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Front separation and 'locking' during hydrocarbons co-combustion in a loop reactor

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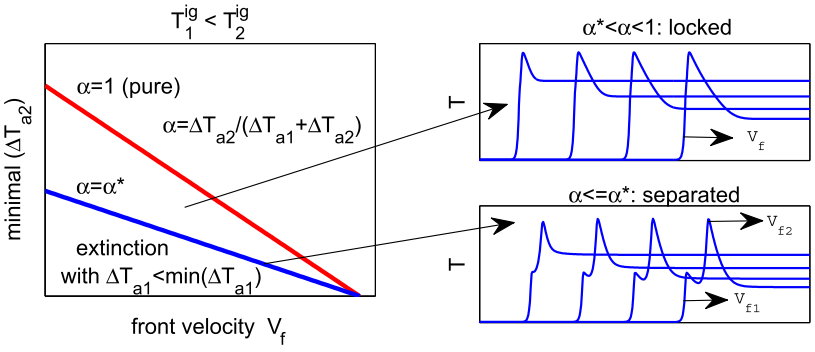
HIGHLIGHTS

- The dynamic patterns of Loop Reactors (LR) fed with two VOC's are analyzed.
- A proper design aims to force locked front patterns, similar to a single reaction.
- Approximations for the maximal temperature and the front velocity are proposed.
- Approximations are verified via once through reactor simulations.
- The operation domain of a forced operated loop reactor is well predicted.

GRAPHICAL ABSTRACT



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ABSTRACT

While previous studies experimentally demonstrated sustained operation in a loop reactor (using ethylene or methane combustion), and analyzed the single-reaction case and suggesting a proper control scheme, an actual implementation of VOC combustion will involve several reactants of varying concentrations. Here we study the dynamics and design implications of a bi-species (methane or ethane and ethylene) and a multi-species combustion. We observe two main structures in which the two fronts are either locked or are separated, with the combustion front of the less reactive component leading the other front. We explain why the locked front structure is favorable as it requires smaller energy investment. We derive approximations for the front properties (maximal temperature, T_{mi}, velocity, v_f) and the conditions for transition and portray these in the plane T_m vs Lev_f in a long once-through reactor. We show that these maps predict well the behavior in loop reactors.

1. Introduction

The loop reactor is composed of several units ($N \geqslant 2$) with a feed port and an exit port that are switched at every predetermined time interval σ. Fig. 1 presents a three-unit system: In the first interval, the feed flow enters the first reactor and exits from reactor N (denoted as units A, C in Fig. 1a). Under proper operation conditions a hot spot propagates within unit A. This pattern will continue as long as the heat front is far from exiting the first reactor. At the second interval, the feed flow enters the second reactor (B), and exits from the first reactor (A), and so on.

The loop reactor is a process that combines a catalytic packed bed with enthalpy recuperation and its main application should be for low-concentration Volatile Organic Carbon (VOC) combustion. The idea was suggested by Matros [1], the simulations for a case of two units were conducted by Haynes and Caram [2] and extended for a three-unit system by Barresi et al [3,4]. An asymptotic solution was suggested by Sheintuch and Nekhamkina [5,6] for an adiabatic reactors based on the analysis of the front

