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Improving vacuum gas oil hydrotreating operation via a lumped parameter dynamic simulation modeling approach

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ABSTRACT

A lumped parameter dynamic model, using both Excel® and HYSYS® software, for industrial refinery/upgrader VGO hydrotreaters has been developed from proprietary and public steady state hydrotreater models. The model is based on industrial plant data to track changes in intrinsic reaction rate based on catalyst deactivation, wetting efficiency, feed properties and operating conditions to provide useful information, such as required operating temperature, outlet sulfur composition and chemical hydrogen consumed. The model credibly simulates local disturbances, and represents the three distinct operating zones during hydrotreater run length (start, middle and end). This correlative, partially predictive model can be applied to demonstrate the tangible economic benefits of increasing hydrogen use to improve the operation of a hydrotreater by increasing run length and/or improving crude processing.

Keywords: Hydrotreating; Lumped parameter; Dynamic simulation; Vacuum gas oil

1. Introduction

Hydrotreating is a process that uses hydrogen and a catalyst to remove contaminants, primarily sulfur and metals from crude oil streams. Hydro-processing has become a key refiner/upgrader operation due to two key developments. First, transportation regulations for refined products have evolved to significantly reduce the maximum amount of sulfur allowed (ex. 30 ppm gasoline for US 2006: US Federal Register, 2000). Secondly, it is becoming necessary for refiners to process heavier, more sour crudes due to reduced availability of "sweeter" (low sulfur) crudes. As a consequence, refiners/upgraders (operators) need to remove more sulfur than previously required. Unfortunately, refiners/upgraders rarely achieve their run lengths and crude through-put objectives for vacuum gas oil (VGO) hydrotreaters (Golden and Martin, 2006 and Robinson, 2004). The performance shortfall is due to the occurrence of disturbances (crude flow, feed compositional, sulfur, metals, and/or hydrogen partial pressure changes) that reduce the effectiveness of the catalysts. Most public domain dynamic hydrotreater research, as noted by Korsten and Hoffmann (1996) and Thakur and Thomas (1985), is based on pilot plant data that does not translate well to industrial applications. A key element of this research project entailed gathering a substantial amount of relevant industrial data (14 operating industrial VGO units, with permission to publish data from six operators) specific to vacuum gas oil hydrotreaters. This paper describes the results from an extensive research by the author (Remesat, 2007) project to create a tool (semi-predictive, correlative dynamic simulation of a vacuum gas oil (VGO) hydrotreater) for refiners/upgraders to use for tracking the performance of a VGO trickle bed hydrotreater and to determine the benefits of increasing hydrogen partial pressure.

The specific objectives presented in this study can be summarized as follows:

1. Illustrate the effectiveness of the developed correlative, partially predictive model that simulates the process over the length of an industrial hydrotreater's operation incorporating the effects of catalyst activity specific to

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Nomenclature

asphaltenes	sum of asphaltenes in the feed (%)
aromatics	sum of aromatics in the feed (%)
A	frequency factor in Arrhenius equation
AF	activity factor
b	temperature effect factor
B	temperature corrected, catalyst fouling factor
Crackstock%	components in crude that will crack
d_p	particle diameter (MM or in.)
D	molecular diffusivity (ft^2/s)
DBT	dibenzothiophene
E_{act}	activation energy (energy/mol)
EF	catalyst efficiency factor
EOR	end-of-run
FR	fouling rate
g	H_2/oil ratio effect factor
g'	gravitational acceleration (ft/s^2)
G	H_2/oil ratio (SCFB)
G_a	Galileo number
HDS	hydro-desulfurization
k	forward reaction rate constant
k_i	equilibrium constant for a reaction
LHSV	space velocity (h^{-1})
M	mass flow (weight/h)
Met%	concentration of metals deposited on catalyst
MOR	middle-of-run
NiMo	nickel molybdenum
P	pressure (PSIA)
p	pressure effect factor
pH_2	hydrogen partial pressure (PSI)
q	percent of blocked sites on catalyst (%)
q_0	maximum percent of blocked sites for completely deactivated catalyst (%)
r_i	reaction rate of component i, mol/(vol.) (time)
R	universal gas constant, energy/(mol) (K)
RNC	catalyst deactivation factor, catalyst properties based
Re	Reynolds number (Ld_p/μ_L)
S	bulk sulfur (wt%)
SOR	start-of-run
T	temperature, °C, unless specifically noted otherwise
t	time
VGO	vacuum gas oil
VPSI	catalyst deactivation factor: activity, efficiency, kinetics
VPSIC	temperature corrected VPSI
WABT	weighted average bed temperature (°F)
Z	packed bed length (ft)

Greek letters

ε	Bed void fraction
ϕ	Ratio of catalyst sites blocked
η	Wetting efficiency
μ	viscosity, N_s/ft^2
ρ	density, LBS/ft^3
τ	Catalyst pellet tortuosity

Subscripts

c	catalyst
f	Feed
HDS	hydrodesulfurization
i	specific component
L	liquid
m	metals
p	product
s	sulfur
0	start-of-run

"start-of-run" (SOR), "middle-of-run" (MOR) and "end-of-run" (EOR).
2. Apply the model to determine economic ways to improve the operation of a VGO hydrotreater.

2. Methods and materials

The VGO hydrotreater model developed:

1. uses lumped parameters that match data available from industrial operations,
2. uses a mix of industrial correlations, kinetic theory and academic research findings,
3. factors in changes in operating conditions in response to disturbances in operation,
4. incorporates changing reaction rate, wetting efficiency, catalyst deactivation in the three zones of the hydrotreater run life,
5. uses parameters for all key process variables (sulfur, hydrogen partial pressure, temperature, hydrogen-to-oil ratio),
6. is run in dynamic mode to track the key variable product sulfur and the representative value of performance weighted average bed temperature (WABT),
7. incorporates familiar software (Excel® and HYSYS®) for easy translation into existing operations and acceptance by users,
8. is correlation based demonstrating semi-predictive tendencies, and
9. is used to represent a trickle bed reactor in operation.

2.1. *Data gathered*

Detailed industrial VGO hydrotreater data, under confidentiality agreement, was obtained and used from six refiners/upgraders. Catalyst, process and laboratory data, and equipment information was among the needed and gathered data. In summary, the following information was compiled for each operating unit modeled:

1. *Operating*: pressures, temperatures, flows over an entire operation (from start-up to shutdown).
2. *Frequent/reliable compositional laboratory data*: crude (including aromatics, cracked gas and olefins) off gas, hydrogen, contaminants (including sulfur, nitrogen, chlorides, and metals (vanadium, nickel and iron), bromine number.
3. *Equipment*: vessel size, pump sizes, piping sizes and control valves.
4. *Catalyst*: suggested equilibrium constants, reaction rates, catalyst physical properties (size and shape).

Tables 1a, 1b and 2 provide a sample of the information gathered from the industrial operating units.