납사 분해로의 모사 속도 향상을 위한 CRACKER 개선

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Fast Simulation for Naphtha Furnaces by Modification of CRACKER

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Introduction

Since ethylene is the basic material in the chemical industry and its market price is rapidly changing, the optimal operation of the ethylene plant is very important. Especially, the thermal cracking furnace is the most important unit in the ethylene plant because it determines the final productivity of the whole plant. The key factor of optimal design and operation in the furnaces is the precise prediction of yields and performance of cracking reactor furnace. Because of the importance of that prediction, development of industrial simulators for furnaces is highly regarded in the ethylene production fields [1].

To find an optimal operation strategy, it is crucial to observe the influence of operating parameters, which can be calculated through the rigorous model with proper reaction mechanisms. In CRACKER, the cracking furnace is modeled based on first principles and solved in practical operation ranges. The base furnace model of this paper is similar to CRACKER's but the calculation procedure is modified to improve the calculation speed and accuracy.

Since numerical difficulties exist due to differences between radical and molecule concentrations and much larger problem size, these decelerate the calculation speed [2]. In this paper, the calculation procedure for radiant box and the reactor sections of CRACKER is modified to increase the simulation speed and accuracy of the results.

This program is written using FORTRAN90. DNSQE, which uses modified Powell method, is applied for nonlinear equations set. For differential algebraic equations set, DASSL, which is made by Linda Petzold, is used [3]. The physical properties, such as heat capacities and heat of reactions, are obtained from CHEMKIN III library [4].

Fundamental Models

For the well-balanced mechanistic models, it is necessary to know the reactions taking place in the reactor. Owing to the complexity of the naphtha feed composition and the radical nature of the reactions, thousands of reactions can occur among the various free radical species [2]. This program uses the free-radical reaction set with the kinetic parameters which is the same as CRACKER. This reaction set has 84 species and 358 reactions.

The governing equations for the cracking coil constitute the two-point boundary value problem which has a significant stiffness in numerical simulation due to the large difference of concentration gradient between radicals and molecules. The general governing equations are represented as a differential algebraic equations set. They are shown in equations (1)~(3).

$$-W\frac{\partial g_i}{\partial z}+\sum_{j=1}^{m} f_{ij} MW_i = 0, \quad \sum_{i=1}^{NC} g_i = 1.0, \quad f_{ij} = k_j \prod_l C_l^{|\nu_{lj}|} \qquad if\ \nu_{lj} < 0 \tag{1}$$

$$\rho C_p V \frac{\partial T}{\partial z} = \sum_{j=1}^{m} (-\Delta H_j) f_j + \frac{UP}{A}(T_a - T), \quad f_j = \sum_i v_{ij} f_{ij}, \quad k_j = A_j \exp(-E_{aj}/RT) \tag{2}$$

$$-W\frac{\partial V}{\partial z} - \frac{\partial p}{\partial z} - \frac{P}{A}\rho V^2 f = 0, \quad V = W/\rho \tag{3}$$

The radiant box supplies heat to the cracking coils by burning fuels. To calculate the fired gas temperature in the radiant box, the one gas zone method is chosen to handle various types of reactor configuration and to simplify the whole problem. The radiant properties are calculated by the weighted sum of gray gases model. [5]

Simulation Procedure

In the current version of CRACKER, the reactor is simulated based on the given CIP (coil inlet pressure) and the CIT (coil inlet temperature). The T_{skin} (tube skin temperature) is calculated using the given fuel and excess air data. But this is impractical in the real plant. In the real ethylene plant, only the coil outlet pressure is known. Because this furnace reactor simulation is a two-point boundary value problem, CIP should be estimated based on outlet pressure to solve this as a initial value problem.

To predict the unknown variables, inlet pressure and T_{skin}, the simulation procedure is divided into two parts. The first part is CIP loop in Fig 1 which finds the CIP with good accuracy. In this part, BISECT method is used to find inlet the pressure under the given outlet pressure condition because the simulation results are very unstable through the predicted inlet pressure ranges. The second part, T_{skin} loop in Fig 1, solves the overall energy balance equations under the condition that the absorbed heat by the reactor is equal to the released heat from the radiant box. The detail procedure for this modification is shown in Fig 1. All the required inputs are furnace geometry, reactor configurations, stream information, and operating conditions. Once all the required data are given properly, the mass, energy, and momentum balance equations with the kinetic reaction mechanisms are simultaneously solved using physical and chemical properties of hydrocarbons and steam.

