ELSEVIER

Chemical Engineering Journal 134 (2007) 3–10

Chemical Engineering Journal

www.elsevier.com/locate/cej

Dimensional analysis for scaling up and down steam cracking coils

Kevin M. Van Geem*, Robert Žajdlík,
Marie-Francoise Reyniers, Guy B. Marin

Laboratorium voor Petrochemische Techniek, UGent, Krijgslaan 281 (S5), B-9000 Gent, Belgium

Abstract

The theory of similarity is applied to scale-up or down steam cracking coils. Dimensional analysis of the model equations shows that scale-up is possible under partial similarity only. Inevitably this leads to differences in product yields between units of different scale. However, careful relaxation of the criteria of similarity can limit scale dependent influences. Two different relaxation strategies are distinguished; the first one aims at realizing the same axial pressure profile neglecting radial non-uniformities, the second focuses on realizing the same radial temperature profile. Neglect of similarity of the radial temperature profile leads to larger differences as compared to differences resulting from neglect of the similarity of the axial pressure profile. In the case of ethane cracking, differences between units of different scale resulting from neglecting the similarity of the radial temperature profile can be up to 4.0% (rel.) for the conversion and up to 1.8% (rel.) for the ethylene yield. This insight is used to design the ideal pilot plant reactor to scale down different industrial reactors.

© 2007 Elsevier B.V. All rights reserved.

Keywords: Scale-up; Chemical reactors; Mathematical modeling; Dimensional analysis

1. Introduction

Designing a pilot plant reactor for steam cracking based on an industrial scale reactor or vice versa is not straightforward. Steam cracking is an endothermic process and is operated at high temperatures. Next to the intrinsic chemical kinetics, heat and mass transport processes, which are scale dependent, affect the product yields. Product yields obtained in a small-scale reactor and in a large-scale reactor will only be identical provided that mass and heat transfer processes are similar and the "chemistry" remains the same. Two different methods are commonly applied in scale-up and scale-down: direct experimental scale-up and mathematical modeling. Mathematical modeling is the most attractive solution because it has the advantage that once the model is developed, results can be gathered easily and computer simulations take only a limited time [1–4]. One of the major challenges in this approach consists of developing a fundamental reaction network. Moreover, fundamental kinetic models require a detailed feedstock composition and obtaining this information for complex hydrocarbon mixtures is not straightforward. Therefore, direct experimental scale-up remains an interesting option and developing a pilot plant installation or an even smaller laboratory scale installation is still practiced [5]. However, the differences in dimensions and typical operating conditions between industrial reactors, pilot plant reactors and laboratory scale reactors result in differences between the obtained conversions and product yields. Generally, the direct scale-up method is based on the "severity" concept. Scale-up is then performed based on experimental data obtained at the same severity [6,7]. The theory of similarity on the other hand focuses on the construction of a small-scale unit similar to an industrial one and operating it under conditions of complete or partial similarity to realize the same product spectrum. According to the theory of similarity, two processes can be defined as similar if they take place in a similar geometrical space, and if all the dimensionless numbers necessary to describe the process, have the same numerical value. If complete similarity cannot be realized, e.g. for an adiabatic reaction preservation of mass, impulse and energy is not possible when the scale is changed [8], working under partial similarity can offer an alternative solution. The latter implies that the influences of "non-similarities" are verified. Only if a negligible influence on scale-up or scale-down is found, the data can be directly transferred to another scale with reasonable accuracy. The main subject of this article is to determine the conditions that allow accurate transfer of data between steam cracking reactors of different scales. Other inter-

---

* Corresponding author. Tel.: +32 9 264 45 17; fax: +32 9 264 49 99.
E-mail address: kevin.vangeem@ugent.be (K.M. Van Geem).

1385-8947/$ – see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.cej.2007.03.065

Nomenclature

c_p	heat capacity (kJ kmol^{-1} K^{-1})
C_j	concentration of component j (kmol m^{-3})
CIP	coil inlet pressure (MPa)
CIT	coil inlet temperature (K)
COP	coil outlet pressure (MPa)
COT	coil outlet temperature (K)
D	diffusion coefficient (m^2 s^{-1})
Da	Damköhler number
d_t	internal tube diameter (m)
Eu	Euler number
f	Fanning friction factor
Fo	Fourier number
$\Delta_r H^\circ$	standard reaction enthalpy (kJ kmol^{-1})
k^0_{ref}	reference reaction rate coefficient (s^{-1})
L	reactor length (m)
M_j	molecular weight of component j (kg kmol^{-1})
n	scale factor
p_t	total pressure (MPa)
Pe	Peclet number
q	heat flux (kJ m^{-2} s^{-1})
r	radial position (m)
r_b	radius of the bend (m)
r_V	reaction rate (kmol m^{-3} s^{-1})
$r_{c\,j}$	coking rate of reaction in which j participates (kg m$^{-2}{}_{reactor}$ s^{-1})
Re	Reynolds number
T	process gas temperature (K)
v	velocity (m s^{-1})
z	axial coordinate (m)

Greek symbols

α	conversion factor depending on the units of p_t
λ	thermal conduction coefficient (kJ m^{-1} s^{-1})
μ	dynamic viscosity (Pa s)
$\nu_{k,j}$	stoechiometric coefficient of the component j in the reaction k
θ	dimensionless temperature
ρ	density of the process gas mixture (kg m^{-3})
τ	residence time (s)
τ_{Dr}	time scale for radial diffusion (s)
τ_w	shear stress (kg s^{-2} m^{-1})
$\tau_{\lambda r}$	time scale for radial conduction (s)
ξ	normalized radial position
ζ	Nekrasov factor for bends

Sub- and superscripts

a	axial
j	component
r	radial
0	initial
′	dimensionless

esting aspects such as the effect of the feedstock, the reactor geometry and the role of coke formation on scale-up are also discussed.