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Notations

Symbols

A_i	pre-exponential factor (8.54×10^9, 7.44×10^9 and 2.18×10^9 for ethylene, ethane and methane, respectively)
B	dimensionless temperature rise
C	molar density (gmole m^{-3})
c	dimensionless mole fraction (ppm)
C_{pg}	gas heat capacity (1.07 kJ kg^{-1} K^{-1})
C_{ps}	solid heat capacity (1.51 kJ kg^{-1} K^{-1})
d	reactor diameter (28.5×10^{-3} m)
D	effective axial mass dispersion (5×10^{-3} m^2 s^{-1})
Da	Damkohler number
E_i	activation energy (93.57, 114 and 147 kJ/mol for ethylene, ethane and methane)
$F(\omega,\kappa)$	function, defined by Eq. (5)
k_s	solid thermal conductivity (1.8×10^{-3} kJ m^{-1} s^{-1} K^{-1})
L	reactor length (L_0 = 0.9 m)
Le	Lewis number ($[(1-\varepsilon)(\rho C_p)_s]/[\varepsilon(\rho C_p)_g]$ = 2139)
Pe	Peclet number for heat
Q_i	kinetic function defined by Eq. (4)
r_i	reaction rate (gmole m^{-3} s^{-1})
R_i	dimensionless reaction rate
R_g	gas constant (8.314 kJ $kmole^{-1}$ K^{-1})
t	time (s)
T	temperature (K)
U	heat transfer coefficient (1.75×10^{-4} kJ m^{-2} s^{-1} K^{-1})
u	gas velocity (0.62 m/s)
v	switching and front velocity (m/s)
x_i	conversion
y	dimensionless temperature
z	axial coordinate (m)

Greek letters

α	less reactivity component fraction defined by Eq. (22)
β	dimensionless heat transfer coefficient ($\beta = 4UL/d(\rho C_p)_g u$ = 0.06)
γ_i	dimensionless activation energy
$\Delta T_{a,i}$	adiabatic temperature rise (K)
$\Delta T_{m,i}$	maximal front temperature rise (K)
ΔH_i	heat of combustion (J mol^{-1})
ε	bed void fraction (0.65)
λ	parameter defined by Eq. (A.4)
κ	parameter defined by Eq. (5)
σ	switching period (s)
ξ, ζ	dimensionless axial coordinate
ρ_g	gas density
ρ_s	solid density (1540 kg m^{-3})
τ	dimensionless time
ω	dimensionless front and switching velocity

Subscripts

ex	exit
f	front
g	gas
in	inlet
ig	ignition
lim	limiting
m	maximal
sw	switching
th	thermal
tot	total

Superscripts

loc	locked
sep	separated
sb	separated boundary

Abbreviates

ATR	adiabatic temperature rise
LR	loop reactor
OD	operation domain

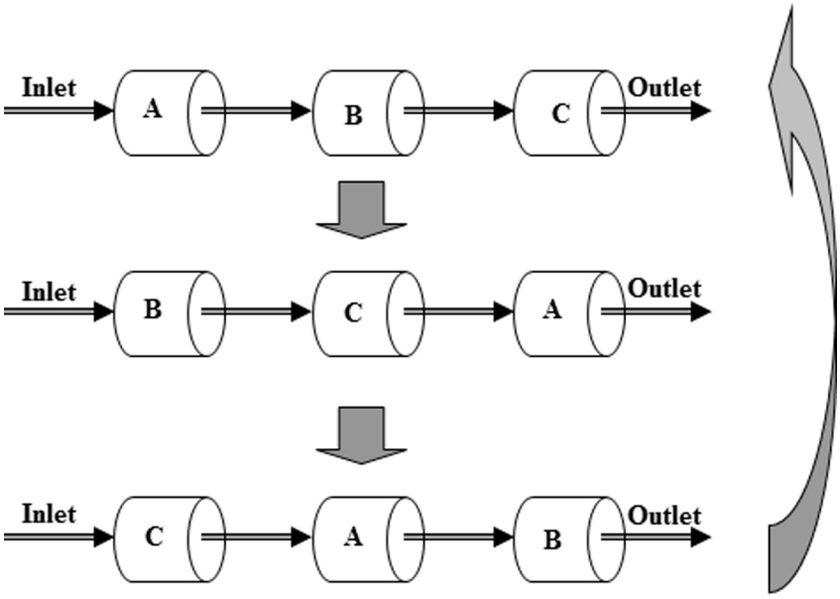

Fig. 1. A scheme of a three-unit (A, B, C) loop reactor: The feed and exit port positions vary periodically.