Non-stationary mathematical modelling of pyrolysis of gasoline fraction

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RELEVANCE

Nowadays, large amounts of ethylene and propylene are obtained with pyrolysis

These alkenes are as feedstock in production of the most common polymers (PET, PVC, polystyrene, etc.)

Thus, there is large and non-decreasing demand for them in the global market and production volumes are to be increased accordingly

THE PROBLEM

The process is complicated by side reactions, which lead to formation of coke deposits on walls of furnace coils

In turn, this causes a number of problems in production line with corresponding consequences

SOLUTION

Thus, creation of a non-stationary model is proposed, which allows to describe changes in properties over time to get ability to predict the state of the process

This will help reduce the accident rate, increase the inter-regeneration cycle, increase the yield of monomers, and also increase the preparedness of personnel for emergency situations

OBJECTIVES

- Obtain control over coke deposition rate by changing process conditions taking in the account time-variant composition of feedstock
- Form a strategy to preserve performance while maximizing the inter-regeneration cycle

THE MODEL

Exponential equations of rate constants:

$$K_j = K_{0j} \cdot \left(\frac{P^2}{T}\right) \cdot \exp\left(\frac{-E_j}{RT}\right)$$

K_{0j} – pre-exponential coefficient, P –pressure, atm., T – temperature, °K, E_j – activation energy, J/mole.

Forth-order Runge-Kutta equations for each of components:

$$A_{1,i} = \sum_j a_{i,j} \cdot K_j \cdot \prod C_k^{\beta_{k,j}}$$

$$A_{2,i} = \sum_j a_{i,j} \cdot K_j \cdot \prod \left(C_k + \frac{h}{2} A_{1,i}\right)^{\beta_{k,j}}$$

$$A_{3,i} = \sum_j \alpha_{i,j} \cdot K_j \cdot \prod \left(C_k + \frac{h}{2} A_{2,i}\right)^{\beta_{k,j}}$$

$$A_{4,i} = \sum_j \alpha_{i,j} \cdot K_j \cdot \prod \left(C_k + h \cdot A_{3,i}\right)^{\beta_{k,j}}$$

α_{ij} – stoichiometric coefficient of component i in reaction j, β_{kj} – stoichiometric coefficient of reactant k in reaction j, C_k – concentration of component k, mole/l., h – integration step, s.

Changes of concentrations are calculated as follows:

$$\frac{dC_i}{d\tau} = \frac{h}{6}\left(A_{1,i} + 2A_{2,i} + 2A_{3,i} + A_{4,i}\right)$$

Coke volume accumulated on each step of integration is calculated in order to calculate its thickness:

$$V = \exp(0.023 \cdot C_{\text{coke}} - 1) \cdot G^{0.8} \cdot (D - 2 \cdot \delta)^{-1.8}$$

$$\delta = \frac{d}{2} - \sqrt{\left(\frac{d}{2}\right)^2 - \frac{V}{\pi \cdot h}}$$