2. Direct experimental scale-up based on the theory of similarity

The theory of similarity enables to determine dimensions and operating conditions for a simulation unit of smaller scale similar to an existing industrial unit (scale-down) or vice versa (scale-up). Complete similarity requires geometrical, material, and process-related similarity [9]. For example material similarity for steam cracking implies that the same feedstock is used, the material of the reactor remains the same, the same diluent is used, etc. Only when complete similarity between a small scale and an industrial unit is achieved, the results of the experimental data obtained in the small-scale unit can be safely transferred to the industrial scale unit. Whether or not two processes are completely similar depends on meeting the criteria of similarity. All corresponding criteria of similarity must have the same value in both systems, e.g. the same Reynolds numbers. These criteria consist entirely of dimensionless numbers and can be found by dimensional analysis. Dimensional analysis is based upon the fact that a mathematical formulation of a chemical or a physical process can only be of general validity if it is dimensionally homogenous, i.e. if it is valid in any system of dimensions [10]. The set of dimensionless numbers resulting from dimensional analysis is called the Π-set. The most efficient way to gather the dimensionless numbers is based on the mathematical description of the process [11]. Traditionally a one-dimensional reactor model is employed in commercial steam cracking software, e.g. SPYRO [12], CRACKER [3] and COILSIM [2]. However, in some cases the implementation of two or three-dimensional reactor models becomes inevitable, e.g. for cracking coils with internally finned tubes [13]. These more-dimensional models are able to give sufficiently accurate results, also for the simulation of reactors operated at extremely high severity [14]. One of the main reasons to use more-dimensional models for simulation is the existence of a significant radial temperature gradient in industrial cracking coils. Elvers et al. [15], Sundaram and Froment [16] and Van Geem et al. [17] showed that for industrial reactors the radial temperature drop from the wall to the gas core is in the order of 100 K. Furthermore, this radial temperature drop is the origin of small but significant differences between the product yields simulated using a one- and two-dimensional reactor model [18]. Therefore, we have opted to determine the complete Π-set based on the two-dimensional reactor model equations. The mass balance for a component j over an annulus with height dz, internal radius r and external radius $r + \mathrm{d}r$ leads to the continuity equation for component j in the process gas mixture [8]:

$$\frac{\partial}{\partial z}(v_a C_j) + \frac{1}{r}\frac{\partial}{\partial r}(r v_r C_j) - \frac{\partial}{\partial z}\left(D_a \frac{\partial C_j}{\partial z}\right) - \frac{1}{r}\frac{\partial}{\partial r}\left(r D_r \frac{\partial C_j}{\partial r}\right) = \sum_i \nu_{i,j} r_i \tag{1}$$

The corresponding energy equation is given by:

$$\frac{\partial}{\partial z}(v_a T) + \frac{1}{r}\frac{\partial}{\partial r}(r v_r T) - \rho c_p \frac{\partial}{\partial z}(r v_r T)\left(\lambda_a \frac{\partial T}{\partial z}\right) - \frac{1}{r}\frac{\partial}{\partial r}\left(r\lambda_r \frac{\partial T}{\partial r}\right) = \sum_i (-\Delta_r H_i^\circ) r_i \tag{2}$$

The momentum equation is obtained by applying Newton's second law on a moving fluid element [18]. For steam cracking, only pressure drops and friction forces have to be considered, while radial pressure gradients can be neglected. Hence, the following momentum Eq. (3) is obtained:

$$\frac{\mathrm{d}p_t}{\mathrm{d}z} = -\alpha\left(\frac{f}{R} + \frac{\zeta}{\pi r_b}\right)\rho v^2 - \alpha\rho v \frac{\mathrm{d}v}{\mathrm{d}z} \tag{3}$$

The boundary conditions for the two-dimensional problem are:

Tube center ($r=0$)	Reactor wall ($r=d_t/2$)	Reactor inlet ($z=0$)
$\frac{\partial T}{\partial r} = 0$	$D_r \rho \frac{\partial}{\partial r}\left(\frac{C_j}{\rho}\right) = \frac{r_{c,j}}{M_j}$	$T = T_0$
$v_r = 0$		$C_j = C_{j0}$
$\frac{\partial}{\partial r}\left(\frac{C_j}{\rho}\right) = 0$	$\frac{\partial T}{\partial r} = \frac{q}{\lambda_r}$	$p_t = p_0$

In the model equations, no terms pertaining to coke layer thickness have been added as the calculations are performed for the initial coke formation rate.

