THE CATALYTIC PELLET:

A Rich Prototype for Engineering Up-Scaling

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In many widely used textbooks in chemical reaction engineering courses, such as Fogler,[1] Levenspiel,[2] and Carberry,[3] the derivation of the conservation equation for the species in a gas mixture, either a pore or pellet domain, is conducted by a "global" approach—where many assumptions and processes are hidden. These assumptions carry significant concepts associated with engineering scaling that (if properly used) offer a powerful learning environment to train students in engineering scaling. This training is useful in handling current chemical engineering problems and it enhances student readiness to find solutions to these practical situations. In fact, an educational environment that introduces scaling as an effective learning tool leads to an excellent understanding of processes at the nano-, micro-, and macro-scales in students. This, in turn, offers an economical training for students as they learn both fundamental principles and up-scaling simultaneously.

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The catalytic pellet has several aspects that make an engineering description of the fundamentals very challenging for untrained readers, *i.e.*, students. Concepts based on transport phenomena are coupled with gas-solid (heterogeneous) catalytic chemical reactions, in addition to geometrical parameters. Students do not seem, however, to have much difficulty in describing (conceptually) the physical chemistry as it happens in the system at the microscale. Chemical engineering students are familiar with hydrodynamics, diffusion, and chemical reactions from freshman and sophomore courses. Thus, a *microscopic* (and even a molecular) description is a logical, and fairly simple, first step for students when describing the physics of transport with chemical reactions inside a catalytic pellet. On the other hand, the development of a description at the *macroscopic* level is problematic. In fact, identifying the proper mathematical language for a useful global or macroscopic description sometimes becomes a bottleneck in the learning process. This aspect, perhaps, led educators in the past to "simplify" the mathematical and physical description so that students are confronted with a simple model. This approach, however, stifles the sequential and evolutionary process of student learning. Instead, a macroscopic description may be easily achieved when the problem is viewed from an up-scaling point of view. Basically, the connection between micro and macroscopic description is an integration of the former in a physical or geometrical domain (see further description, below). This approach will produce a mixture of "averaged" quantities and "point" variables. In order to close the problem description, a connection between the two is required. These concepts are rooted in general principles of scaling and engineering approximations that are the subject matter of this contribution. A byproduct of the approach is that concepts from freshman and sophomore mathematics courses become relevant and of enormous practical value for the students. This leads to a successful marriage, rather than to a divorce, between mathematics and physics for the engineer in training.

TRANSPORT AND REACTION IN CATALYTIC PORES AND PELLETS: BRIEF SYNOPSIS OF THE LEARNING APPROACHES

An analysis of the literature shows that heterogeneous reactions and catalysis are very popular subjects. Traditional textbooks such as Levenspiel[4] introduce students to models using an intuitive approach (see more below) that allows them to compute concentration profiles and effectiveness factors. Other textbooks with more sophisticated mathematics concentrate on an *a priori* analysis with implications to practical aspects[5-8]; within this framework, Aris[9] reported useful techniques for obtaining information from reaction-diffusion equations without actually solving such equations. The spectrum of contributions could accommodate all levels of trained readers between these two limits, and it would appear that there is nothing to be added from the expert point of view.

Nonexperts, however—the students—may fare less well. They may wonder how a complicated problem in two phases with reaction on the walls may be modeled as a domain with homogeneous reactions (see section below) by a simplistic and intuitive approach. Those more mathematically gifted may explore a more sophisticated description, but will not survive the mathematical machinery in Aris.[10] Therefore, despite expert contributions on the subject of transport and reaction in heterogeneous media, there is a need for a systematic approach to introducing nonexperts to the subject. This approach must be based on first principles, must conclude with the overall or macro-transport equations, and must be followed by the complete and logical sequence of steps at the heart of the scaling process. These concepts are so important in training the future engineer, from both fundamental and practical points of view, that disguising them does not seem to be a useful and effective strategy.

The classic and intuitive approach to up-scaling used in the literature for a porous domain (*e.g.*, Levenspiel[4]) usually leads to confusion concerning homogeneous and heterogeneous catalytic reactions. This approach is based on a global[1] balance for species A in an incremental volume of the pore domain. If this balance is applied to Cartesian geometry,[11] then the result leads to the following differential equation after the limiting process is invoked:

$$\frac{\partial c_A}{\partial t} = -\nabla \cdot N_A + R_A(c_A) \qquad (1)$$

Eq. (1) in one dimension yields the following result after a vague reference to Fick's law with an effective diffusivity, D_{eff}:

$$\frac{\partial c_A}{\partial t} = D_{eff} \frac{\partial}{\partial z}\left(\frac{\partial c_A}{\partial z}\right) + R_A \qquad (2)$$

In many cases, a first order consumption is considered and Eq. (2) reduces to:

$$\frac{\partial c_A}{\partial t} = D_{eff} \frac{\partial}{\partial z}\left(\frac{\partial c_A}{\partial z}\right) - a_v k c_A \qquad (3)$$