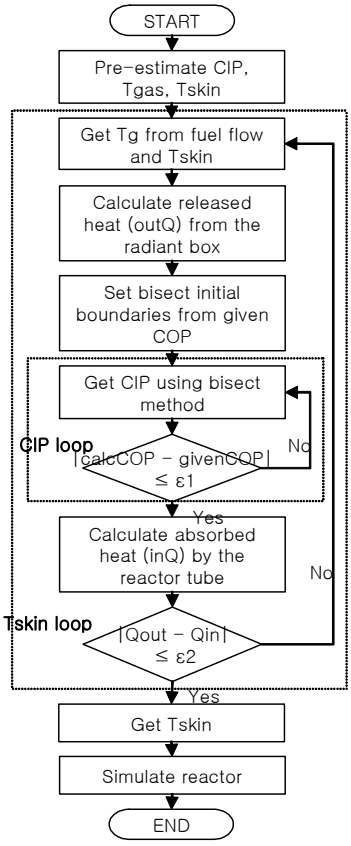

Fig. 1. Modified simulation procedure flow diagram

Examples

(1) Example 1: Calculation time for CIP and Tskin estimation

Since the original CRACKER calculates T_{skin} based on the given CIP, the simulation time of modified program is compared for only T_{skin} loop calculation. In this case, CPU time required for a solution ranges between 50 and 800 seconds on Pentium 4 1.7G computer depending on the reactor length and convergence option selected.

Table 1. Calculation times for loop conditions

Case	Calculation time (sec)
One-cycle	11.59
CIP-loop-only	216.83
T_{skin}-loop-only	89.81
CIP+T_{skin}-loop	3326.80

To test the total simulation time, we compared 4 cases: one-cycle, CIP-loop-only, T_{skin}-loop-only, and CIP+T_{skin}-loop cases. In one-cycle case, both of the CIP and the T_{skin} are given. This case roughly shows the calculation time for one reactor

loop. CIP-loop-only case simulates using given T_{skin} datum. In this case, only the CIP loop in Fig 1 is used. T_{skin}-loop-only case is same as CIP loop only case except that the CIP is given instead of the T_{skin}. CIP+T_{skin}-loop estimates both of the inlet pressure and T_{skin}. Table 1 shows the calculation time for each case.

In this example, we can notice that the CIP loop spends much time through all calculation of cracking reactor simulation. The reason of this time consumption is that the cracking reactor system is very unstable and sensitive to the change of CIP. If the user knows the exact inlet pressure, this modified program shows fast calculation speed.

(2) Example 2: Ethane cracker

In this example, the simulation results for the ethane cracker are compared with the reactor design data and the results of original CRACKER. The ethane cracking reactor which is used for this example has the reactor coil of 73.794m length. The results for the design, the original CRACKER, and the prediction by the modified program are compared in Table 2. The predicted results of the modified program shows good agreement with the furnace design data. Figures 2 and 3 shows the temperature, pressure and composition profiles through the reactor length for the original and the modified programs. While the modified program shows almost same pattern of profiles in these figures. it requires shorter calculation time than the original CRACKER. The calculation times are shown in Table 2.

Table 2. Ethane cracking: results comparisons

	Design	CRACKER	Modified
TMT (K)	-	1270.26	1332.62
CIT (K)	946.00	946.00	946.00
COT (K)	1124.00	1120.93	1123.95
CIP (kPa)	270.54	270.54	270.54
COP (kPa)	174.28	176.53	174.20
Conversion (%)	65.00	65.5	66.0
C2H4 (%)	-	48.0	48.4
C3H6 (%)	-	3.2	3.2
Calculation time (sec)		734.13	45.38