As illustrated in Fig. 1, the model Eqs. (1)–(3) can be easily transformed into a dimensionless form. The dimensionless equations for the continuity equation and the energy equation are obtained by dividing each term in the original equations by the coefficient of the convective term and rendering variables such as the temperature and concentrations dimensionless. The convective term is chosen because this term is the most important term in the continuity and energy equations. The following dimensionless variables can thus be introduced:

$$z' = \frac{z}{L},\quad \xi = \frac{2r}{d_t},\quad y_i = \frac{C_i}{C^0},\quad r_i' = \frac{r_{Vi}}{r_V^0},\quad \theta = \frac{T}{T^0},$$

$$v_a' = \frac{v_a}{v_a^0},\quad v_r' = \frac{v_r}{v_r^0},\quad D_r' = \frac{D_r}{D_r^0},\quad \lambda_r' = \frac{\lambda_r}{\lambda_r^0},$$

$$-\Delta_r H_i' = \frac{-\Delta_r H_i^\circ}{|\Delta_r H_{\mathrm{ref}}^\circ|}$$

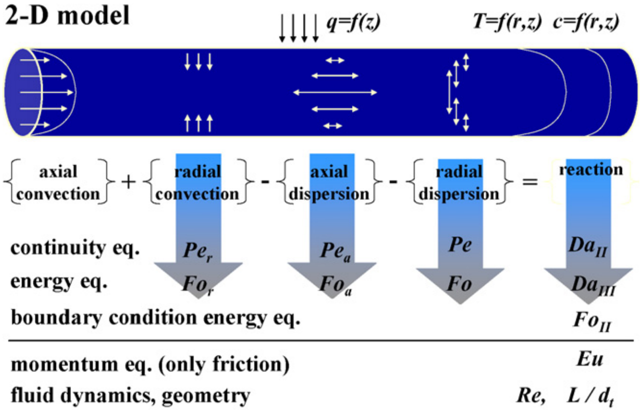

Fig. 1. Schematical representation of the dimensionless model equations and origin of the dimensionless numbers.

Fig. 1 shows that transforming the continuity equation for a specific component into a dimensionless form leads to the introduction of four dimensionless numbers: three Peclet numbers (Pe, Pe_r and Pe_a) and one Damköhler number Da_{II}. Generally for steam cracking, the values for the radial Peclet number Pe_r are very low [$Pe_r \rightarrow 0$] [8–18] and ideal macro-mixing along the cross-section of the tube can be assumed. In contrast, the values for the axial Peclet number Pe_a are very high [$Pe_a \rightarrow \infty$] and back mixing can be neglected [8–18]. If ideal macro-mixing in the radial direction is assumed and back mixing is neglected, the dimensionless continuity equation for a component j is given by:

$$\frac{\partial}{\partial z'}(v_a' y_j) - \frac{1}{Pe}\frac{1}{\xi}\frac{\partial}{\partial \xi}\left(\xi D' \frac{\partial y_j}{\partial \xi}\right) = Da_{II}\sum_i \nu_{i,j} r_i' \tag{4}$$

Also in the dimensionless energy Eq. (4) dimensionless numbers are defined: three Fourier numbers (Fo, Fo_r and Fo_a) and one Damköhler number Da_{III} (see Fig. 1). As for the continuity equation, the contributions of the terms of axial conduction and radial convection can be neglected, resulting in the following dimensionless energy equation:

$$\frac{\partial}{\partial z'}(v_a' \theta) - Fo\frac{1}{\xi}\frac{\partial}{\partial \xi}\left(\xi \lambda' \frac{\partial \theta}{\partial \xi}\right) = Da_{III}\sum_i (-\Delta_r H_i') r_i' \tag{5}$$

If only friction is taken into account, the momentum equation can be transformed into the following dimensionless form:

$$\frac{\mathrm{d}p'}{\mathrm{d}z'} = \frac{1}{Eu}(v_a')^2 \tag{6}$$

with Eu the Euler number. The dimensionless boundary conditions are:

Tube center ($\xi=0$)	Reactor wall ($\xi=1$)	Reactor inlet ($z'=0$)
$\frac{\partial \theta}{\partial \xi} = 0$	$\frac{\partial y_j}{\partial \xi} = \frac{r_{c,j}}{D_r M_j} = Pe_{II}$	$\theta = 1$
$v_r' = 0$		$y_j = 1$
$\frac{\partial y_j}{\partial \xi} = 0$	$\frac{\partial \theta}{\partial \xi} = \frac{2}{d_t}\frac{q}{T^0 \lambda_r} = Fo_{II}$	$p' = 1$

In Table 1 all the dimensionless numbers are given. This Π-set differs from the Π-set derived by Zlokarnik [11] and Damköhler [8] because these authors used a one-dimensional reactor model for the mathematical description.

3. Complete versus partial similarity

The theory of similarity states that if the dimensionless numbers defined in Table 1 are the same for two reactors then the temperature profile and the pressure profile are similar and the product distribution is identical. However, Damköhler [8] showed that it is impossible for two different tubular reactors to have identical values for the three dimensionless numbers Da_{II}, Re and L/d_t-ratio. Hence, for tubular reactors scale-up under

Table 1
Dimensionless numbers originating from process-related, geometrical and hydrodynamic similarity