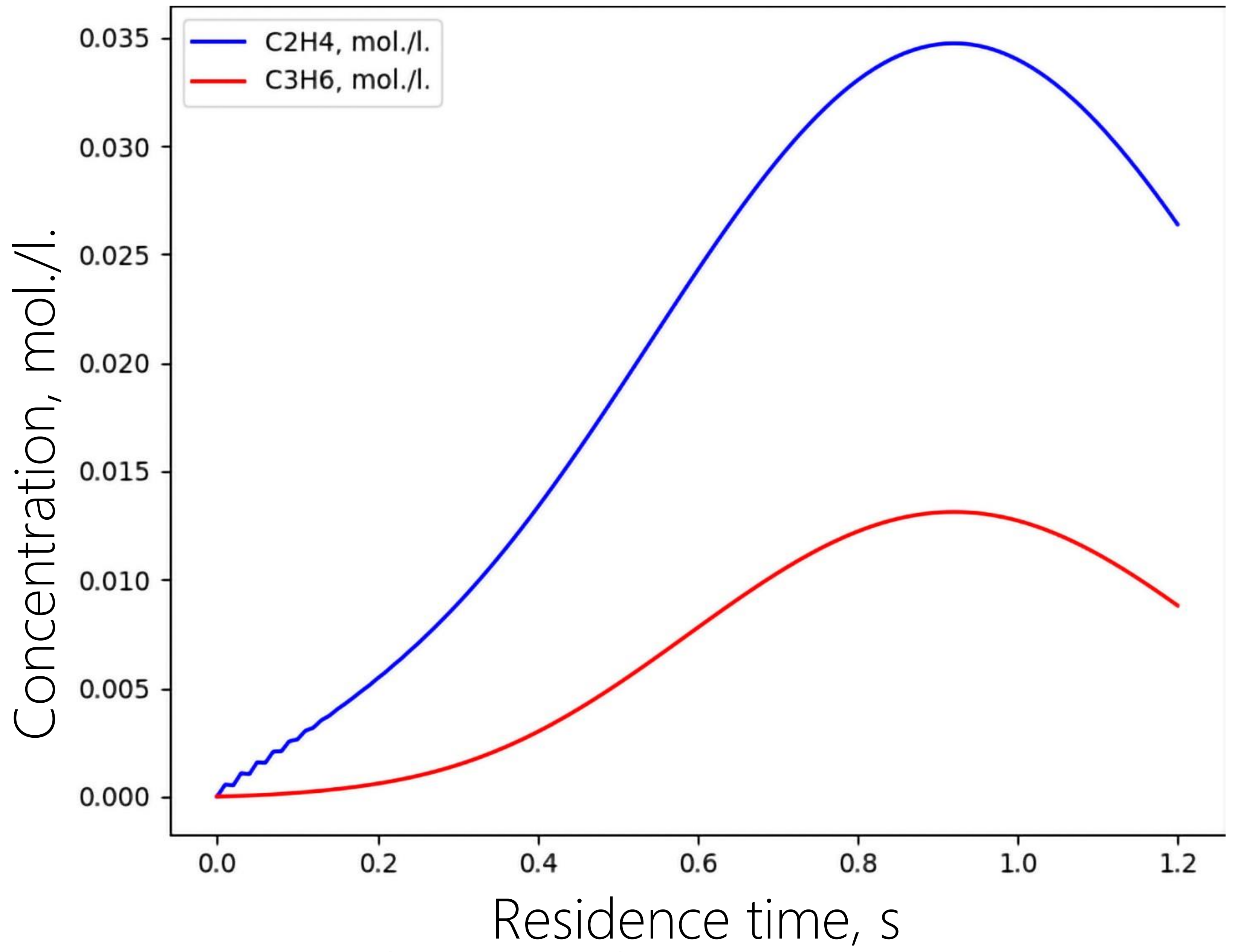

Fig 1. Ethylene and propylene concentration dynamics along the furnace coil

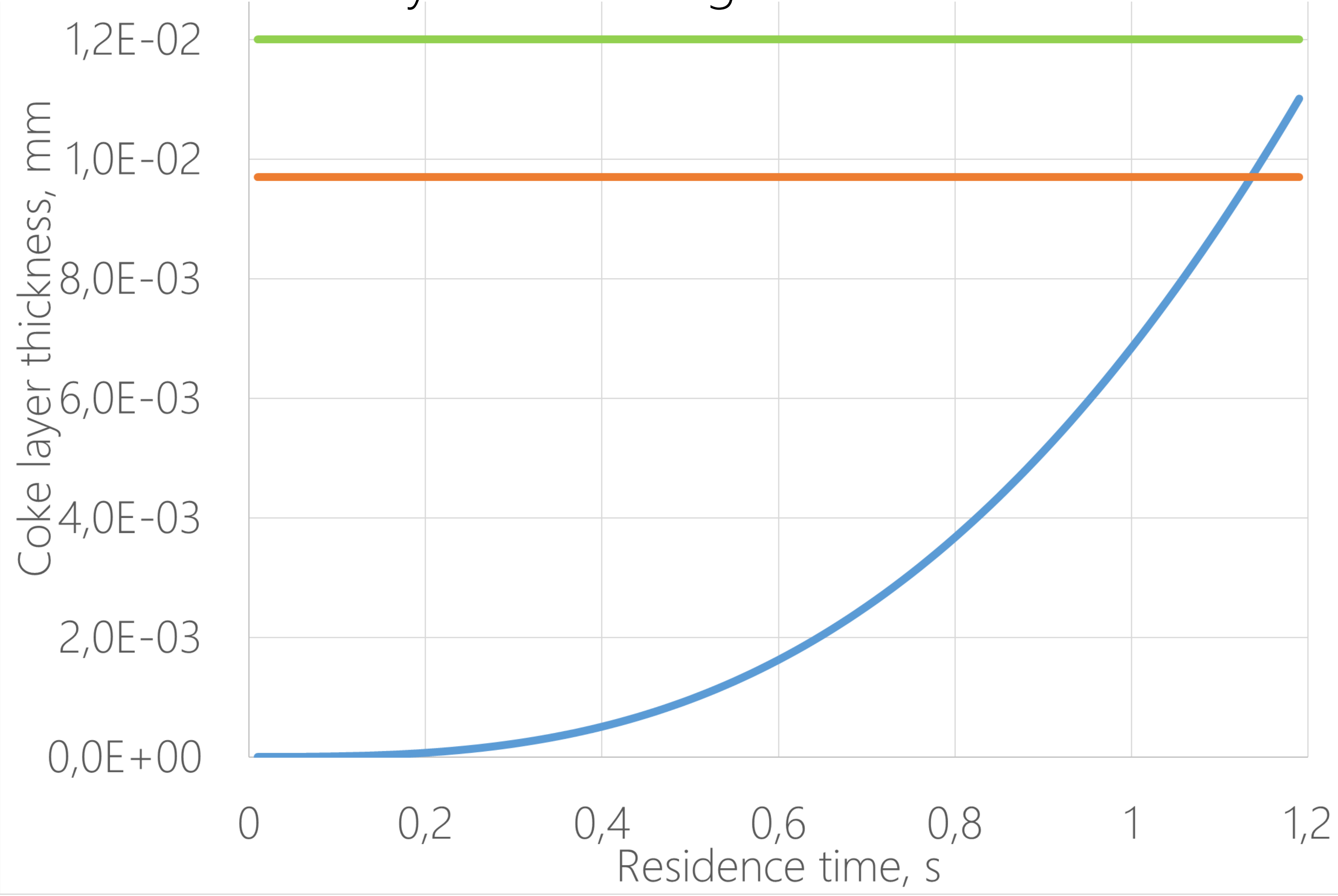

Fig 2. Comparison of calculated coke layer growth vs estimates via experimental data

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