This equation should describe, according to the traditional approach, a diffusion process with a heterogeneous catalytic reaction in a pore domain. In many cases, a modified constant is defined as $k' = a_v k$. Students in mass transfer courses, however, have found an equation that closely mimics Eq. (3):

$$\frac{\partial c_A}{\partial t} = D \frac{\partial}{\partial z}\left(\frac{\partial c_A}{\partial z}\right) - k' c_A \qquad (4)$$

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[1] *The word global is frequently used to hide the actual scaling process in deriving the macrotransport or up-scaled equation for the domain under consideration.*

The pseudo-similarity between Eqs. (3) and (4) is obvious because untrained students are not usually concerned with specific details at this point; learning problems appear as soon as students begin to compare the two equations. Eq. (4) has been derived for the case of homogeneous reactions taking place in the entire volume and with molar concentrations, c_A, expressed per unit of the entire volume. This is a remarkable contrast with the situation in a catalytic pore domain, in which reactions are heterogeneous, *i.e.*, located on the surface and not within the bulk of the domain. In addition, we face two types of concentrations of species A—surface and bulk. Obviously, if what a student has learned in the case of Eq. (4) is correct, something else must be playing a role in Eq. (3). One conclusion is obvious: Eq. (3) is totally misleading since, from the point of view of the untrained reader, we have a chemical reaction homogeneously distributed in the domain and with concentrations of species A per unit volume of such volume. No surface reaction, surface concentration, and connection with bulk concentration are identified at this point in the learning process.

In order to highlight the reasons why Eq. (3) is misleading, an analysis of the chemical and physical situation at a catalytic cavity or pore (see Figure 1) is performed at the microscopic[2] level. We consider here a two-phase system consisting of a fluid phase, identified as the γ-phase, and a solid phase, identified as the κ-phase. The analysis foundations of diffusion and reaction in this two-phase system call for the use of the species continuity equation in the γ-phase and the species jump condition at the catalytic γ-κ interface. The species continuity equation for this system, in the form of molar fluxes[12]), can be written as:

$$\frac{\partial c_{A\gamma}}{\partial t} = -\nabla \cdot N_A + R_{A\gamma} \qquad A = 1,2,3,....,N \quad (5)$$

This equation, however, fails to identify the species velocity as a crucial part of the species transport equation. To avoid confusion about the mechanical aspects of multicomponent mass transfer, Eq. (5) is suggested to be written in the following form[11]:

$$\frac{\partial c_{A\gamma}}{\partial t} = \nabla \cdot (c_{A\gamma} v_{A\gamma}) + R_{A\gamma} \qquad A = 1,2,3,....,N \quad (6)$$

Eq. (6) needs boundary conditions, and, when surface transport[14] can be neglected, the jump condition takes the form:

$$\frac{\partial c_{As}}{\partial t} = \left(c_{A\gamma} v_{A\gamma}\right) \cdot n_{\gamma\kappa} + R_{As}, \quad \text{at the } \gamma - \kappa \text{ interface,} \qquad A = 1,2,3,....,N \quad (7)$$

This equation can be easily written in terms of the molar flux by recognizing that $N_A = c_{A\gamma}\, v_{A\gamma}$. Furthermore, Eq. (7) can be derived by a shell balance around the interfacial region,[13, 14] and the jump condition can be viewed as a surface transport equation that forms the basis for various mass transfer boundary conditions that could take place at the phase interface.[15]

At this point, several observations are in order. First, the microscopic transport and reaction model presented in terms of Eq. (5) or, alternatively, Eq. (6) and Eq. (7) implies and describes a very different situation with respect to the one that seems to be implied by Eq. (3), which has obvious differences with respect to Eq. (4). Second, a reaction term in the microscopic model is located in the jump condition given by Eq. (7) and therefore implies a reaction located at the fluid-solid interface. An additional reaction term is also present in the species continuity equation. Third, there are two different types of concentrations in the model, *i.e.*, a surface concentration (moles per unit area), c_{AS}, is used in the jump condition of Eq. (7) while a bulk concentration (moles per unit volume), $c_{A\gamma}$, is used in the species continuity equation. A similar pattern has been used for the two reaction terms, one in Eq. (6) and the other in Eq. (7).

The dilemma, for students or apprentices, becomes clear by comparing the so-called global approach and the microscopic approach presented above. While the microscopic approach seems to capture the essential physicochemical situation in the pore domain, it leads to a very different description than one based on the global approach. This description, however, is consistent with the physical chemistry involved in the process. On the other hand, the global approach seems to arrive at an equation that fails to capture the key aspects of the transport and reaction process. The objective of the next section is to reconcile these two results by introducing a process of *upscaling* the microscopic model to arrive systematically and