	Dimensionless numbers		
Process-related similarity	$Pe = \frac{d_{\mathrm{t}}^2}{4D^0}\frac{v_{\mathrm{a}}^0}{L} = \frac{\tau_{Dr}}{\tau}$ $Fo = \frac{4L}{v_{\mathrm{a}}}\frac{\lambda^0}{c_{\mathrm{p}}\rho_{\mathrm{g}}d_{\mathrm{t}}^2} = \frac{\tau}{\tau_{\lambda r}}$	$Da_{\mathrm{II}} = \frac{L}{v_{\mathrm{a}}^0}\frac{r_{\mathrm{V}}^0}{C^0} = k_{\mathrm{ref}}^0\tau$ $Da_{\mathrm{III}} = \frac{Lr_{\mathrm{V}}^0}{v_{\mathrm{a}}^0}\frac{\lvert \Delta_{\mathrm{r}}H_{\mathrm{global}}\rvert}{c_{\mathrm{P}}\rho_{\mathrm{g}}T^0}$ $Eu = \frac{d_{\mathrm{t}}p_{\mathrm{t}}^0}{2f\rho_{\mathrm{g}}(v_{\mathrm{a}}^0)^2L}$	$Pe_{\mathrm{II}} = \frac{r_{\mathrm{c,j}}}{D_{\mathrm{r}}M_{\mathrm{j}}}$ $Fo_{\mathrm{II}} = \frac{2}{d_{\mathrm{t}}}\frac{q}{T^0\lambda_{\mathrm{r}}}$
Geometrical similarity	$\frac{L}{d_{\mathrm{t}}}$		
Hydrodynamic similarity	$Re = \frac{v_{\mathrm{a}}d_{\mathrm{t}}\rho_{\mathrm{g}}}{\mu}$		

complete similarity is excluded, but working under partial similarity might be an option. A judicious choice of the criterion of similarity to be abandoned is necessary. As the value of the Reynolds number has only a slight influence on the hydrodynamics in the turbulent flow regime, hydrodynamic similarity is abandoned. In industrial tubular reactors, Reynolds numbers easily reach values of 10^5 while in typical pilot plant reactors the Reynolds number is limited to about 10^4. However, abandoning hydrodynamic similarity only is not sufficient and therefore also geometrical similarity is neglected. Still problems remain, in particular in realizing a similar radial temperature and concentration profile. This can be illustrated by considering the dimensionless energy equation and the corresponding dimensionless Fourier number Fo in Table 1. This number is the ratio of the residence time τ to the time scale for radial heat dispersion $\tau_{\lambda\mathrm{r}}$. Table 1 also shows that maintaining the same value for the Damköhler number Da_{II} implies that the residence time τ should remain fixed upon a change of scale. Hence, to realize a similar radial temperature profile, the time scale for radial heat dispersion $\tau_{\lambda\mathrm{r}}$ should also remain unchanged upon a change in scale. However, $\tau_{\lambda\mathrm{r}}$ can only be the same in two reactors if they have the same diameter. Moreover, according to the dimensionless number stemming from the boundary condition of the energy equation Fo_{II} not only the diameter of the reactor must remain unchanged, but also the axial heat flux profile must be similar to realize a similar radial temperature profile. However, realizing the same radial temperature and concentration profile is not the only problem. An analysis of the momentum equation shows that problems pertaining to the pressure profile are to be expected too. If identical pressure drops have to be obtained in two different tubular reactors, the Euler number has to be the same. If the friction factor is calculated according to the Blasius equation for smooth tubes [19]:

$$f = \frac{0.079}{Re^{1/4}} \tag{7}$$

The resulting Euler number is then given by:

$$Eu = \frac{d_{\mathrm{t}}^{1.25}p_{\mathrm{t}}^0}{0.158\rho_{\mathrm{g}}(v_{\mathrm{a}}^0)^2L} = \frac{d_{\mathrm{t}}^{1.25}p_{\mathrm{t}}^0\tau^2}{0.158\rho_{\mathrm{g}}L^3} \tag{8}$$

From this equation it is obvious that the same Euler number can be obtained in two different tubular reactors if the length and the diameter are chosen wisely. Using a different expression for the friction factor, such as Prandtl's equation, leads to similar conclusions; a similar pressure profile can be obtained by a carefully chosen combination of the length and the diameter of the reactor. However, a decrease of the tube diameter inevitably leads to a decrease of the radial temperature drop. Hence, it is not possible to obtain both the same radial temperature and axial pressure profile in two different steam cracking coils. Two options for scale-up under partial similarity thus remain:

- Maintaining a similar axial pressure profile [i.e. the same value of the Euler number, *Eu*] and abandoning similarity of radial transport [i.e. allowing different values of the Peclet number, *Pe*, and the Fanning friction factor, *Fo*].
- Maintaining similar radial transport properties [i.e. the same values for *Pe* and *Fo*] and abandoning a similar axial pressure profile [i.e. allowing different values of *Eu*].

In what follows, these two options for scaling up steam cracking coils under partial similarity are discussed in more detail.

4. Influence of relaxation of criteria of similarity on scale-up and scale-down

In this work, we have opted to use theoretical calculations to estimate the highest accuracy that can be reached upon a change of scale for a tubular steam cracking reactor. The differences found for reactant conversions and for the predicted yields of the main products obtained in different scale units are generally used as a measure for the accuracy of scale-up [11]. A detailed microkinetic model is used to estimate the differences resulting from a change in scale [17]. The simulation results obtained with this mathematical model allow estimating the overall accuracy. We have opted to use a two-dimensional reactor model for simulating the steam cracking process. This enables a straightforward evaluation of both the role of the radial temperature profile and the effect of the axial pressure profile on the conversion and the product yields. The reactor model equations are given by Eqs. (1)–(3). More details about how the model equations are solved are given in Van Geem et al. [17]. The reactor model is coupled to a radical kinetic model for the cracking of naphtha and ethane [2].

