# Fischer-Tropsch Reactor Model in VBA for Excel

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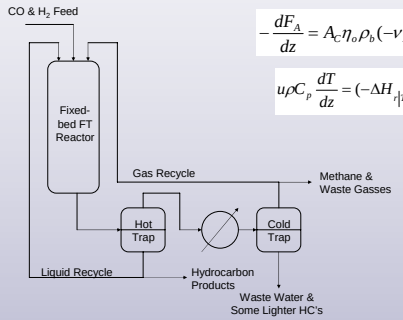
Objective: Develop and validate a 1-D Fixed-bed reactor model that accurately reflects industrial reactor behavior

## Model Description

The reactor model is a shell and tube heat exchanger with catalyst pellets on the tube side and high-pressure boiling water on the shell side. The user specifies the final CO conversion and the VBA code solves the design equations[1,2] by a 4th order Runge-Kutta algorithm at fixed steps (typically 3 mm) down the reactor until the desired conversion has been reached. Kinetic equations, catalyst geometry, catalyst properties, and reactor conditions are user inputs.




$$-\frac{dF_A}{dz} = A_C \eta_o \rho_b (-\nu_A) r \qquad \frac{dP}{dz} = \frac{\delta_{GW}}{(1-\varepsilon_L/\varepsilon)^3} - \rho_g g_c$$

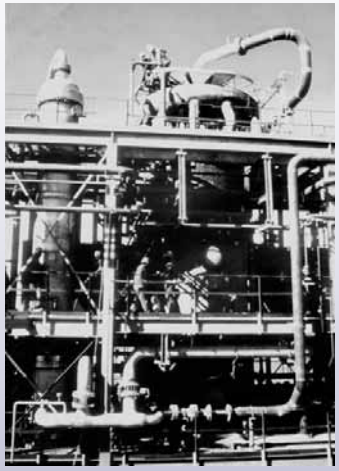
$$u\rho C_p \frac{dT}{dz} = (-\Delta H_{r|T^0})\eta_o \rho_b (-\nu_A) r - \frac{4U}{d_t}(T - T^*)$$

www.icat.dtu.dk/intro/index.html

Table 1. Representative Kinetic Models For Co and Fe Used in Model Validation

| Data Source | Rate Expression Form | A ($atm^{-1.25}s^{-1}$) | $E_A$ (J/mol) | B ($atm^{-1}$) | $\Delta H_R$ (J/mol) |
|---|---|---|---|---|---|
| Generalized kinetics | $-r_{CO} = \frac{A P_{CO}^{1/2} P_{H_2}^{1/2}}{\left(1 + B P_{CO}^{1/2} P_{H_2}^{1/2}\right)^2}$ | 1.27E+08 | 90,927 | 0.0750 | -6,753 |
| GH Kinetics | $-r_{CO} = \frac{A P_{CO}^{1/2} P_{H_2}^{1/2}}{\left(1 + B P_{CO}^{1/2} P_{H_2}^{1/2}\right)^2}$ | 1.70E+08 | 84,800 | 0.0180 | -26,100 |
| Unpublished kinetics | $-r_{CO} = \frac{A P_{CO}^{1/2} P_{H_2}^{1/2}}{\left(1 + B P_{CO}\right)^2}$ | 6.49E+05 | 73,000 | 3.05E-04 | -23,629 |

## Industrial Significance



http://www.engin.umich.edu/~cre/01chap/html/reactors/sasol.htm

- Fischer-Tropsch (FT) synthesis has been commercial since WWII
- FT technology has become a viable alternative source of liquid fuels due to concern over foreign oil dependence and fuel prices
- Feed stocks include natural gas, coal, biomass, and garbage.
- Fixed-bed design is simplest and most economical for smaller scale production
- This model demonstrates ability to:
  - –Develop relatively cheap, robust codes
  - –Gain insight into reactor design issues
  - –Explore ranges of operating parameters