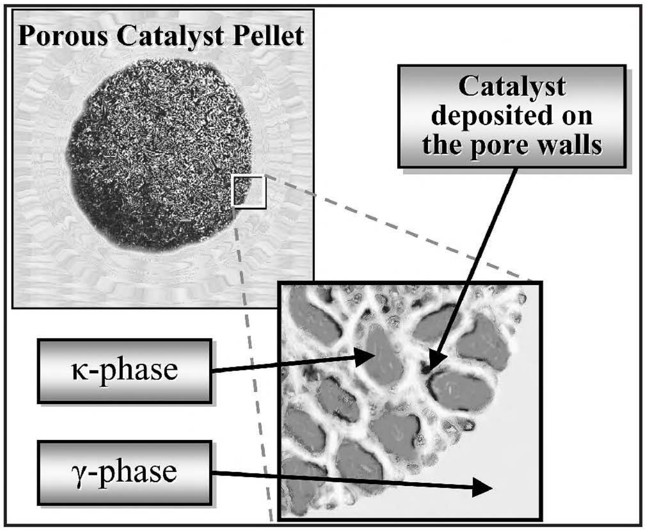

Figure 1. *Sketch and basic nomenclature of the pellet and pore domain.*

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[2] *The term microscopic here is used in the sense of continuum mechanics,* i.e., *local means a point in the finite domain of analysis.*

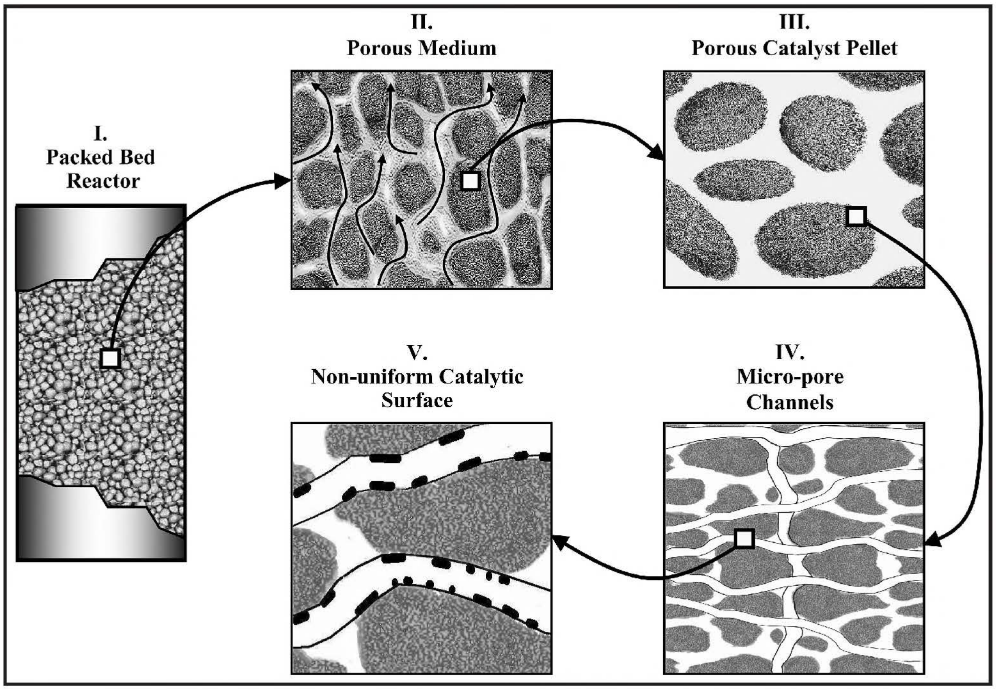

Figure 2. *Different scales associated with a catalytic reactor.*

without confusion at the correct macro transport equation for the pore domain.

UPSCALING OF THE MICROSCOPIC MODEL: A SOUND AND ROBUST APPROACH

In this section, we present two of the different scales involved in a catalytic process. Students are usually familiar with the reactor scale that produces a given chemical, but may not be aware of other scales also associated with this process. Figure 2 shows the rich spectrum of scales associated with packed-bed reactors, *i.e.*, the five-level hierarchy involved in a catalytic process. Level I is the packed-bed reactor scale, and a closer look inside the reactor domain reveals a Level II scale, associated with the different regions in the reactor domain. These regions could be different either in their morphology or in their function (see Arce and Ramkrishna[16]), although in many cases they are considered uniform (see Froment and Bischoff[17]). An analysis of these different regions shows they are made of individual catalyst pellets, *i.e.*, Level III is the catalyst pellet. Level IV is the one associated with the structure of individual pellets, *i.e.*, the domain of the micropores. Finally, each micropore could be actually different and, therefore, Level V constitutes the individual pore domain. The flow of information goes from the smallest length scale to the largest length scale. In other words, the process of up-scaling starts at Level V and finishes at Level I, the packed-bed reactor. In this contribution we will show how to proceed with the up-scaling only with Level V, *i.e.*, the pore domain, and Level IV, *i.e.*, the catalytic pellet domain. Other considerations on up-scaling can be found in Whitaker[18] and Arce, et al.[11]

In order to accomplish the up-scaling process in a rigorous manner, without confronting all the geometric complexities, we will consider the catalytic pellet made of a capillary bundle.[19-21] This capillary bundle is assumed to be made of cylindrical tubes 2L long, with a radius, r_o, and within a pellet of a square section b^2 (see Figure 3). This pellet domain therefore has a porosity given by $\pi r_o^2/b^2$.