4.1. Case 1: similar axial pressure profile

As mentioned above, a first analysis of the dimensionless numbers shows that the radial temperature profile can be similar in two reactors only if they have the same diameter and if they are operated under a similar axial heat flux profile. Generally, this is not the case and the diameter of the small-scale reactor is typically an order of magnitude smaller than that of the large-scale reactor. Consequently, the radial temperature drop is also an order of magnitude smaller in the small-scale reactor as compared to the large-scale reactor, i.e. of the order of 10 K in the small-scale reactor and 100 K in the large-scale reactor (see Fig. 2). The worst-case scenario is the situation in which the radial temperature drop is almost non-existing [$d_t \rightarrow 0$; $Pe \rightarrow 0$; $Fo \rightarrow \infty$] in the small-scale reactor, i.e. a one-dimensional situation, and is strongly pronounced in the large-scale reactor. In that case, the effect on the conversion and the product yields is maximal. This maximal difference can thus be estimated by comparing the two-dimensional simulation results for an industrial reactor, exhibiting an important radial temperature profile, with the results obtained from a one-dimensional reactor model under the same conditions. In the one-dimensional simulation, the radial temperature profile is completely ignored. Hence, the one-dimensional simulation can be considered as a measure for a pilot plant reactor working under completely the same operation conditions as the industrial reactor, i.e. the same residence time, similar axial temperature and pressure profile. The reactor used in the simulations is a traditional Lummus SRT-I reactor with a uniform diameter of 0.12 m and a length of 101 m. As it requires both high heat fluxes and has a large-reactor diameter; the radial temperature profile can thus be expected to be pronounced. As feedstock pure ethane is chosen because this feedstock requires high heat fluxes to crack. The axial temperature profile used in the one-dimensional reactor model is the same as the average two-dimensional temperature profile. To calculate the average two-dimensional temperature at a certain axial position the cup mixing temperature is applied [20]:

$$T_{\mathrm{av}} = \frac{\int_0^R T(r)v(r)r\mathrm{d}r}{\int_0^R v(r)r\mathrm{d}r} \tag{9}$$

The results obtained with both reactor models then allow to compare the influence of abandoning the radial dispersion terms in Eqs. (4) and (5). In Fig. 2 the radial temperature profile and the average temperature at the middle of the Lummus SRT-I reactor are shown. The process conditions used in the different simulations and the simulation results are summarized in Table 2. Using a similar axial pressure profile but neglecting the radial temperature profile in reactors of different scale can lead to significant differences; 4.0% (rel.) on the conversion and 1.8% (rel.) on the ethylene yield. The simulation results show that using the two-dimensional reactor model [2D ref.] a higher ethane conversion (1.9%) is simulated than with the one-dimensional reactor model [1D]. On the other hand, the difference between the ethylene yield simulated with the one-dimensional [1D] and the two-dimensional reactor model [2D ref.] is less pronounced (0.4%). For the other important products

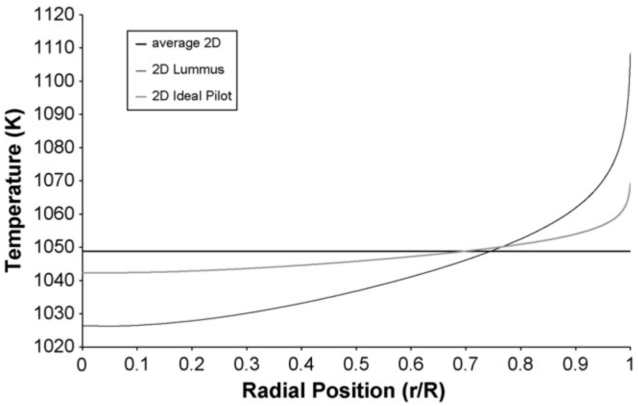

Fig. 2. Influence of the reactor diameter on the radial temperature profile for the same average temperature. Radial temperature profile in the middle of an industrial Lummus SRT-I reactor (01.0 m long and with a diameter of 0.12 m) and in the ideal pilot plant reactor (20.0 m long and with a diameter of 2.5 10^{-2} m). [—, 2D simulation of ethane steam cracking in Lummus SRT-I reactor, Feed flow rate: 0.97 kg s^{-1}, dilution: 0.35 kg steam/kg HC, CIP: 0.34 MPa, COT: 1100 K, $Fo = 7$; ▬ 2D simulation of ethane steam cracking in pilot plant reactor, Feed flow rate: 5.1×10^{-3} kg s^{-1}, dilution: 0.35 kg steam/kg HC, CIP: 0.30 MPa, COT: 1100 K, $Fo = 170$].

