$$\frac{df_C}{dz} = -A_{\text{rgn}}(r_{11} + r_{12}) \quad (\text{A.54})$$

$$\frac{dT_{\text{dil}}}{dz} = \frac{A_{\text{rgn}}}{C_{\text{p,tot}}f_{\text{tot}}} [H_{CO}(r_{11} - r_{13}) + H_{CO_2}(r_{12} + r_{13})] \quad (\text{A.55})$$

$$C_{\text{ptot}} = \left(\frac{C_{\text{pN}_2}f_{\text{N}_2} + C_{\text{pO}_2}f_{\text{O}_2} + C_{\text{pCO}}f_{\text{CO}} + C_{\text{pCO}_2}f_{\text{CO}_2} + C_{\text{pH}_2O}f_{\text{H}_2O} + C_{\text{pC}}F_{\text{ent}}}{f_{\text{tot}}} \right) \quad (\text{A.56})$$

$$F_{\text{ent}} = \frac{0.453WA_{\text{rgn}}}{16} \quad (\text{A.57})$$

$$\rho_f = 0.06243\rho_g \text{MW}_{\text{g,rgn}} \quad (\text{A.58})$$

$$W = \rho_f Yu_1 \quad (\text{A.59})$$

$$\log_{10}Y = \log_{10}60 + 0.69\log_{10}X - 0.445(\log_{10}X)^2 \quad (\text{A.60})$$

$$X = \frac{u_1^2}{gD\rho_p^2} \quad (\text{A.61})$$

$$\varepsilon_{\text{dil}} = 1 - \frac{\rho_{\text{dil}}}{\rho_s} \quad (\text{A.62})$$

$$\rho_{\text{dil}} = \frac{F_{\text{ent}}}{0.3048A_{\text{rgn}}u_1} \quad (\text{A.63})$$

$$Z_{\text{dil}} = Z_{\text{rgn}} - Z_{\text{bed}}. \quad (\text{A.64})$$

Carbon mass balance

Under the assumption that all the entrained catalyst returns to the dense bed, it is possible to write an overall carbon balance for the regenerator:

$$\frac{dC_{\text{rgc}}}{dt} = \frac{1}{W_{\text{rgn}}} [(F_{\text{sc}}C_{\text{sc}} - F_{\text{rgc}}C_{\text{rgc}})(1 - C_{\text{h}}) + (f_{\text{CO}}(Z_{\text{bed}}) + f_{\text{CO}_2}(Z_{\text{bed}}))\text{MW}_{\text{C}}] \quad (\text{A.65})$$

But C_{rgc} is constant in the dense bed, as the catalyst is considered to be well mixed

$$F_{\text{sc}}C_{\text{sc}}(1 - C_{\text{h}}) = F_{\text{rgc}}C_{\text{rgc}}(1 - C_{\text{h}}) - (f_{\text{CO}}(Z_{\text{bed}}) + f_{\text{CO}_2}(Z_{\text{bed}}))\text{MW}_{\text{C}} \quad (\text{A.66})$$

$$\therefore C_{\text{rgc}} = \frac{[F_{\text{sc}}C_{\text{sc}}(1 - C_{\text{h}}) + (f_{\text{CO}}(Z_{\text{bed}}) + f_{\text{CO}_2}(Z_{\text{bed}}))\text{MW}_{\text{C}}]}{F_{\text{rgc}}(1 - C_{\text{h}})} \quad (\text{A.67})$$

As the process is in steady state

$$C_{\text{rgc}} = \frac{[F_{\text{sc}}C_{\text{sc}}(1 - C_{\text{h}}) + (f_{\text{CO}}(Z_{\text{bed}}) + f_{\text{CO}_2}(Z_{\text{bed}}))\text{MW}_{\text{C}}]}{F_{\text{sc}}(1 - C_{\text{h}})} \quad (\text{A.68})$$

Nomenclature related to the Appendix [7, 19]