The first step in the scaling analysis of the model pellet described above is to identify the microscopic description of the transport and reaction process taking place at the pore (capillary) level. This description is based on the capillary model described above and is restricted to the case of dilute solutions of species A. Since the pore domain is "sealed" at one end, convective transport can be neglected and the general species continuity [Eq. (5)] takes the form:

$$\frac{\partial c_{A\gamma}}{\partial t} = D_\gamma \left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_{A\gamma}}{\partial z}\right) + \frac{\partial^2 c_{A\gamma}}{\partial z^2}\right], \quad \text{in the } \gamma-\text{phase} \qquad (8)$$

Eq. (8)[3] also assumes that a homogeneous circumferential distribution of catalyst is on the internal surface of the pore domain and therefore a symmetrical condition on the angular direction can be assumed. Also, there is no homogeneous reaction, *i.e.*, $R_{A\gamma} = 0$. In addition, Eq. (8) requires boundary conditions that can be obtained from the jump condition given by Eq. (7). This condition implies, for the different boundaries, that:

$$c_{A\gamma} = c^0_{A\gamma} \qquad @ \qquad z = 0 \qquad (9)$$

$$\frac{\partial c_{A\gamma}}{\partial z} = 0 \qquad @ \qquad z = L \qquad (10)$$

$$-D_\gamma \frac{\partial c_{A\gamma}}{\partial r} = kc_{AS} \qquad @ \qquad r = r_o \qquad (11)$$

$$\frac{\partial c_{A\gamma}}{\partial r} = 0 \qquad @ \qquad r = 0 \qquad (12)$$

The initial condition is not stated, but could be any symmetric concentration distribution present initially within the

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[3] *For the steady-state version of this equation, using the concept of molecular flux, N_A, one can write Eq. (13) as $\nabla \cdot N_A = 0$. This is a similar looking equation to the incompressibility condition in fluid mechanics, $\nabla \cdot v = 0$, where v is the hydrodynamic velocity of the fluid (see, for example, Whitaker[22]).*

pore domain. Eq. (9) assumes very good mixing at the pore mouth with the implication that the mass transfer coefficient, k_g, or alternatively, the Sherwood number, is very large. Eq. (10) represents a symmetry condition associated with a capillary tube of length 2L. Eq. (11) clearly captures the interfacial nature of the boundary, as we observe both type of concentrations $c_{A\gamma}$ and c_{AS} playing a role in the equation.

The microscopic model described in Eqs. (8)-(12) is a rigorous description of the physical chemistry process taking place at the pore domain, and students can identify this type of model successfully and without confusion. Students can apply the knowledge acquired in physical chemistry and engineering mathematics to successfully achieve the model.

The next step in the up-scaling process is to recognize what geometrical dimensions are most relevant to describe the pore domain in less detail. For example, the change of the concentration, along the axial direction, z, is important information needed to describe the performance of the pore domain. From this point of view, the "local" variation of the concentration related to the cross-sectional area may be averaged. This approach has been inherently associated with an integration of the microscopic model to reach a macroscopic model in the domain. In short, the student is looking to achieve an elimination of the *explicit* presence of some of the independent variables to obtain a less detailed description of the domain.[4] The process mimics closely the concept of average values of a function, as opposed to the point or local values for such a function. This is another concept already used by the students in applied mathematics or statistics courses. Thus, students are once more introduced to the notion of an average value of a function, f(x) – a concept encountered previously in calculus. In addition, averaging approaches and the connection between averaging and integrals is reviewed, as well as the relation between macroscopic description and integrals. The connection between micro, differential, and local concepts is also discussed. By the end, students are well aware that a microscopic-level model is connected by integration, *i.e.*, by up-scaling, to a macroscopic-level model that applies to the domain, *i.e.*, the control line, surface, or volume that is of interest.

Now, the following definition of area-average for the concentration is useful:

$$\left\langle c_{A\gamma}\right\rangle^{\gamma} = \frac{1}{\pi r_0^2}\int_{r=0}^{r=r_0} 2\pi r c_{A\gamma} dr \tag{13}$$

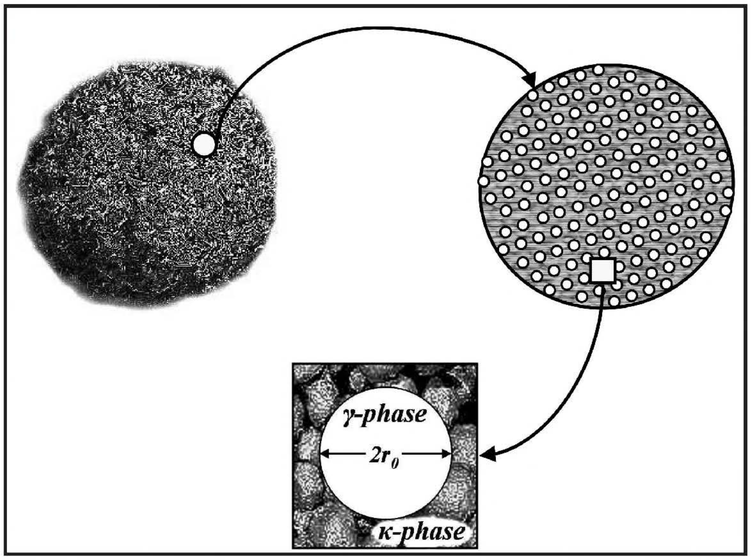

***Figure 3**. Cylindrical pore domain and its nomenclature.*

Eq. (13) is a useful averaging tool[5] to conduct an integration of the species continuity in Eq. (8). The procedure involves algebraic steps where students have the chance to apply what they learned in the supporting mathematics courses of the engineering curriculum (see Arce, et al.,[10]). The final result is the following area-averaged equation:

$$\frac{\partial\left\langle c_{A\gamma}\right\rangle^{\gamma}}{\partial t} = D_{\gamma}\frac{\partial^2\left\langle c_{A\gamma}\right\rangle^{\gamma}}{\partial z^2} - \frac{2k}{r_0}c_{AS} \tag{14}$$

In arriving at Eq. (14), the use of the boundary condition given by Eq. (11) was invoked and, therefore, the heterogeneous reaction present in this equation has been integrated with the governing differential equation. The process just described has led a *heterogeneous* reaction to look like a *homogeneous*-type reaction, given in Eq. (4). The omission of this aspect of the analysis is a crucial learning failure for the students and will undoubtedly lead to confusion. The up-scaling approach used above successfully highlights the source of the reaction term in Eq. (14). The process of integrating boundary conditions with differential equations to produce area-averaged or macro-transport equations is typical of all transport process in multiphase systems.

If students wish to solve Eq. (14), they will encounter difficulty because the equation shows two types of variables, *i.e.*, the area-averaged bulk concentration, $\langle c_{A\gamma}\rangle^{\gamma}$, and the surface concentration, c_{AS}. Therefore, we need to find a relation between these two variables. Otherwise, the up-scaling approach would fail and we would need to return to the original microscopic model in pore domain. In fact, the approach would fail without a method of closure. There are several options to implement such a method.[24-28] We will use a rather elementary approach here based on approximations that enhance the student's engineering training.

By using the flux boundary conditions at the interface of the pore domain, the following estimation can be made:

$$D_{\gamma}\left(\frac{c_{A\gamma}\big|_{r=0} - c_{A\gamma}\big|_{r=r_0}}{r_0}\right) = O\left(kc_{A\gamma}\big|_{r=r_0}\right) \tag{15}$$

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[4] *This process is related to the homogenization of the porous medium.*[23]

[5] *The equation may be viewed, in fact, an integral operation for the function $c_{A\gamma}$ that yields an averaged value, $\langle c_{A\gamma}\rangle$, of such function in the cross sectional area.*

This equation can be rearranged into the form:

$$\frac{c_{A\gamma}\big|_{r=0} - c_{A\gamma}\big|_{r=r_0}}{c_{A\gamma}\big|_{r=r_0}} = O\left(\frac{kr_0}{D_\gamma}\right) \tag{16}$$

From this result, it is possible to identify certain limiting situations. If $kr_o/D_\gamma << 1$, then the following result would hold:

$$\langle c_{A\gamma}\rangle^\gamma \approx c_{AS} \tag{17}$$

Therefore, in the limiting situation, one could use $\langle c_{A\gamma}\rangle^\gamma \approx c_{AS}$[6] to obtain the area averaged equation given by:

$$\frac{\partial\langle c_{A\gamma}\rangle^\gamma}{\partial t} = D_\gamma \frac{\partial^2\langle c_{A\gamma}\rangle^\gamma}{\partial z^2} - \frac{2k}{r_0}\langle c_{A\gamma}\rangle^\gamma \tag{18}$$

If the condition $kr_o/D_\gamma << 1$ fails, other closure procedures are available (see Payne, *et al.*,[29] and Oyanader & Arce[30]).

We are now in a position to offer several useful observations from the student learning point of view. First, a comparison between Eq. (18) and Eq. (3) highlights several differences. Eq. (18) is in terms of area-averaged concentrations and Eq. (4) fails to identify this important difference. Second, equation (18) is only valid for certain cases, *i.e.*, slow reactions, and therefore has limitations. It is also not of a general validity as Eq. (3) seems to indicate. This limitation is the same type of constraint found, for example, in the case of the well-mixed model for CSTR. It is only valid if this particular limit holds, and many practical situations need a more realistic type of reactor model (see, for example, Levenspiel[2]). Third, the reaction term in Eq. (18) is a source term rooted in the heterogeneous, catalytic reaction present at the wall of the pore domain, as was clearly captured by Eq. (11). An up-scaling procedure located this reaction term in the macro-transport Eq. (18). For example, if other homogeneous reactions were also present in the γ-phase, they would appear in Eq. (18) after originally being captured by Eq. (8). The rate coefficient for these reactions would differ from that of heterogeneous processes. For example, the rate coefficient $2k/r_o$ in the reaction term identified in Eq. (18) shows the pore radius indicating that this coefficient is something other than a true homogenous rate constant. Fourth, by introducing an up-scaling approach and avoiding misconceptions, we have created a very rich learning environment for the students where approximations, closure procedures, and limitations of the resulting up-scaled or macro-transport equations are all transparent to the students. Moreover, all basic mathematical skills learned in courses required as prerequisites for the engineering curriculum are now of practical use, and no mathematical skills beyond these are necessary!