Table 2
Reactor geometry, process conditions and simulation results for ethane cracking in an industrial Lummus SRT-I reactor

	Lummus SRT-I reactor
Reactor length (m)	101.0
Tube diameter (m)	1.2×10^{-1}
CIT (K)	873
COT (K)	1100
Dilution (kg steam/kg HC)	0.35
Flow rate (kg s^{-1})	9.7×10^{-1}
Residence time (s)	0.7

	1D	2D CIP	2D av.	2D COP	2D ref.
CIP (MPa)	0.34	0.34	0.30	0.26	0.34
COP (MPa)	0.22	0.30	0.26	0.22	0.22
Eu	8.3	25	25	25	8.3
Pe	0	1.4×10^{-1}	1.4×10^{-1}	1.4×10^{-1}	1.4×10^{-1}
Fo	∞	7	7	7	7
	Steam cracking products (wt.%)				
H_2	3.0	3.1	3.1	3.1	3.1
CH_4	2.5	2.7	3.0	2.5	2.9
C_2H_2	0.3	0.3	0.3	0.4	0.4
C_2H_4	40.0	40.5	40.7	40.5	40.8
C_3H_6	0.7	1.0	0.8	0.7	0.7
C_4H_6	0.8	1.2	1.1	1.0	1.0
C_4H_{10}	0.9	0.9	0.8	0.8	0.8
C_2H_6-conversion	48.7	51.8	50.9	49.7	50.6

1D, one-dimensional simulation with same average axial T-profile as 2D ref.; 2D, CIP: same T-profile and CIP as 2D ref.; 2D av., same T-profile and average pressure as 2D ref.; 2D COP, same T-profile and COP as 2D ref.; 2D ref., two-dimensional simulation for reference conditions.

such as hydrogen, methane or propylene the differences remain relatively small (0.1–0.3%). Van Geem et al. [17] showed that the radial temperature profile increases the ethane conversion but decreases the ethylene selectivity because light olefins are removed by secondary reactions generating species with higher molecular weight such as propylene and butadiene.

Overall the differences are quite important especially for the conversion, and hence, it can be concluded that neglecting the radial temperature profile has a significant influence on the yields of the main products. Hence, when the scale is changed it is important to keep the radial temperature profile as similar as possible; otherwise the product yields will differ significantly although both different scale reactors are operated under similar conditions.

4.2. Case 2: similar radial temperature profile

Estimating the effect of differences in the axial pressure profile on the yields is more difficult than estimating the effect of differences in the radial temperature profile. Generally, the pressure drop in the small-scale reactor is significantly lower than the pressure drop observed in long industrial reactors such as the Lummus SRT-I reactor used in the previous simulations. For example the pressure drop in a pilot reactor of a length of 12.4 m and with a diameter of 0.01 m is typically 0.04 MPa, while in the Lummus SRT-I reactor the pressure drop is over 0.12 MPa under similar operating conditions. By increasing the length of the pilot plant reactor the pressure drop can be increased but for practical reasons the length of a pilot plant reactor is typically limited to 20 m. To estimate the effect of relaxing the similarity of the axial pressure profile for a given radial temperature profile simulations have to be performed with different axial pressure profiles in the reactor but similar radial temperature profiles. Therefore, the simulation results obtained for the base case of the Lummus SRT-I reactor with a pressure drop of 0.12 MPa [2D ref.] are compared with the simulation results obtained for the Lummus SRT-I reactor in which the same radial and axial temperature profile exists but with a pressure drop that matches the one observed in the pilot plant unit, i.e. 0.04 MPa. This last simulation case can be considered as a measure for a pilot plant reactor working under similar operation conditions as the industrial reactor, i.e. the same residence time, similar axial and radial temperature profile, but with a different axial pressure profile. However, different alternatives are available to realize the reduced pressure drop. One alternative is to maintain the same coil inlet pressure (CIP) as in the reference case [2D CIP]. Other alternatives consist in maintaining the same average pressure [2D av.] or in maintaining the same coil outlet pressure (COP) as the reference case [2D COP]. The conditions and the simulation results for the three different cases are summarized in Table 2. The results in Table 2 show that scale-up using equal *Pe* and *Fo* numbers but loosing similarity for the axial pressure profile, i.e. different *Eu* number, can also lead to significant differences. Especially when the same CIP [2D CIP] or the same COP [2D COP] is used the differences can become important. The smallest differences resulting from differences in pressure are found for the reactor that operates under the same average pressure [2D av.] as the reference case [2D ref.]. Table 2 shows that although the *Eu* numbers differ significantly ($Eu = 25$ in 2D ref.; $Eu = 7$ in 2D av.) the simulated conversion and ethylene yield differ less than 0.3%. The differences resulting from relaxing the similarity of the axial pressure profile are then at best 0.6% (rel.) on the conversion and 0.2% (rel.) on the ethylene yield. Thus, if the scale is changed and the pressure drop is different in the reactors of different scale this should not necessarily lead to differences if the average pressure in the small-scale unit is the same as in the industrial unit. However, the errors induced by relaxing the similarity of the axial pressure profile can be in the same order as the one from neglecting the radial temperature profile if this rule of thumb is neglected. The same conclusion is found if instead of ethane another feedstock is used and if instead of the Lummus SRT-I reactor another reference reactor is chosen.