A_{comb}	combustor cross-sectional area, m^2	E_{13c}	activation energy for heterogeneous CO combustion, kJ/kmol
A_{rgn}	regenerator cross-sectional area, m^2	E_{13h}	activation energy for homogeneous CO combustion, kJ/kmol
A_{ris}	riser cross-sectional area, m^2	E_{β}	activation energy for CO/CO ₂ at the catalyst surface, kJ/kmol
CCR	catalyst circulation rate, kg/s	Fr	Froude number
C_{c}	coke on catalyst, kg coke/kg catalyst	F_{ent}	entrained catalyst flow rate, kg/s
C_{h}	weight fraction of hydrogen in coke, kg H ₂ /kg coke	F_{feed}	oil feed flow rate, kg/s
C_i	concentration of i^{th} component, kmol i/m^3 mixture	F_j	molar flow rate of the j^{th} lump in the riser, kmol/s
C_{pair}	mean heat capacity of air, kJ/kg K	F_{rgc}	catalyst circulation rate (CCR), kg/s
C_{pC}	catalyst heat capacity, kJ/kg K	F_{sc}	spent catalyst flow rate, kg/s
C_{pCO}	mean heat capacity of CO, kJ/kg K	F_{st}	molar flow rate of steam in the riser feed, kmol/s
C_{pCO_2}	mean heat capacity of CO ₂ , kJ/kg K	f_{air}	air molar flow rate to the regenerator, kmol/s
C_{pfl}	mean heat capacity of liquid feed, kJ/kg K	$f_{\text{c}}, F_{\text{C}}$	molar flow rate of carbon at any location in the regenerator or riser, kmol/s
C_{pfv}	mean heat capacity of vapour feed, kJ/kg K	f_{CO}	molar flow rate of CO in the regenerator, kmol/s
$C_{\text{pH}_2\text{O}}, C_{\text{pst}}$	mean heat capacity of H ₂ O, steam, kJ/kg K	f_{CO_2}	molar flow rate of CO ₂ in the regenerator, kmol/s
C_{pN_2}	mean heat capacity of N ₂ , kJ/kg K	$f_{\text{H}_2\text{O}}$	molar flow rate of H ₂ O in the regenerator, kmol/s
C_{pO_2}	mean heat capacity of O ₂ , kJ/kg K	f_i	molar flow rate of the i^{th} component in the regenerator, kmol/s
C_{rgc}	coke on regenerator catalyst, kg coke/kg catalyst	f_{N_2}	molar flow rate of N ₂ in the regenerator, kmol/s
C_{sc}	coke on spent catalyst at any location in the regenerator, kg coke/kg cat	f_{O_2}	molar flow rate of O ₂ in the regenerator, kmol/s
C_3^-	C ₃ alkanes	f_{tot}	molar flow rate of the vapour (total) in the regenerator, kmol/s
$C_3^=$	C ₃ alkenes	G-A	gasoline aromatics
C_4^-	C ₄ alkanes	G-iP	gasoline iso-paraffins
$C_4^=$	C ₄ alkenes	G-N	gasoline napthenes
D	diameter of the catalyst sphere, m	G-NP	gasoline n-paraffins
D_{comb}	diameter of the combustor, m	G-O	gasoline olefins
D_{reg}	diameter of the regenerator, m	G_s	solid mass flux in the riser (independent of axial location), kg/m ² s
E_i	activation energy for the i^{th} reaction in the riser, kJ/kmol	g	acceleration due to gravity, m/s ²
		H_{CO}	heat of formation of CO, kJ/kmol
		H_{CO_2}	heat of formation of CO ₂ , kJ/kmol
		$H_{\text{H}_2\text{O}}$	heat of formation of H ₂ O, kJ/kmol
		H_{ris}	riser height, m
		HN	heavy napthenes
		HP	heavy paraffins
		ΔH_{evap}	heat of vaporization of oil feed, kJ/kg
		ΔH_i	heat of cracking of the i^{th} lump, kJ/kmol
		h	dimensionless riser height ($= z/H_{\text{ris}}$)
		LA	light aromatics
		LN	light napthenes
		k_{i0}	frequency factor for the i^{th} reaction in the riser, m ³ /kg cat s
		k_{co}	frequency factor for coke combustion, 1/atm s K