Moreover, all basic mathematical skills learned in courses required as prerequisites for the engineering curriculum are now of practical use, and no mathematical skills beyond these are necessary!

Once we have up-scaled the smallest level, V (the pore domain), it will be useful to show how this information can be used in up-scaling the system to the next level, IV (the catalytic pellet domain). We realize the porosity of the pellet is a parameter that plays an important role and the intrinsic averaged, scaled-up Eq. (18) is perhaps not the most useful from a reactor design point of view, since the reactor term $\frac{2k}{r_0}\langle c_{A\gamma}\rangle^\gamma$ is the unit volume of the fluid phase. In the description of transport and reaction processes of real porous systems,[31-33] it is traditional to work with the reaction per unit volume of the porous medium since the ratio of the fluid volume to the volume of the porous medium is the porosity, *i.e.*, $\varepsilon_\gamma = V_\gamma / V$; $V \equiv V_\gamma + V_\kappa$ in the notation of Figure 1. By using the porosity in Eq. (18), one can find the reaction rate per unit volume of porous media:[12]

$$R_\gamma = \varepsilon_\gamma \frac{2k}{r_0}\langle c_{A\gamma}\rangle^\gamma \tag{19}$$

Eq. (19) represents the usual reaction term found in the reaction design literature.[31,34] If one identifies $2\varepsilon_{\gamma\kappa}/r_o$ as the unit surface area per unit volume of the porous medium (catalysts phase) and denotes it by a_v, Eq. (19) can be written in the usual form, $R_\gamma = a_v k \langle c_{A\gamma}\rangle^\gamma$. Another important quantity that appears in the process of up-scaling is the diffusivity modified by the porous medium. The diffusive flux of "A," per unit volume of porous media for the z-direction of the porous domain of Figure 1, can be written as.[12]

$$N_\gamma = -\varepsilon_\gamma D_\gamma \frac{d\langle c_{A\gamma}\rangle^\gamma}{dz} \tag{20}$$

Traditionally, a tortuosity factor, τ,[34] is included to accommodate the geometry of the porous medium. Thus, Eq. (20) is expressed as:

$$N_\gamma = -\varepsilon_\gamma \frac{D_\gamma}{\tau}\frac{d\langle c_{A\gamma}\rangle^\gamma}{dz} \tag{21}$$

The term D_γ/T can be defined as an effective diffusivity of the medium, D_{eff}, that leads to the usual equation for the flux in a porous medium:

$$N_\gamma = -\varepsilon_\gamma D_{eff} \frac{d\langle c_{A\gamma}\rangle^\gamma}{dz} \tag{22}$$

By using Eq. (19), written in terms of a_v, and Eq. (22), Eq. (18) leads to the up-scaled version of the conservation equa-

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[6] *This type of approximations is very popular in cases of reaction engineering problems in homogenous systems such as the "well-mixed" model for the CSTR that educators have used widely. Unfortunately, the same approach seems to have been overlooked in multiphase systems.*

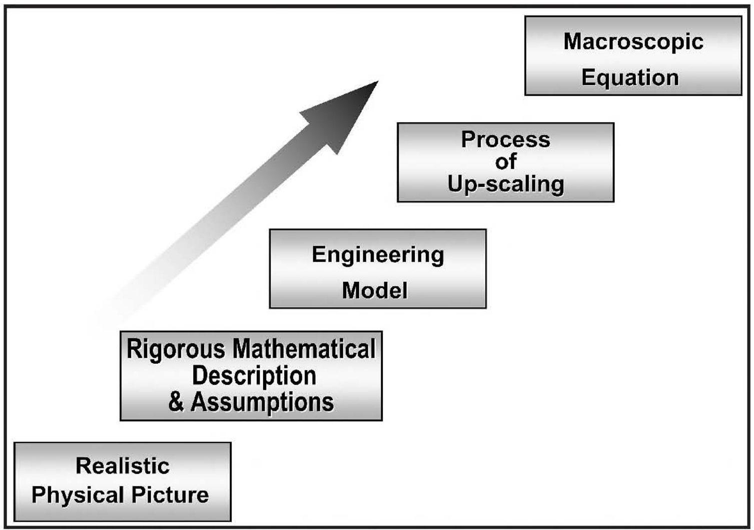

***Figure 4**. Pedagogical sequential steps associated with up-scaling.*

tion for the catalyst pellet (porous medium) usually seen in textbooks:[11,35,36]

$$\varepsilon_\gamma \frac{\partial \langle c_{A\gamma} \rangle^\gamma}{\partial t} = \varepsilon_\gamma D_{eff} \frac{\partial^2 \langle c_{A\gamma} \rangle^\gamma}{\partial z^2} - a_v k \langle c_{A\gamma} \rangle^\gamma \qquad (23)$$

Eq. (23) has been derived by a very systematic and progressive-learning up-scaling approach based on the species continuity equation and a microscopic description of the transport and reaction processes at the pore and pellet domain levels. The approach followed methods well-rooted in a sound pedagogical environment (see section IV, below) and used a level of mathematics originating in courses engineering students are required to take. In fact, students are surprised by the level of usefulness of the concepts used in the up-scaling approach outlined in this section. Comments and discussion of the pedagogical aspects are presented in the section below.