## Model Validation

- Partial validation using Shell Bintulu plant data
- 9 design parameters constrained by the Shell report
- 7 design parameters assumed/adjusted
- 3 of 4 performance parameters matched within 10% of reported values

| Parameter | $Co/ZrO_2/SiO_2$ (Shell) Reported[3] | Assumed |
|---|---|---|
| **Input/Operating Parameters** | | |
| HC Production (bbl/day) | 6,700 | |
| % CO | – | 32.3 |
| $H_2$/CO Ratio | 2.15 | |
| Inlet Temp (K) | – | 468 |
| Pressure in (bar) | 40 | |
| Recycle Ratio | – | 3.0 |
| CO conversion (%) | – | 75 |
| $C_{5+}$ Selectivity | 96 | |
| $CH_4$ Selectivity | 4 | |
| $CO_2$ Selectivity (% of CO converted) | 1 | |
| **Reactor/Catalyst Characteristics** | | |
| Tube diameter (cm) | 5.0 | |
| Number of tubes | 8,000 | |
| Cooling water Temp (K) | – | 460.5 |
| Catalyst particle diameter (mm) | 2 | |
| Bed void fraction | – | 0.40 |
| Catalyst activity | – | 0.20 |

http://www.bda.gov.my/investment/Projects.htm

| Output/Performance Parameters | Reported | Calculated |
|---|---|---|
| Effectiveness factor | – | 0.96 |
| Space velocity ($h^{-1}$) | – | 1,139 |
| Pressure drop (atm) | – | 0.28 |
| Tube length (m) | **20** | **19.4** |
| Catalyst charge ($m^3$) | **310** | **301** |
| Catalyst productivity ($g_{C_{5+}}/g_{cat}$-h) | **0.092** | **0.12** |
| Outlet or Maximum Temp (K) | **510** | **474** |

## Model Characterization

### Kinetic Model Study

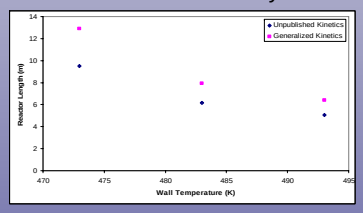



Figure 1. Inlet T vs. Reactor Length for Generalized & Unpublished Co kinetics

### Recycle Ratio Study

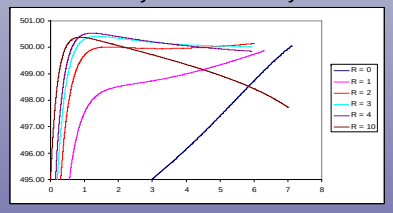



Figure 2. Parametric study of recycle ratio for Generalized Co Kinetics

### Pressure Study

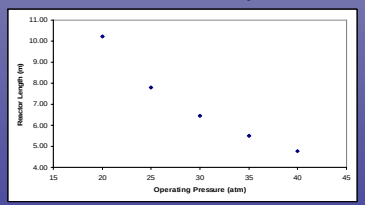



Figure 3. Operating P vs. Reactor Length

### Particle Diameter Study

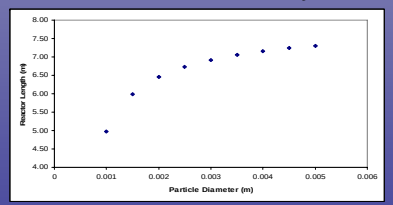



Figure 4. Particle Diameter vs. Reactor Length (effective diffusion length held constant)

[1]Davis, M. E. *et al, Fundamentals of Chemical Reaction Engineering*; McGraw Hill: Boston, 2003.
[2]Froment, G. F.; Bischoff, K. B. *Chemical Reaction Analysis and Design*; 2nd Edition; Wiley Series in Chemical Engineering: New York, 1990; pp. 620-625.
[3]C. H. Bartholomew and R. J. Farrauto, *Industrial Catalytic Processes*; 2nd Edition; John Wiley & Sons, Inc., New Jersey, 2006. Chapter 6 & p. 459