$k_{\text{reg,c}}$	rate constant for oxidation of carbon to CO in the regenerator, 1/atm s	T_{sc}	temperature of the spent catalyst, K
$k_{\text{reg,11}}$	rate constant for oxidation of carbon to CO in the regenerator, 1/atm s	T_{st}	temperature of the steam fed with the riser feed, K
$k_{\text{reg,12}}$	rate constant for oxidation of carbon to CO ₂ in the regenerator, 1/atm-s	ΔT_{st}	drop in temperature in the stripper (assumed 10°C), K
$k_{\text{reg,13c}}$	rate constant (heterogeneous) for oxidation of CO to CO ₂ in the regenerator, kmol CO/m ³ cat-atm ² -s)	U_0	superficial velocity of the vapour at any axial location in the riser, m/s
$k_{\text{reg,13h}}$	rate constant (homogeneous) for oxidation of CO to CO ₂ in the regenerator, kmol CO/m ³ cat-atm ² -s)	u_1	superficial velocity, m/s
$k_{\text{reg,14}}$	rate constant for oxidation of H ₂ to H ₂ O in the regenerator, kmol/m ³ cat atm ² s	V_p	velocity of the catalyst particle in the riser, m/s
$k_{13c,0}$	frequency factor for heterogeneous CO combustion, kmol CO/m ³ atm ² s	W	catalyst inventory in the regenerator, kg catalyst
$k_{13h,0}$	frequency factor for homogeneous CO combustion, kmol CO/m ³ atm ² s	x_i	mole fraction of the i^{th} lump
MW_C	molecular weight of coke, kg/kmol	x_{pt}	relative catalytic CO combustion rate
MW_{H_2}	molecular weight of H ₂ , kg/kmol	Z_{bed}	bed height of the dense phase in the regenerator, m
MW_g	average molecular weight of the gas oil feed, kg/kmol	Z_{comb}	height of the combustor, m
$MW_{g,\text{rgn}}$	average molecular weight of the vapour (O ₂ , CO, CO ₂ , H ₂ O, N ₂) in the regenerator, kg/kmol	Z_{dil}	bed height of the dilute phase in the regenerator, m
MW_i	molecular weight of the i^{th} lump, kg/kmol	Z_{rgn}	bed height of the regenerator, m
P_{CO}	average CO partial pressure in the regenerator, atm	z	axial height from the entrance of the riser or regenerator, m
P_{O_2}	average O ₂ partial pressure in the regenerator, atm		
P_{rgn}	combustor-regenerator pressure, atm		
P_{ris}	riser pressure at any location in the riser, atm		
Q_{air}	heat flow rate with air, kJ/s		
Q_C	heat released by carbon combustion, kJ/s		
Q_{ent}	heat input to the dense bed from entrained catalyst returning from the cyclone, kJ/s		
Q_H	heat released by hydrogen combustion, kJ/s		
$Q_{\text{loss,rgn}}$	heat loss from the regenerator, kJ/s		
$Q_{\text{loss,ris}}$	heat loss from the riser base, kJ/s		
Q_{rgc}	heat flow with the regenerated catalyst, kJ/s		
Q_{sc}	heat flow rate with the spent catalyst, kJ/s		
Q_{sg}	heat flow rate with gases from the dense bed of the regenerator, kJ/s		
R	universal gas constant, kJ/kmol K or atm m ³ /kmol K		
r_i	rate of the i^{th} reaction, kmol/kg cat s		
ROT	riser outlet temperature, K		
T	temperature in the riser at any axial location, K		
T_{air}	temperature of air to the regenerator, K		
T_{base}	base temperature for heat balance calculations (assumed to be 866.6 K), K		
T_{feed}	temperature of the gas oil feed, K		
T_{rgn}	temperature in the combustor/dense bed regenerator (= ROT), K		

Greek letters

$(\alpha_{ij})_k$	stoichiometric coefficient characterizing $k \rightarrow j$ in the i^{th} reaction
α, β, γ	parameters characterizing the deactivation of the catalyst
β_c	CO/CO ₂ ratio at the catalyst surface in the regenerator ($\equiv k_{\text{reg,11}}/k_{\text{reg,12}}$)
β_{c0}	frequency factor in β_c expression
ε	void fraction in the riser or regenerator
θ	residence time of the catalyst, s
ρ_{den}	density of the solids in the regenerator dense bed, kg solids/m ³ bed
ρ_{dil}	density of the solids in the regenerator dilute bed, kg solids/m ³ bed
ρ_g	molar density of the vapour in the regenerator, kmol/m ³
ρ_p	density of the porous catalyst, lb/ft ³
ρ_s	density of the porous catalyst, kg porous catalyst/m ³ porous catalyst
ρ_v	density of the vapour mixture at any location in the riser, kg/m ³
φ	catalyst activity
ψ	slip factor

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