PEDAGOGICAL ASPECTS: ROLE OF THE CATALYTIC PELLET AS AN EFFECTIVE POK

The concept "Principal Objects of Knowledge," or POK's, was introduced in the *Colloquial Approach Environments*[37] to enhance student learning and promote a more efficient study habit in engineering students, in order to master difficult concepts. The tool was extended to include a variety of subjects[38,39] in fluid mechanics, mass and energy balances, and continuum theory. The role of the catalyst particle or pellet as a rich example of POK for students interested in learning about transport in porous media and heterogeneous reactions is identified in this contribution. Principle Objects of Knowledge are learning enhancers, at an intermediate level of complexity, that help students by building blocks of knowledge. By looking at Figure 2, catalytic pellets are located at a level (IV) within the spectrum of scales. Studying transport and reaction at this level allows students to work efficiently at all levels. In fact, if packed-bed reactors are assumed uniform, level IV (the macro-transport equation of the catalytic pellet) becomes the prototype-design equation for the packed-bed reactor.[11]

The catalytic pellet is an incubator of learning for many situations relevant in current chemical reacting systems. For example, the macroscopic equations derived in Section III, may be viewed as the design equations of a micro-reactor housed in the pellet domain. This has obvious implications for processes that inherently have associated many scales ranging from the molecular-, nano-, and micro-scale processes, such as in transcellular transport, tissue engineering, pharmaceutical, environmental, and microelectronic applications. Examples of porous domains related to these applications may include soils, membranes in separation and purifications, fuel cells and high performance batteries, biological porous and fibrous media (such as human tissues and materials in drug delivery), and air-cleaning devices. In other words, the catalytic pellet is a multiscale-domain environment that offers a powerful prototype for efficiently studying many multiphase and multicomponent systems (see, for example, Arce[40] and Arce, *et al.*,[11]). Today, these applications are very relevant to many engineering majors – including chemical, biomedical, and environmental engineering. In short, the catalytic pellet becomes a very flexible POK to help students learning in many multiphase and multiscale systems of practical interest.

Therefore, appropriate student training in up-scaling various scale levels identified in a catalytic process (see Figure 2) gives them a sound background to attack problems within a wide range of multiphase systems. In short, by following this up-scaling approach, students will learn about connecting physics and mathematics, understanding the role of different scales, and realizing that the new and frontier chemical engineering applications of today's technology are not so far from the classical ones – when viewed from an up-scaling perspective.

The sequence identified in Figure 4 represents a sound pedagogical environment that follows a systematic and progressive approach[41,42] to derive engineering equations in a catalyst pellet that can be up-scaled to yield macrocoscopic equations. This approach is more efficient and yields much less confusion than those currently used in textbooks based on a more "unit-operation" point of view.

General concepts at the microscopic level of the porous domain dominate the first two steps of the sequence identified in Figure 4, as it was illustrated in Sections II and III of this contribution. Specific microscopic details related to the pore domain are addressed in the next step (the engineering equation[38,42]) of the sequence. The last step of the sequence is focused on the up-scaling process. The engineering model becomes a rigorous mathematical description of the physical and chemical processes taking place in the domain. This model is clearly valid at every point of the domain and, therefore, is undoubtedly connected with the idea of a microscopic level of the physical system. Solution approaches should not be emphasized here, just the correct description of the physics and chemistry taking place is enough. The last step deals with possible ways to obtain information from the engineering model.

What is interesting and useful, from the pedagogical point of view in the sequence of Figure 4, is that students in engineering majors are quite comfortable with describing (conceptually) basic or microscopic physical aspects of a problem, and identifying a mathematical model afterward that mimics closely the physics that they have visualized. For example, it is quite rational to introduce students to geometrical and physical chemistry concepts in a pore domain, within a catalytic pellet, where diffusion and (heterogeneous catalytic) reactions take place. Heterogeneous reactions and catalysis must, of course, be introduced separately from the kinetic concepts, as they usually are in physical chemistry courses. Diffusion is present as the only transport mechanism inside the pore cavity, so that reactants can travel from the bulk to the surface of the pore domain only by gradients of concentrations. Since the reaction is catalytic, students have no problem recognizing it is located at the walls of the pore domain and, therefore, no reaction is present in the bulk of such pore, unless by-products of the process are present. These could be produced by homogenous reactions.