5. Design of the "ideal" pilot plant reactor

The main objective in what follows is to explore how the previous conclusions can contribute to the design of the ideal pilot plant reactor, i.e. a pilot reactor that, if operated under similar process conditions as the industrial reference unit, results in an almost identical product distribution. The simulation results indicate that it is more important to focus the design of a pilot plant reactor on obtaining a similar radial temperature profile, then on obtaining a similar axial pressure profile. Creating a unit with a similar radial temperature profile requires that the reactors have the same diameter and a similar heat flux profile. The length of the reactor can be chosen freely, as long as the reactor is operated under the same average pressure as the industrial unit. However, practical considerations also affect the design of a pilot plant reactor. The minimum diameter of the pilot reactor tube is limited by the need to measure process variables, such as gas phase temperature. As the available dimensions of the furnace are limited too, the reactor length should not be more than 20 m. Also the reactor diameter of pilot plant reactors is limited to 2.5×10^{-2} m because, as pointed out by Van Damme et al. [21], the dimensions of the pilot reactor should be chosen so as to achieve turbulent flow conditions in the coil with reasonable flow rates. Too high diameters require very high flow rates. Taking into account these practical limitations results in a length of 20 m and a diameter of 2.5×10^{-2} m for an ideal pilot plant reactor for the Lummus SRT-I reactor. Using these dimensions reduces the differences for direct experimental scale-up. The differences between this pilot reactor and the industrial reactor are 2.0% (rel.) for the conversion and 1.0% (rel.) for the ethylene yield under the reference conditions specified in Table 2. The total flow rate (hydrocarbons + steam) should be about 6.5×10^{-3} kg s^{-1} to obtain the same residence time as in the Lummus SRT-I reactor (1s). These conditions also guarantee a turbulent flow regime ($Re > 4000$) in the pilot reactor. Also for other feedstocks than ethane these dimensions remain unchanged. Table 3 shows that the design of the ideal pilot plant reactor remains valid if instead of a Lummus SRT-1 reactor another industrial reactor is to be scaled down. Only in the case that a Millisecond reactor needs to be scaled down, a shorter length of the pilot plant reactor is

Table 3
Design and typical operation conditions of the ideal pilot plant reactor for scale down of several industrial reactors (Lummus SRT-I, Split coil, Millisecond U tube Stone & Webster) and a gradient free reactor for studying coke formation

	Lummus SRT-I	Split coil	Millisecond	U tube	Gradient free
Industrial reactor characteristics					
Diameter (cm)	12	8/12/16	3	8	–
Length (m)	100	45	10	20	–
Feed flow rate (kg s^{-1})	1	0.33	3.3×10^{-2}		–
COT (K)	1060–1120	1060–1140	1150–1230	1080–1160	–
CIP (Mpa)	0.35	0.35	0.3	0.3	–
Residence time (s)	1	0.4	0.1	0.3	–
Ideal pilot plant characteristics					
Diameter (cm)	2.5	2.5	2.5	2.5	0.5
Length (m)	20	20	10	20	20
Feed flow rate (kg s^{-1})	6.0×10^{-3}	9.0×10^{-2}	2.0×10^{-2}	1.3×10^{-2}	5.0×10^{-4}
COT (K)	1060–1120	1060–1140	1150–1230	1080–1160	950–1170
CIP (Mpa)	0.3	0.3	0.25	0.27	0.40–0.22
Re	1.0×10^{4}	2.0×10^{4}	5.0×10^{4}	2.0×10^{4}	5.0×10^{3}
Residence time (s)	1	0.4	0.1	0.3	0.5

recommended because a length of 20 m would require too high flow rates to realize a residence time of 0.1 s used in the industrial Millisecond reactor. Note in Table 3 that in this case the reactor length of the ideal plant reactor is equal to the length of the corresponding industrial reactor, and the term scale-down or scale-up is no longer appropriate. These are almost identical reactors because a Millisecond in practice exists of a large number (160–200) of short, parallel tubes, and hence, only the diameter varies.

Table 3 further shows that for a gradient free pilot plant reactor the diameter is a lot smaller than the one found for the “ideal” pilot plant reactor. In this case the radial temperature gradient should be kept as small as possible, and thus, the diameter should be kept as small as possible. If turbulent flow needs to be realized in this reactor the diameter should best not be smaller than 5 mm. Hence, this value is selected for the gradient free pilot plant reactor. Furthermore, it should be mentioned that until now only operation under initial conditions, i.e. when no coke is formed on the reactor surface, has been considered. To transfer data on coke formation from one reactor to another the conditions at the reactor wall/process gas interface, i.e. pressure, temperature and species concentrations have to be identical.

However, analysis of the dimensionless model equations shows that realizing a similar radial temperature profile and similar axial pressure profile in two tubular reactors for steam cracking is only possible if these reactors are identical. Consequently, direct experimental scale-up to industry of results obtained for coke formation is not possible. The only solution is developing a fundamental coke formation model and predicting the run length based on a simulation model. The role of a pilot plant reactor for studying coke formation is thus limited to developing fundamental coke formation models. An accurate measurement of the process gas temperature and the temperature at the reactor wall/process gas interface is crucial. Hence, to study coke formation in a pilot plant reactor the radial temperature drop should be kept as small as possible. The gradient free reactor is thus also an appropriate reactor for developing a fundamental coke formation model.