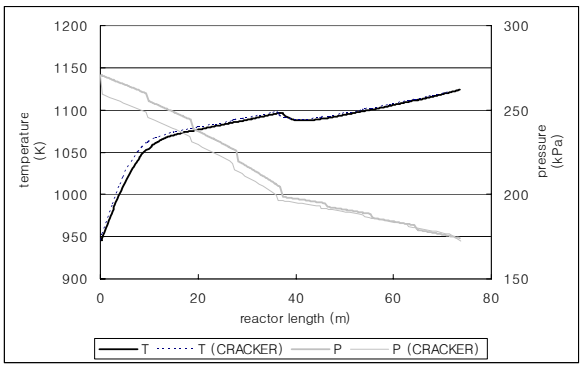

Fig 2. Temperature and pressure profile for ethane cracker

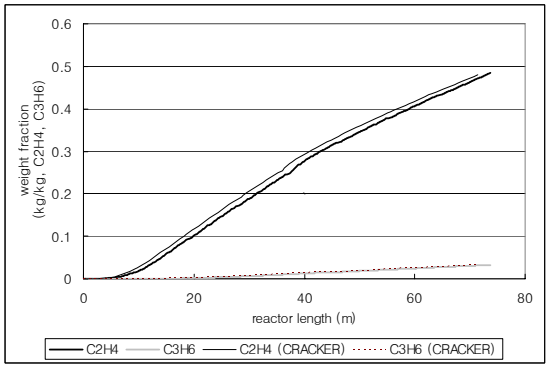

Fig 3. Composition profiles of C_2H_4 and C_2H_4 for ethane cracker

(3) Example 3: Naphtha cracker

in this naphtha cracker example, one of the industrial naphtha cracking furnaces is simulated. the naphtha cracking reactor length is 25.618m which is shorter than the length of the ethane cracking reactor in example 2. The results of CRACKER and modified program are reported with the operating data in Table 3. The modified program shows well fitted results with the operating conditions. The modified program shows shorter calculation time than the original CRACKER. In this simulation, the calculation time is shorter than the previous ethane cracker example because the reactor length of the naphtha case is shorter than the ethane case. The detail composition, temperature and pressure profiles along the reactor length are presented in Figures 4 and 5.

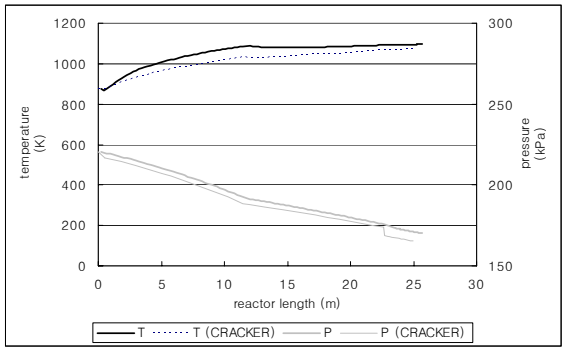

Fig 4. Temperature and pressure profile for naphtha cracker

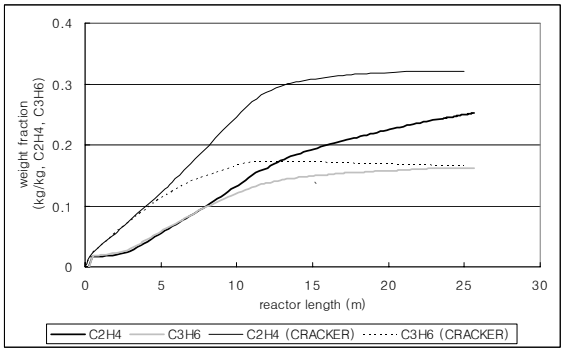

Fig 5. Composition profiles of C_2H_4 and C_2H_4 for naphtha cracker

Conclusion

Because coil outlet pressure and coil inlet temperature are given from the real plant data, coil inlet pressure should be estimated for the furnace simulation. To estimate it, the cracking furnace simulator, CRACKER, is modified by the proposed procedure. In this procedure, the simulation speed is faster than the existing CRACKER. The modified program shows the well estimated coil inlet pressure and the cracking results profiles.

Table 3. Naphtha cracking: results comparisons

	Design	CRACKER	Modified
TMT (K)	-	1157.98	1284.13
CIT (K)	874.00	874.00	874.00
COT (K)	1095.00	1071.49	1095.89
CIP (kPa)	220.50	220.50	220.50
COP (kPa)	168.56	165.47	168.87
C2H4 (%)	-	32.1	25.2
C3H6 (%)	-	16.6	16.3
Calculation time (sec)		1157.98	30.72

Due to the improved simulation speed and the accuracy of this program, the modified program can be used for determining the optimal operation of cracking furnaces. This can be expected to help to maximize the plant efficiency and profit.

Acknowledgement

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