Furthermore, students who are familiar with thermal surface sources can trivially associate the transport and reaction situation in the pellet with a process at the boundary of the domain where conductive fluxes and sources (*i.e.*, reaction) must be involved. In other words, the catalytic pellet is the equivalent situation to that of the heat conduction and heat generation with heterogeneous sources (see, for example, Whitaker[43]), a concept already introduced in the heat transfer course. In fact, students who have already taken the proper heat and mass transfer courses usually find the pore and pellet situation a simple variation of the examples they already encountered in these subjects. Moreover, the analysis and study of the catalytic pore and pellet by following the sequence listed in Figure 4 reinforces the concepts previously learned.

Aris[9] stated that there are many useful ways to extract information from a model without actually solving the model equations. In the case under analysis, up-scaling approaches are an effective way to accomplish this. Although the detailed solution of the model is not achieved in the process of up-scaling, students learn a great deal about the system behavior by implementing the approach. Another important point to make is that the mathematics required in the process are of the same level learned in undergraduate-level courses. Thus, a marriage between mathematics and physics has been born in students' minds. This connection fosters an excellent integration of otherwise divorced components or pieces of the engineering curriculum.

STUDENT FEEDBACK AND QUALITATIVE ASSESSMENT

The qualitative assessment, based on the feedback from students on the implementation of up-scaling approach in two different courses at the FAMU-FSU College of Engineering, has shown a very promising trend. The students have been able to clearly perform better in exercises that involve conceptually the identification of quantities related to bulk parameters – such as averaged concentrations, as opposed to local concentration values – in a fluid phase interacting with a solid phase through a catalytic reaction. Also, students learn sequentially about effective diffusivity in a porous domain and its differences with respect to molecular and Knudsen type diffusivities.

Student interviews at the end of the course have confirmed they mastered the concepts and achieved, in general, a deeper understanding of the different aspects in a heterogeneous system with diffusion and reaction. A similar outcome was observed in the kinetic courses taught at Tennessee Tech. Students felt very comfortable obtaining the description of the system and identifying boundary conditions for the model. In addition, they welcomed the discussion of the closure process and the implication to the approximations involved in applying the results of the model. Furthermore, the platform of knowledge developed seems to be a very good tool to attack other more sophisticated systems, such as a collection of pores in a catalytic particle. In addition, students have expressed their satisfaction in using concepts of engineering mathematics to develop applied or engineering models that are efficient in handling complex situations in transport and reaction. One aspect useful to determine is how much the approach has increased their ability to handle systems with transport and heterogeneous reactions, and with several scales involved such as those in biological systems. This aspect will be a subject matter for future assessment.

SUMMARY AND CONCLUDING REMARKS.

This contribution presents an analysis of the importance of a pellet as an environment where multi-scale transport processes take place, and introduced a systematic and progressive approach to derive differential models of the up-scaled or macroscopic type in a pore domain and catalyst pellet. The up-scaling approach promotes the explicit use of methods rooted in scaling concepts, and avoids unit operation views followed in many classical textbooks. The same approach can be extended to include engineering equations valid for the entire reactor (see, for example, Whitaker[18]).

Once this approach has been introduced, the student can extend the analysis from one-single porous cavity to a complete pellet. The procedure enhances the student's ability to understand how a macroscopic type of description can be used as a useful approximation for describing the process of diffusion and reaction that takes place in a heterogeneous domain at the microscopic level. Furthermore, students do not seem to show any confusion about the assumptions and limitations of the macroscopic model once they have followed a systematic approach for the derivation and averaging of the microscopic model.

Some of the key benefits introduced by the approach presented here, from the student's point of view, include:

a. *A realistic description of the physics and chemistry of the process.*

b. *A clear identification of the role of the molecular diffusion and surface reaction, and the need for identifying an effective diffusivity.*

c. *A chance to reinforce concepts already learned in previous engineering and chemistry courses.*

d. *The opportunity for the students to apply mathematical concepts learned in the engineering math courses effectively.*

e. *A clear opportunity for building blocks of knowledge in a sequential approach.*

f. *Avoiding the use of "hidden" up-scaling arguments to derive macroscopic engineering equations directly,* i.e., *without using the micro-scale description for chemical/physical processes.*

The up-scaling approach also allows students to find things out.[44] In fact, based on what we saw in our courses, the process of connecting basic physics with mathematical description creates a powerful learning environment that helps the students to become confident and alert life-long learners. In all instances, the mathematical level required does not go beyond the one reached by students in undergraduate mathematics courses, quite contrary to what many educators claim.

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ChE letter to the editor

The recent article "Turning New Faculty Members into Quick Starters"[1] made a lot of sense to me on a first reading. New faculty members are under immense pressure and they need all the help they can get, but if I may be allowed to sound a note of criticism, the article contains no mention whatsoever of industry.

The great pioneers of chemical engineering education such as Donald F. Othmer had strong links with professional practice but in recent decades the academic community in chemical engineering has developed its own culture which has grown away from that of industry. This column[1] gives the impression that young engineering faculty are expected to perform in the same way as their scientific and mathematical colleagues in terms of lectures and supervisions, publications and grants. Industrial contacts and practice, however, can provide many educational and research benefits.[2] Such contacts should be encouraged among our "quick-starting" young faculty members, despite the pressures on their time.

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