6. Conclusions

In this paper the theory of similarity is applied to scale-up and scale down steam cracking reactors. The dimensionless model equations show that it is impossible to reach complete similarity for two different tubular reactors. Scale-up is thus only possible under partial similarity and inevitably this leads to differences. However, if the criteria of similarity are relaxed with care only small differences between units of different scale can be obtained. Further analysis of the dimensionless model equations shows that neglecting hydrodynamic and geometrical similarity is still insufficient. Problems remain, in particular with realizing a similar radial temperature and axial pressure profile. Realizing a similar radial temperature profile and similar axial pressure profile in two tubular reactors for steam cracking is only possible if these reactors are identical. Hence, two different relaxation strategies are applied; the first one aims at realizing a similar axial pressure profile neglecting radial nonuniformities, the second focuses on realizing a similar radial temperature profile. Neglecting the similarity of the radial temperature profile leads to more important differences as compared to the differences resulting from neglecting the similarity of the axial pressure profile. The errors made for ethane cracking in a Lummus SRT-I reactor for neglecting the radial temperature profile are 4.0% (rel.) for the conversion and 1.8% (rel.) for the ethylene yield, while for neglecting the axial pressure profile 0.6% (rel.) for the conversion and 0.2% (rel.) for the ethylene yield. The preceding rules make it possible to design a so-called ideal pilot plant reactor based on a specific industrial reactor, i.e. a reactor with a similar radial temperature profile as the reference reactor. On the one hand the reactors should have similar diameters. On the other hand the heat flux profile in the two reactors should be as similar as possible. However, for practical limitations it is not possible to create pilot reactors with diameters of over 2.5×10^{-2} m. The length of the reactor can be chosen freely, as long as the reactor is operated under an average pressure as in the industrial unit. Applying the preceding rules on the Lummus SRT-I reactor leads to a pilot plant reactor with a diameter of 2.5×10^{-2} m and a length of 20 m. Also for other industrial reactors the diameter of the “ideal” pilot plant reactor remains unchanged. Only for a gradient free reactor a smaller diameter is recommended because in this case the radial non-similarities should be kept as small as possible. Direct experimental scale-up of results obtained for coke formation is not possible. Only simulations using a fundamental coke formation model are able to provide accurate run lengths of industrial installations.

Acknowledgment

Kevin M. Van Geem holds a Ph.D. grant of the IWT-Vlaanderen.

References

[1] M. Dente, S. Pierucci, E. Ranzi, New improvements in modeling kinetic schemes for hydrocarbon pyrolysis, Chem. Eng. Sci. 47 (1992) 2629–2634.

[2] P.J. Clymans, G.F. Froment, Computer generation of rate equations for thermal cracking of normal and branched paraffins, Comp. Chem. Eng. 8 (1984) 137–142.

[3] E. Joo, K. Lee, M. Lee, S. Park, CRACKER—a PC based simulator for industrial cracking furnaces, Comp. Chem. Eng. 24 (2000) 1523–1528.

[4] Z. Belohlav, P. Zamostny, T. Herink, E. Eckert, T. Vanek, A novel approach for the prediction of hydrocarbon thermal cracking product yields from the substitute feedstock composition, Chem. Eng. Technol. 28 (2005) 1166–1176.

[5] A. Pinter, A. Tungler, L. Nagy, L. Vida, I. Kovacs, J. Kerezsi, A laboratory steam cracking reactor to characterize raw materials, Int. J. Chem. React. Eng. 2 (2004) A15.

[6] W.R. Shu, L.L. Ross, Cracking severity index in pyrolysis of petroleum fractions, Ind. Eng. Chem. Proc. Des. Dev. 21 (1982) 371–377.

[7] K.M. Van Geem, M.F. Reyniers, G.B. Marin, Two severity indices for scale-up of steam cracking coils, Ind. Eng. Chem. Res. 44 (2005) 3402–3411.

[8] G.Z. Damköhler, Einflüsse der Strömung, Diffusion und des Wärmeübergenges auf die Leistung von Reactionsöfen, Electrochemie 42 (1936) 846–862.

[9] M. Zlokarnik, Scale-up of processes using material systems with variable physical properties, Chem. Biochem. Eng. Q. 15 (2001) 43–47.

[10] M. Zlokarnik, Scale-up in Chemical Engineering, Wiley-VCH, Weinheim, 2002.

[11] D.M. Himmelblau, K.B. Bishoff, Process Analysis and Simulation, J. Wiley, New York, 1968.

[12] M. Dente, E. Ranzi, A.G. Goossens, Detailed prediction of olefin yields from hydrocarbon pyrolysis trough a fundamental simulation-model (SPYRO), Comp. Chem. Eng. 3 (1979) 61–75.

[13] J.J. De Saegher, T. De Temmerman, G.F. Froment, Three dimensional simulation of high severity internally finned cracking coils for olefins production, Revue de l’Institut Français du Petrole 51 (1996) 245–260.

[14] G.F. Froment, Kinetics and reactor design in the thermal cracking for olefins production, Chem. Eng. Sci. 47 (1992) 2163–2177.

[15] B. Elvers, S. Hawkins, G. Schulz, Tubular reactors, Ullmann’s Encyclopedy Ind. Chem. (1992) 181–198.

[16] K.M. Sundaram, G.F. Froment, 2 Dimensional model for the simulation of tubular reactors for thermal cracking, Chem. Eng. Sci. 35 (1980) 364–371.

[17] K.M. Van Geem, G.J. Heynderickx, G.B. Marin, A comparison of one and two-dimensional reactor models for steam cracking: effect on yields and coking rate, AIChE J. 50 (2004) 173–183.

[18] G.F. Froment, K.B. Bishoff, Chemical Reactor Analysis and Design, J. Wiley, New York, 1990.

[19] R.H. Perry, D.W. Green, Perry, McGraw-Hill, New York, 1997.

[20] R.B. Bird, E.N. Lightfood, W.E. Stewart, Transport Phenomena, J. Wiley, New York, 2001.

[21] P.S. Van Damme, S. Narayanan, G.F. Froment, Thermal cracking of propane and propane–propylene mixtures: pilot plant versus industrial data, AIChE J. 21 (1975) 1065–1073.